Mathematical Modeling in the Natural Sciences

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Documentation and Literature:

`https://imsc.uni-graz.at/keeling/teaching.html`

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What is Modeling?

- A lecture about the relevance of mathematics for medicine
  - was recently planned in Graz, and
  - and at the beginning came the constraint:

    Please no Models.
  - But it would not have been possible to satisfy this.

    Why?
- At the Styrian Modeling Week it is often asked by novices:
  - Did the project group get the

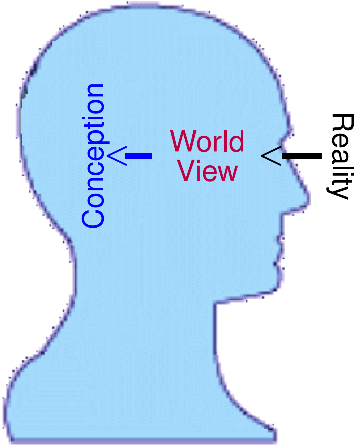
    right answer

    to the problem?
  - But this does not fit to the context.

    Why?

What is Modeling?

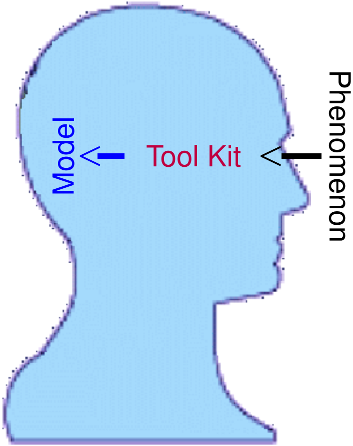
- First answer: Everyone models daily!



- A new-born child gets flooded with perceptions.
- Slowly these must be processed more efficiently, so that the child can function.
- The world gets simplified: Depending on assumptions most details get swept away, the most important ones emphasized.
- The person developes a *world view* – a filter – with which reality gets mapped into conceptions.
- Whether or not the mapping is exact is not important, rather whether it is sufficient for certain purposes.

What is Modeling?

- Mathematically: process is similar!



- A modeler can get flooded with details of a task.
- These must be prioritized,
- e.g., how does one get from A to B in Graz?
  - The most exact model is the city of Graz itself.
  - A map or a sketch is sufficient for the goal.
- The world gets simplified, one makes assumptions.
- One uses ones own *tool kit*, in order to map a phenomenon into a model.
- Whether or not the mapping is exact is not important, rather whether it is sufficient for certain purposes.

What is Modeling?

- A lecture about the relevance of mathematics for medicine
  - was recently planned in Graz, and
  - and at the beginning came the constraint:

    Please no Models.
  - But it would not have been possible to satisfy this.

    Why?

Because mathematics can only be a tool to map medical phenomena, and such mappings are by definition models.

- At the Styrian Modeling Week it is often asked by novices:
  - Did the project group get the

    right answer

    to the problem?
  - But this does not fit to the context.

    Why?

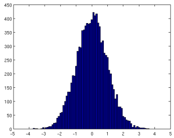
The model is a mapping of a phenomenon. Whether the mapping is exact is not important, rather whether it is sufficient for certain goals (?).

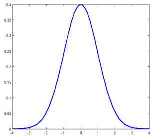
What is Modeling?

- The way of thinking to *give up*: *The equations in textbooks represent discovered natural laws.*
- Example: Are these unconditionally valid?

$$E = mc^2 \quad \text{or} \quad F = ma \quad ?$$

- Examples: Samples of ones own weight measured daily and represented with a histogram (left):





Is the deeper *reality* a smooth approximated curve (right)? What *are* probabilities?

- Main point: These descriptions are only provisional *models*, which have limits to their validity.
- Can a model ever be complete and final?

Steps of Modeling

Example: the documentary film *Supersize Me!*

- A man eats only at McDonalds
  - 30 days long, three times daily,
  - every product at least once,
  - to the question “Supersized?” he always answers “yes”,
  - less that 5000 steps daily,
  - consumes approximately 5000 kcal/day.
- He gains weight (mass): 84kg$\rightarrow$ 95.5kg.
  - Could one have predicted this weight gain?
  - If he were to have continued this program, what would have been his steady state weight?

To the modeling:

- How does one even begin to develop a model?
- Are there appropriate principles which one can use?
- Are there known directions?

Steps of Modeling

For the documentary film *Supersize Me!*

Recall that one simplifies and makes assumptions depending upon goals.

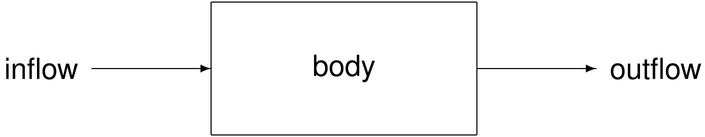
- Goal 1: To predict the weight gain.
- Goal 2: To anticipate a steady state weight.

Recall that one must prioritize the details of a task.

- The film maker gains weight over 30 days: 84kg $\rightarrow$ 95.5kg.
- consumes about 5000 kcal/day,
- less than 5000 steps daily (i.e., no exercise).

Step 1 of Modeling

Step 1: Definition of a physical domain,

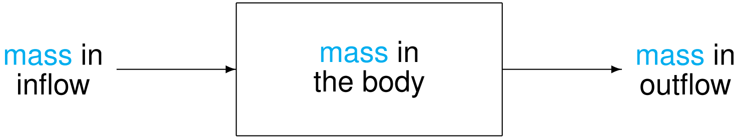


Collection of assumptions,

- As simple as possible. There is currently no reason to do anything more complicated:
- Inflow, outflow and body are homogeneous units.
- Further physical details are neglected, e.g.,
  - cells in the body,
  - stars in the sky,
  - number of employees at McDonalds,
  - time of day of the meals, etc.

Step 2 of Modeling

Step 2: Symbolic description of the system,



Identification of an applicable principle: mass balance or conservation of mass

$$\begin{array}{c}\text{mass change in}\\ \text{the body (1 day)}\end{array} = \begin{array}{c}\text{mass inflow}\\ \text{(1 day)}\end{array} - \begin{array}{c}\text{mass outflow}\\ \text{(1 day)}\end{array}$$

Step 2 of Modeling

$$\frac{\text{mass change in}}{\text{the body (1 day)}} = \frac{\text{mass inflow}}{\text{(1 day)}} - \frac{\text{mass outflow}}{\text{(1 day)}}$$

Mathematical formulation of the principle:

$$m(1) - m(0) = z(0) - a(0)$$

where

$$\begin{aligned} m(1) &= \text{mass at the end of the 1. day} \\ m(0) &= \text{mass at the beginning (84kg)} \\ z(0), a(0) &= \text{inflow, outflow for the forthcoming 1. day} \end{aligned}$$

and similarly for the subsequent days.

Symbolic answers to the goal-questions:

$$m(30) = \ ? \quad m(\infty) = \ ?$$

Step 2 of Modeling

Detailed description of the system: inflow?

- energy inflow is 5000 kcal/day (given).
- mass inflow? conversion through density, kcal/kg?
- known densities:

  fat 9 $\frac{\text{kcal}}{\text{g}}$, carbohydrates 4 $\frac{\text{kcal}}{\text{g}}$, protein 4 $\frac{\text{kcal}}{\text{g}}$
- density for a typical McDonalds mixture:
  $$7.8\frac{\text{kcal}}{\text{g}} = 7800\frac{\text{kcal}}{\text{kg}}$$
- mass inflow: energy inflow / density
  $$5000\frac{\text{kcal}}{\text{day}} \Big/ 7800\frac{\text{kcal}}{\text{kg}} = \frac{5000}{7800}\frac{\text{kg}}{\text{day}}$$

Step 2 of Modeling

Detailed description of the system: outflow?

- Rule of thumb:

$$\text{kcal needs per day} = (21.6 \times \text{mass})\ \frac{\text{kcal}}{\text{day}}$$

- So if (21.6 × Masse) kcal/day are consumed, exactly this much energy is lost, and the mass remains the same.
- If more energy is consumed, still just this much energy is lost, i.e.,

$$\text{energy outflow} = (21.6 \times \text{mass})\ \frac{\text{kcal}}{\text{day}}$$

- With conversion through density

$$\begin{aligned} \text{mass outflow} &= \text{energy outflow} \Big/ \text{density} = \\ (21.6 \times \text{masse})\ \frac{\text{kcal}}{\text{day}} \Big/ 7800\,\frac{\text{kcal}}{\text{kg}} &= \left(\frac{21.6}{7800} \times \text{mass}\right) \frac{\text{kg}}{\text{day}} \end{aligned}$$

- In particular for the forthcoming 1. day,

$$a(0) = \frac{21.6}{7800} \times m(0) = \frac{21.6}{7800} \times 84$$

Step 3 of Modeling

Step 3: Solution of the mathematical problem – *numerically*!

- Summary for the 1. day,

$$m(1) = m(0) + z(0) - a(0) = 84 + \frac{5000}{7800} - \frac{21.6}{7800} \times 84 = 84.8736$$

- For the 2. day,

$$m(2) = m(1) + z(1) - a(1) = 84.8736 + \frac{5000}{7800} - \frac{21.6}{7800} \times 84.8736$$
$$= 85.7497$$

- etc, until the 30. day,

$$m(30) \approx 95.8\text{kg}.$$

- At steady state the mass does not change, so it holds,

$$0 = z(\infty) - a(\infty) = \frac{5000}{7800} - \frac{21.6}{7800} \times m(\infty)$$

or

$$m(\infty) = \frac{5000}{7800} / \frac{21.6}{7800} \approx 231\text{kg}$$

Step 3 of Modeling

Step 3: Solution of the mathematical problem – *exactly*!

- The mass balance,

$$m(t+1) - m(t) = z(t) - a(t)$$

  for 1 day at the beginning of the t-th day.

- Now for the fraction Δt of a day,

$$m(t+\Delta t) - m(t) = \Delta t \cdot (z(t) - a(t))$$

- With $\Delta t \to 0$,

$$\underbrace{m'(t)}_{\substack{\text{instantaneous} \\ \text{rate of change}}} \quad \xleftarrow{\Delta t \to 0} \quad \frac{m(t+\Delta t) - m(t)}{\Delta t} = z(t) - a(t)$$

cf. instantaneous and average speed.

Step 3 of Modeling

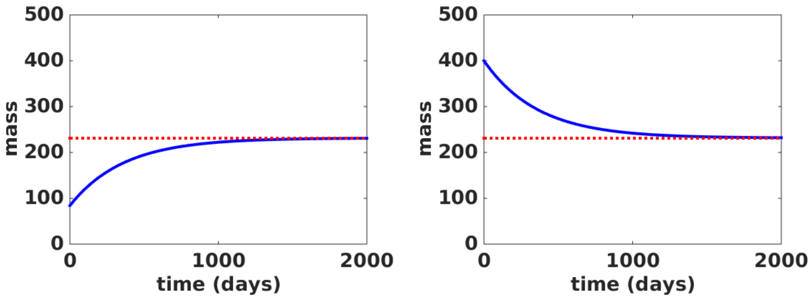
- With the inflow $z(t) = \epsilon/\kappa$ ($\epsilon = 5000$, $\kappa = 7800$) and outflow $a(t) = m(t)\phi/\kappa$ ($\phi = 21.6$) there results the *differential equation*,

$$m'(t) = \epsilon/\kappa - m(t)\phi/\kappa \quad \begin{cases} > 0, & m(t) < \epsilon/\phi \ (\approx 231.5) \\ < 0, & m(t) > \epsilon/\phi \ (\approx 231.5) \end{cases}$$

with solution

$$m(t) = \epsilon/\phi + (m(0) - \epsilon/\phi)\exp(-\phi t/\kappa).$$

- Solutions with $m(0) = 84$ and $m(0) = 400$,



Step 4 of Modeling

Step 4: Qualitative investigation of the mathematical model

- Are the computed values even comprehensible?
- Is the sequence $m(0), m(1), m(2), \ldots$ always increasing, as expected?
- Does this sequence approach the computed steady state $m(\infty)$?
- Do results depend upon the initial weight $m(0)$?

Step 5 of Modeling

Step 5: Comparison with data, validation

- The computed value is $m(30) = 95.8$ kg.
- The measured value is 95.5 kg.

difference significant?

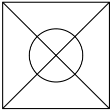
- What would one conclude if daily oscillations in the weight data had been measured?
  - If these are randomly scattered about the predicted sequence?
  - If departures from the predicted sequence were not randomly scattered but were instead systematic?
- If differences between measured and predicated values are significant, which changes in the model should be considered next?

Model Types

- Structural models
  - Relationships among components are considered.
  - Example (above): weight gain
    $$m(t) = \epsilon/\phi + (m(0) - \epsilon/\phi)\exp(-\phi t/\kappa).$$
  - Example (below): Fall of a stone
    $x'' = -g$, $x(0) = h$, $x'(0) = 0 \Rightarrow x(t) = -gt^2/2 + h$.
    $x(\tau) = 0 \Rightarrow \tau = \sqrt{2h/g} \Rightarrow v = -x'(\tau) = \sqrt{2gh}$.
- Empirical models
  - Measured data $\{(t_n, m_n)\}_{n=1}^N$,
    empirical curve $M(t; a, b, c) = a + b\exp(ct)$.
  - Determination of parameters through minimization of a merit function $E(a, b, c) = \sum_{n=1}^N [M(t_n; a, b, c) - m_n]^2$.
- Models through dimensional analysis
  - Impact-velocity v of a falling stone? Relevant quantities: mass m, height h, fall-time τ, acceleration g, ...?
  - Dimensional analysis: $v = f(h, m, g, \tau)$. (L/T, L,M,L/T^2,T)
    dimensionally correct possibilities: $v = k\sqrt{gh}$, $v = k' g\tau$,
    $v = k'' h/\tau$, where k, k', k'' are dimensionless.

Model Types

- Deterministic
  - Examples (above): weight gain and fall of a stone.
  - Example: thermodynamics with macroscopic properties, e.g., pressure, temperature, density.
  - Example: discovery of treasures in a landscape:
    - $\beta =$ fraction of surface containing treasures.
    - $E(t) =$ number of treasures discovered by a simple area-covering walk up to time t.
    - Model: $E' = \beta$, $E(0) = 0 \Rightarrow E(t) = \beta t$.
- Stochastic
  - Example: statistical mechanics with microscopic properties, e.g., positions and velocities of molecules, collisions, forces.
  - Example: discovery of treasures in a landscape:
    - $p_n(t) =$ probability that n in t already found
    - $P(n_t \to (n+1)_{t+dt}) = \beta dt, \forall n$
    - $P(n_t \to n_{t+dt}) = 1 - P(n_t \to (n+1)_{t+dt}) \cdots = 1 - \beta dt$
    - $p_n(t + dt) = P(n_t \to n_{t+dt}) \cdot p_n(t)$ (Bayes)
      $+P((n-1)_t \to n_{t+dt}) \cdot p_{n-1}(t)$ + negligible
    - $p_n(t + dt) = (1 - \beta dt)p_n(t) + \beta dt p_{n-1}(t)$



Model Types

- Stochastic
  - Example: discovery of treasures in a landscape
    - $p_n(t+dt) = (1-\beta dt)p_n(t) + \beta dt p_{n-1}(t)$
    - $p_n'(t) \leftarrow [p_n(t+dt) - p_n(t)]/dt = -\beta p_n(t) + \beta p_{n-1}(t)$
    - expected value of treasures found by t is $E(t) = \sum_{n=0}^{\infty} np_n(t) = \sum_{n=1}^{\infty} np_n(t)$
    - solutions $\{p_n'(t)\}_{n=0}^{\infty}$ continuous and sums converge uniformly means

$$
\begin{aligned}
E'(t) = \sum_{n=1}^{\infty} np_n'(t) &= -\beta \sum_{n=1}^{\infty} np_n(t) + \beta \sum_{n=1}^{\infty} np_{n-1}(t) \\
&= -\beta E(t) + \beta \left. \sum_{n=1}^{\infty} (n-1)p_{n-1}(t) \right|_{=E(t)} + \beta \left. \sum_{n=1}^{\infty} p_{n-1}(t) \right|_{=1}
\end{aligned}
$$

or $E'(t) = \beta$, and $E(0) = 0 \Rightarrow E(t) = \beta t$.

- In this way macroscopic quantities emerge through expected values of microscopic stochastic quantities.

Model Types

- Lumped parameters
  - It is assumed that certain spatial dependencies can be neglected.
  - Example: The temperature $T(t)$ in the body at time t is modeled with Newton's cooling law,

$$\rho c V T'(t) = \alpha A[T_\infty - T(t)], \quad T(0) = T_0$$

ρ	$=$	density	c	$=$	specific heat
α	$=$	heat transfer coefficient	A	$=$	interface area
V	$=$	volume	T_∞	$=$	external temperature

  - Such models are typically described with ordinary differential equations.
- Distributed parameters
  - Spatial dependencies are not neglected.
  - Example: The temperature $T(t, \boldsymbol{x})$ in the body at time t and at position $\boldsymbol{x}$ satisfies the heat equation,

$$\rho c T_t = \nabla \cdot (\lambda \nabla T), \quad T(t, \mathrm{skin}) = T_\infty(t), \quad T(0, \boldsymbol{x}) = T_0(\boldsymbol{x})$$

λ	$=$	thermal conductivity	$a = \lambda/(\rho c)$	$=$	thermal diffusivity
λ	$=$	$\delta\alpha$	δ	$=$	skin thickness

  - Such models are typically described with partial differential equations.

Model Types

- Dynamic Models
  - Continuous time models
    - Evolution depends continuously on time.
    - Example: logistic growth,
      $$P'(t) = \alpha P(t)[K - P(t)]$$
      Solutions are simply S-shaped.
  - Discrete time models
    - State jumps discretely to the next generation.
    - Example: logistic evolution,
      $$P_{n+1} = \tilde{\alpha} P_n[\tilde{K} - P_n]$$
      Solutions can be periodic and even chaotic!
- Static models
  - State does not depend upon time.
  - Example: a membrane with tension T is loaded in its interior over Ω with a force $f(\boldsymbol{x})$ and clamped at its boundary over $\partial\Omega$. The Poisson equation is a distributed model for the deformation $u(\boldsymbol{x})$,
    $$-T\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

Purposes of Modeling

- Most of all: to answer the motivating goal-question.
  - Length of time until the house temperature $T(t)$ sinks $100(1-p)\%$ of its way to the outside temperature T_∞?
  - Model with Newton cooling:
    $\rho c V T'(t) = \alpha A[T_\infty - T(t)], \quad T(t_0) = T_0.$
  - Solution:
    $T(t) = T_\infty + (T_0 - T_\infty)\exp[-\alpha A t/(\rho c V)]$
  - Length of time: $t^\star = \ln(1/p)\rho c V/(\alpha A)$.

ρ = density
c = specific heat capacity
V = volume
A = surface area
λ = thermal conductivity
$a = \lambda/(\rho c)$ = thermal diffusivity
δ = wall thickness
$\alpha = \lambda/\delta$ heat transfer coefficient

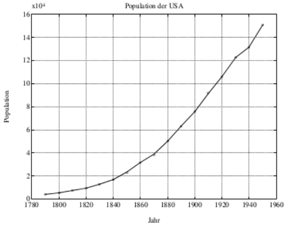
- To better understand the modeled system.
  - effect of insulation (α)? house surface area (A)?
- To estimate system parameters.
  - determination of $\rho c V/(\alpha A)$? of α?
- To control and to optimize the modeled system.
  - minimize surface area A?
- Optimal control
  - How many fishing boats from a fleet should be in operation?
- Optimal decision making
  - How many goods should be purchased and stored?
  - Should one buy a tram ticket?

Empirical Models

- Example: prediction of population growth

Population
of the USA

$\{(t_i, P_i)\}_{i=1}^N$
are given



- Possible models
  - $P(t) = kt + d$ (linear)
  - $P(t) = Ce^{kt}$ (exponential)
  - $P(t) = K/[1 + \exp(-(t - t_0)/\tau)]$ (logistic)
- For the linear model, $P(t; k, d) = kt + d$, one can easily minimize the merit function,

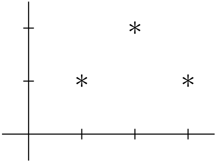
$$E(k, d) = \sum_{i=1}^{N} |P(t_i; k, d) - P_i|^2$$

Linear Regression

- **Homework**: Show that E is globally minimized at

$$k^\star = \frac{\overline{t \cdot P} - \overline{t} \cdot \overline{P}}{\overline{t^2} - \overline{t}^2}, \quad d^\star = \overline{P} - k^\star \overline{t}, \quad \text{e.g.,} \quad \overline{t \cdot P} = \frac{1}{N} \sum_{i=1}^{N} t_i P_i$$

- Simple example in which the regression line is clear?



$k = 0$, $d = 4/3$

- Should the merit function

$$E(k,d) = \left[\sum_{i=1}^{N} |P(t_i; k, d) - P_i|^p \right]^{\frac{1}{p}}$$

$$\|\boldsymbol{x}\|_{\ell_\infty} = \max_{1 \le i \le N} |x_i|$$

$$\|\boldsymbol{x}\|_{\ell_p} = \left[\sum_{i=1}^{N} |x_i|^p \right]^{\frac{1}{p}}$$

be minimized with $p = 1, 2$ oder ∞?

- Easier to solve with $p = 2$, but $p = 1$ is more robust!

Robust Merit Functions

Homework: For $\mathbf{1} = \langle 1, \ldots, 1 \rangle$, $\boldsymbol{f} = \langle a, b, \ldots, b \rangle \in \mathbb{R}^{n+1}$ show

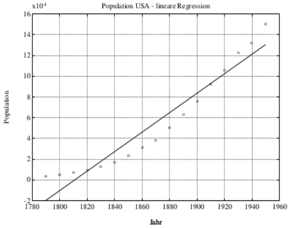
$$\frac{a + nb}{1 + n} = \underset{c \in \mathbb{R}}{\operatorname{argmin}} \|\boldsymbol{f} - c\mathbf{1}\|_{\ell_2}^2 \quad \text{while} \quad b = \underset{c \in \mathbb{R}}{\operatorname{argmin}} \|\boldsymbol{f} - c\mathbf{1}\|_{\ell_1}$$

Message: The easier $\|\cdot\|_{\ell_2}$-norm is vulnerable to outliers, but the harder $\|\cdot\|_{\ell_1}$-norm is less so.

- The empirical result,

  Population of the USA

  approximated through linear regression



  manifests systematic departures from the data!
- The linear model is therefore not suitable.

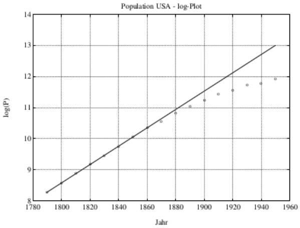
Exponential Regression

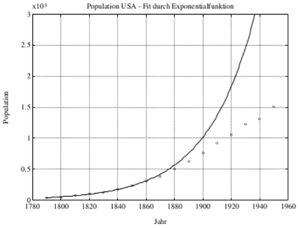
- For the exponential Model, $P(t;k,C) = Ce^{kt}$, one can implement methods to minimize the merit function,
$$E(k,C) = \sum_{i=1}^{N} |P(t_i;k,C) - P_i|^2$$
but another solution can be computed more easily with regression.
- With the transformation,
$$Q(t;k,d) = \ln P(t;k,C) = \ln C|_{=d} + kt$$
the merit function
$$F(k,d) = \sum_{i=1}^{N} |Q(t_i;k,d) - \ln P_i|^2$$
can be minimized easily:
$$k = \frac{\overline{t \cdot \ln P} - \bar{t} \cdot \overline{\ln P}}{\overline{t^2} - \bar{t}^2}, \quad d = \overline{\ln P} - k\bar{t}, \quad C = e^d$$
- Notice that the minimizing solution for F is not necessarily the minimizing solution for E!

Non-Linear Regression

- The empirical result,

Population
of the USA
approximated through
linear regression
of exponentially
transformed data





manifests systematic departures from the data!

- The exponential model is therefore not suitable.
- For the logistic model,

$$P(t; K, t_0, \tau) = K/[1 + \exp(-(t - t_0)/\tau)]$$

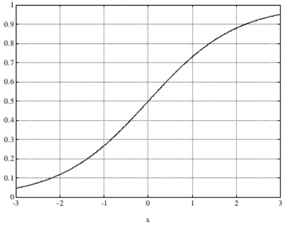
one can minimize the merit function,

$$E(K, t_0, \tau) = \sum_{i=1}^{N} |P(t_i; K, t_0, \tau) - P_i|^2$$

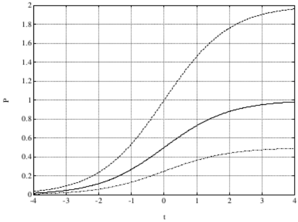
but optimization methods are necessary for this.

The Logistic Function

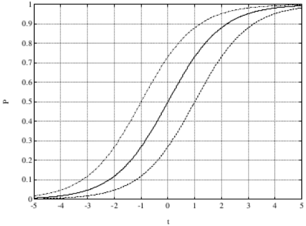
- Qualitative properties:



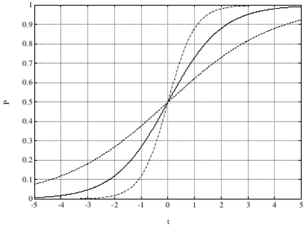
$P(t; K, t_0, \tau) = K/[1 + \exp(-(t - t_0)/\tau)]$



K varies



t_0 varies



τ varies

- K = capacity, $(t_0, K/2)$ = inflection point, τ = time scale

Introduction to Optimization

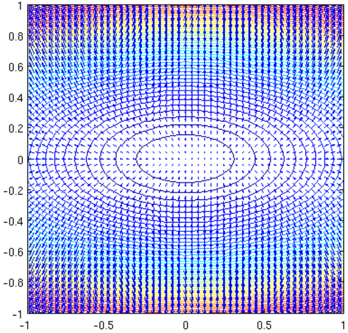
- Example:

$$f(x,y) = \frac{1}{4}x^2 + y^2$$

- Level curves: $f(x,y) =$ constant.
- Gradient:

$$\nabla f(x,y) = \begin{bmatrix} f_x \\ f_y \end{bmatrix} = \begin{bmatrix} x/2 \\ 2y \end{bmatrix}$$

is orthogonal to a level curve.



- Steepest descent: $\boldsymbol{x} = \langle x, y \rangle^{\mathrm{T}}$

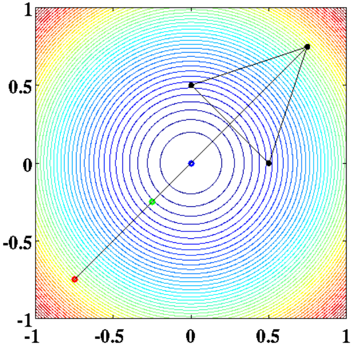
$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha \nabla f(\boldsymbol{x}_k)$$

where stepsize α is chosen so that $f(\boldsymbol{x}_{k+1}) < f(\boldsymbol{x}_k)$.

- The method requires access to ∇f, and it can get trapped in a local minimum.

Nelder-Mead Method

- The method is also called the *Simplex Method*, particularly in higher dimensions. MATLAB: `fminsearch`.
- Example: In $\mathbb{R}^2$ one begins with 3 start-points, e.g.,
$$\boldsymbol{x}_1 = (\tfrac{3}{4}, \tfrac{3}{4}), \quad \boldsymbol{x}_2 = (0, \tfrac{1}{2}), \quad \boldsymbol{x}_3 = (\tfrac{1}{2}, 0)$$
and finds here, $f(\boldsymbol{x}_1) \geq f(\boldsymbol{x}_2) \geq f(\boldsymbol{x}_3)$. (contours unknown)



With the midpoint
$$\boldsymbol{x}_\mathrm{m} = \frac{\boldsymbol{x}_2 + \boldsymbol{x}_3}{2}$$
the next reasonable samples are:
$$\boldsymbol{x}_\mathrm{m} - \tfrac{1}{2}(\boldsymbol{x}_1 - \boldsymbol{x}_\mathrm{m})$$
$$\boldsymbol{x}_\mathrm{m} - (\boldsymbol{x}_1 - \boldsymbol{x}_\mathrm{m})$$
and
$$\boldsymbol{x}_\mathrm{m} - 2(\boldsymbol{x}_1 - \boldsymbol{x}_\mathrm{m})$$

One replaces $\boldsymbol{x}_1 \leftarrow \boldsymbol{x}_\mathrm{m} - \tfrac{1}{2}(\boldsymbol{x}_1 - \boldsymbol{x}_\mathrm{m})$, and then repeats, etc.

Nelder-Mead Method

- The method has difficulties when the simplices are not regular, i.e., very thin or very flat.
- For this reason the parameters should be scaled to have comparable orders of magnitude.
- Example: For the population data, $K \approx 180000$

$$\text{inflection point} = (t_0, K/2) \approx (1910, 90000), \quad t_0 \approx 1910$$
$$4000 = P(1790) \approx 180000e^{(1790-1910)/\tau}, \quad \tau \approx 30$$

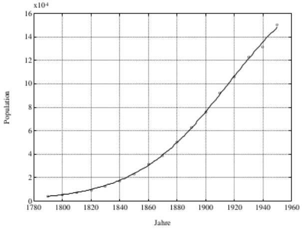
- With the optimization parameters x_1, x_2 and x_3

$$K = x_1 \cdot 10^5, \quad t_0 = x_2 \cdot 10^3, \quad \tau = x_3 \cdot 10^1$$
$$t = [\cdots], \quad P = [\cdots], \quad f = K./(1 + \mathtt{exp}(-(t - t_0)/\tau))$$
$$E = \mathtt{sum}((f - P).\hat{}2)$$

- The empirical result,

$$K \approx 200070$$
$$t_0 \approx 1915.8$$
$$\tau \approx 32.496$$

fits rather well.



Parameter Estimation through Regression Analysis

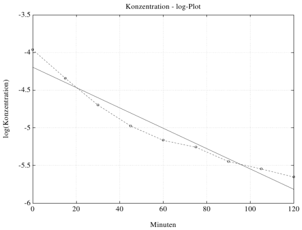
- A chemical reaction proceeds, and chemical data $\{(t_i, u_i)\}_{i=1}^{N}$ are measured: concentrations u_i (mole per liter) at time t_i.

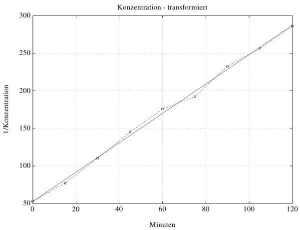
t	0	15	30	45	60	75	90	105	120
$u(t)$	0.0190	0.0130	0.0091	0.0069	0.0057	0.0052	0.0043	0.0039	0.0035

- The *order* (m) of a reaction:
  - $m = 1$: $U \to \tilde{U}$ $\quad (u' = -ku)$
  - $m > 1$: $mU \to U_m$ $\quad (u' = -\kappa u^m)$
- The empirical model for a reaction of m-th order:
  - $m = 1$: $u(t) = Ce^{-kt}$.
  - $m > 1$: $u(t) = (kt + d)^{-\frac{1}{m-1}}$. $\quad (\kappa = k/(m-1))$
  - Notice: $\lim_{m\to 1}[(m-1)kt + u_0^{1-m}]^{-\frac{1}{m-1}} = u_0 e^{-kt}$.
- The order of the above reaction should be determined.
- Regression can be carried out using the following order dependent transformations:
  - $m = 1$: $\ln u(t) = \ln C - kt$.
  - $m > 1$: $u(t)^{1-m} = kt + d$.

Parameter Estimation through Regression Analysis

- The result for $m = 1$ and $m = 2$:





$\{(t_i, \ln u_i\}_{i=1}^N$ left and $\{(t_i, 1/u_i\}_{i=1}^N$ right.

- For $m = 1$ the data points are not randomly scattered around the regression curve.
- For $m = 2$ the scatter does seem random, but
- (exercise) is the fit better for $m = 3$?
- Measures of the data fit: $\|\text{distances}\|_{\ell_2}$, $\|\text{distances}\|_{\ell_1}$, correlation coefficient für the data $\{(x_i, y_i)\}_{i=1}^N$,

$$r = \frac{\overline{x \cdot y} - \overline{x} \cdot \overline{y}}{[\overline{x^2} - \overline{x}^2]^{\frac{1}{2}} [\overline{y^2} - \overline{y}^2]^{\frac{1}{2}}}, \quad r^2 \to 1 \Rightarrow \text{ perfect fit.}$$

A Good Model

- Before optimizing: What is even a *good* Model?
- Properties:
  - Few independent interpretable parameters.
  - Model can be used for predictions, e.g.,

$$P(t) = \frac{K}{1 + (\frac{K}{P_0} - 1)e^{-\frac{t-t_0}{\tau}}}, \quad u(t) = \begin{cases} u_0 e^{-kt}, & m = 1 \\ (kt + u_0^{1-m})^{-\frac{1}{m-1}}, & m > 1 \end{cases}$$

- Disadvantages of many parameters, e.g., $P(t) = \sum_{j=0}^{n} a_j t^j$,
  - Unknown parameters are: $\{a_j\}_{j=0}^{n}$
  - determined with data: $P_i = P(t_i) = \sum_{j=0}^{n} a_j t_i^j$, $0 \leq i \leq n$,

$$\begin{bmatrix} 1 & t_0 & t_0^2 & \cdots & t_0^n \\ \vdots & & & & \vdots \\ 1 & t_n & t_n^2 & \cdots & t_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} P_0 \\ \vdots \\ P_n \end{bmatrix}$$

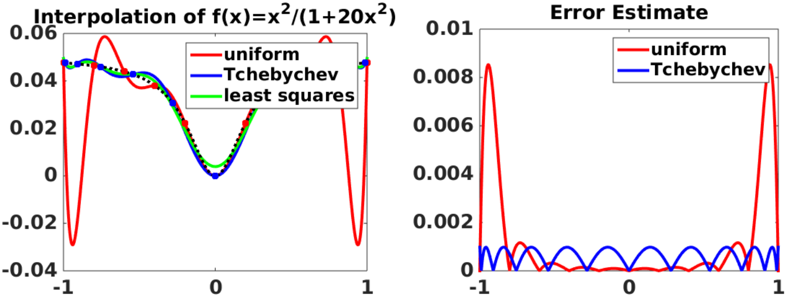
  - or through $\min = \sum_{j=0}^{m} [P(t_j) - P_j]^2$, $m \geq n$,

$$A = \begin{bmatrix} 1 & t_0 & t_0^2 & \cdots & t_0^n \\ \vdots & & & & \vdots \\ 1 & t_m & t_m^2 & \cdots & t_m^n \end{bmatrix}, \quad A^{\mathrm{T}} A \boldsymbol{a} = A^{\mathrm{T}} \boldsymbol{P}$$

Accuracy of Global Interpolation

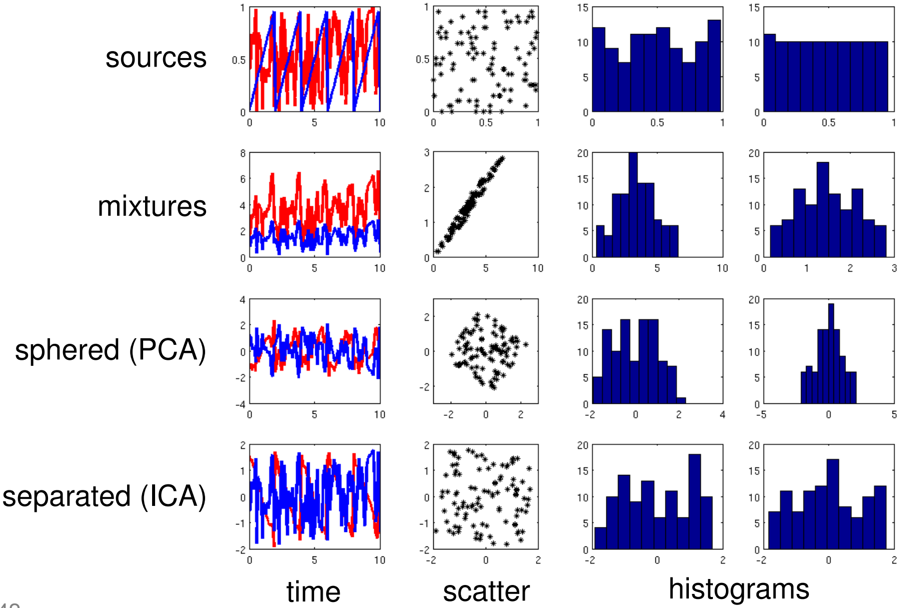
- Example: The function $f(x) = x^2/(1+20x^2)$ is interpolated with $n = 10$ or $m = 100$ as follows:
  - (uniform) $P(x_i) = f(x_i)$, $x_i = -1 + 2i/n$, $i = 0, \dots, n$
  - (Tchebychev) $Q(t_j) = f(t_j)$, $t_j = \cos(\pi(j+1/2)/(N+1))$, $j = 0, \dots, n$
  - (least squares) $\sum_{k=0}^{m} |R(y_k) - f(y_k)|^2 = \min$, $y_k = -1 + 2k/m$, $k = 0, \dots, m$

- The results look like this:



where the theoretical error is shown to the right.

Graphical Overview of PCA/ICA



Formulation of PCA/ICA

- The source signals $\boldsymbol{z}_1, \boldsymbol{z}_2 \in \mathbb{R}^n$ are the rows of

$$Z = \begin{bmatrix} \boldsymbol{z}_1^{\mathrm{T}} \\ \boldsymbol{z}_2^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} z_1(t_1) & z_1(t_2) & \cdots & z_1(t_n) \\ z_2(t_1) & z_2(t_2) & \cdots & z_2(t_n) \end{bmatrix}$$

  These are independent and not Gauss distributed.

- The measured signals $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \mathbb{R}^n$ are unknown mixtures of the sources

$$\begin{bmatrix} \boldsymbol{y}_1^{\mathrm{T}} \\ \boldsymbol{y}_2^{\mathrm{T}} \end{bmatrix} = Y = AZ, \quad A \in \mathbb{R}^{2\times 2}$$

  These are not independent and tend to be Gauss distributed.

- The goal is to minimize *Gaussianity* in order to determine estimates $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^n$ of the sources,

$$\begin{bmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \end{bmatrix} = X = WY, \quad W \in \mathbb{R}^{2\times 2}$$

  stepwise through $W = (\text{rotation}) \cdot (\text{scale}) \cdot (\text{rotation}) \approx A^{-1}$.

Formulation of PCA/ICA

Steps:

- Centering: $\overline{Y} \in \mathbb{R}^m, \mathbf{1} \in \mathbb{R}^n$

$$Y_\mathrm{c} = Y - \overline{Y}\mathbf{1}^\mathrm{T}, \quad \overline{Y}_i = \frac{1}{n}\sum_{j=1}^{n} Y_{ij}, \quad \mathbf{1}_i = 1$$

- Sphering:

$$K = \frac{1}{n} Y_\mathrm{c} Y_\mathrm{c}^\mathrm{T}, \quad KV = V\Lambda, \quad Y_\mathrm{s} = \Lambda^{-\frac{1}{2}} V^\mathrm{T} Y_\mathrm{c}$$

- Rotation:

$$X_\mathrm{c} = UY_\mathrm{s}, \quad U^\mathrm{T} = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m\}$$

  where every $\boldsymbol{u}_k$ minimizes the Gaussianity.

  $\boldsymbol{x} = \{x_i\}$ & $M_1(\boldsymbol{x}) = 0$

  e.g., Kurtosis $\Rightarrow M_k(\boldsymbol{x}) = \frac{1}{n}\sum_{i=1}^{n} x_i^k$

$$\mathcal{K}(\boldsymbol{x}) = M_4(\boldsymbol{x}) - 3M_2^2(\boldsymbol{x})$$

  satisfies $\mathcal{K}(\boldsymbol{n}) = 3\sigma^4 - 3\sigma^4 = 0$ for $\boldsymbol{n} \sim N(\mu, \sigma^2)$.

  So the merit function $J(\boldsymbol{u}) = \mathcal{K}^2(Y_\mathrm{s}^\mathrm{T}\boldsymbol{u})$ can be maximized under the constraint $\boldsymbol{u}_k^\mathrm{T}\boldsymbol{u}_l = \delta_{kl}$.

- Translation:

$$X = X_\mathrm{c} + U\Lambda^{-\frac{1}{2}} V^\mathrm{T} \bar{Y}\mathbf{1}^\mathrm{T} = U\Lambda^{-\frac{1}{2}} V^\mathrm{T} Y = WY$$

Formulation of PCA/ICA

(PCA) Let the data be so decomposed,

$$Y_{\mathrm{c}} = Y - \bar{Y}\mathbf{1}^{\mathrm{T}}, \quad K = \frac{1}{n} Y_{\mathrm{c}} Y_{\mathrm{c}}^{\mathrm{T}}, \quad KV = V\Lambda, \quad Y_{\mathrm{s}} = \Lambda^{-\frac{1}{2}} V^{\mathrm{T}} Y_{\mathrm{c}}$$

Let $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_m\}$ with $\lambda_1 \geq \cdots \geq \lambda_m$. With $P \in \mathbb{R}^{r \times m}$, $r < m$, $P_{i,j} = \delta_{i,j}$, the data Y are thus projected to the r strongest principle components,

$$Y \approx Y_P = \bar{Y}\mathbf{1}^{\mathrm{T}} + V\Lambda^{\frac{1}{2}} P^{\mathrm{T}} P Y_{\mathrm{s}} = \bar{Y}\mathbf{1}^{\mathrm{T}} + \frac{1}{n} Y_{\mathrm{c}} (P Y_{\mathrm{s}})^{\mathrm{T}} (P Y_{\mathrm{s}})$$

(ICA) Let the data be so decomposed,

$$X_{\mathrm{c}} = U Y_{\mathrm{s}}$$

With $Q \in \mathbb{R}^{r \times m}$, $r < m$, $Q_{i,j} = \delta_{q_i,j}$, the data Y are thus projected to the r independent components $\{q_1, \ldots, q_r\}$,

$$Y \approx Y_Q = \bar{Y}\mathbf{1}^{\mathrm{T}} + V\Lambda^{\frac{1}{2}} U^{\mathrm{T}} Q^{\mathrm{T}} Q X_{\mathrm{c}} = \bar{Y}\mathbf{1}^{\mathrm{T}} + \frac{1}{n} Y_{\mathrm{c}} (Q X_{\mathrm{c}})^{\mathrm{T}} (Q X_{\mathrm{c}})$$

A Bad Model

Disadvantages of empirical models with many parameters:

- Information cannot be extracted easily from the many parameters $\{a_j\}_{j=0}^n$.
- Every data set can be exactly interpolated with enough parameters.
  - Is the result *between* data points reasonable?
  - *outside* of the data points?
- The parameters of the result do not necessarily depend stably upon the data: $\boldsymbol{P} = \{P_i\}_{i=0}^n$, $\boldsymbol{a} = \{a_j\}_{j=0}^n$,
$$\|\boldsymbol{P} - \tilde{\boldsymbol{P}}\| \text{ small } \not\Rightarrow \|\boldsymbol{a} - \tilde{\boldsymbol{a}}\| \text{ small}$$
e.g., $A\boldsymbol{a} = \boldsymbol{P}$, $A\tilde{\boldsymbol{a}} = \tilde{\boldsymbol{P}}$,
$$\frac{\|\boldsymbol{a} - \tilde{\boldsymbol{a}}\|}{\|\boldsymbol{a}\|} \leq \kappa(A) \frac{\|\boldsymbol{P} - \tilde{\boldsymbol{P}}\|}{\|\boldsymbol{P}\|}$$
where $\kappa(A) = \|A\|\|A^{-1}\|$ can be very large.
- Computational overhead is not cost effective.

Rewriting a Model in Dimensionless Form

- Temperature evolution in an unheated house:
$$\rho c V T'(t) = \alpha A[T_\infty - T(t)], \quad T(0) = T_0$$
- Dimensionless quantities:
$$\theta = T/T_0, \quad \tau = \alpha A t/(\rho c V)$$
- Differential equation with these,
$$\begin{aligned}
\rho c V \frac{dT}{dt} &= \rho c V \frac{d}{dt}(\theta T_0) = \rho c V T_0 \frac{d\theta}{d\tau}\frac{d\tau}{dt} = \alpha A T_0 \frac{d\theta}{d\tau} \\
\alpha A[T_\infty - T] &= \alpha A[T_\infty - T_0\theta] = \alpha A T_0[T\infty/T_0 - \theta] \\
\Rightarrow \quad \alpha A T_0 \frac{d\theta}{d\tau} &= \alpha A T_0[T\infty/T_0 - \theta] \quad \Rightarrow \quad \frac{d\theta}{d\tau} = \theta_\infty - \theta
\end{aligned}$$
where $\theta_\infty = T_\infty/T_0$ and $\theta(0) = T(0)/T_0 = 1$.
- *Dynamic Similarity*: For an experiment with all parameters scaled ($\tilde{\alpha}\tilde{A}/(\tilde{\rho}\tilde{c}\tilde{V}) = \alpha A/(\rho c V)$, $\tilde{T}_\infty/\tilde{T}_0 = T_\infty/T_0$), the behavior in θ is the same.

Realistic Example: Navier-Stokes

- Conservation of Momentum for an incompressible fluid:

$$\rho \partial_t \boldsymbol{v} + \rho(\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\nabla p + \nu \nabla^2 \boldsymbol{v} + \boldsymbol{f}$$

ρ = density, $\boldsymbol{v}$ = velocity, p = pressure, ν = viscosity, $\boldsymbol{f}$ = force

- Dimensionless quantities:

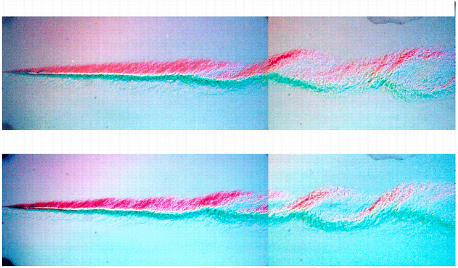
$$\tilde{\boldsymbol{x}} = \boldsymbol{x}/L, \quad \tilde{\boldsymbol{v}} = \boldsymbol{v}/U, \quad \tilde{t} = tU/L, \quad \tilde{p} = p/(\rho U^2), \quad \tilde{\boldsymbol{f}} = \boldsymbol{f}L/(\rho U^2)$$

where L and U are characteristic length and velocity.

- Rewritten dimensionless where $\mathrm{Re} = \rho LU/\nu$

$$\partial_{\tilde{t}} \tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \tilde{\nabla})\tilde{\boldsymbol{v}} = -\tilde{\nabla}\tilde{p} + \frac{1}{\mathrm{Re}} \tilde{\nabla}^2 \tilde{\boldsymbol{v}} + \tilde{\boldsymbol{f}}$$

- High and low speed flows, but the Reynolds Number (Re) is the same:



Models Through Dimensional Analysis

- Measured quantity:

$$G = \underbrace{m(G)}_{\text{measured value}} \cdot \underbrace{[G]}_{\text{measurement unit}}$$

- Base quantities:

$$\{g_i\}_{i=1}^r \quad \text{e.g.} \quad g_1 = \text{length}, \quad g_2 = \text{time}, \quad g_3 = \text{mass}$$

- Base units:

$$\{[g_i]\}_{i=1}^r \quad \text{e.g.} \quad [g_1] = \text{meter}, \quad [g_2] = \text{sec}, \quad [g_3] = \text{kg}$$

  SI System:

  meter, second, kilogram, Ampere, Kelvin, candela, mole

- Derived quantities:

$$\{G_j\}_{j=1}^n \quad \text{e.g.} \quad G_1 = g_1/g_2 \text{ (speed)}$$
$$[G_1] = [g_1]/[g_2] = \text{meter/sec}$$

- In general,

$$G_j = \prod_{i=1}^r g_i^{\alpha_{ij}}, \quad [G_j] = \prod_{i=1}^r [g_i]^{\alpha_{ij}}$$

- Dimensionless if $[G] = 1$.

Models Through Dimensional Analysis

Def: The quantities $\{\mathcal{G}_k = \prod_{j=1}^{n} G_j^{\lambda_{jk}}\}_{k=1}^{m}$ are *independent combinations of* $\{G_j\}_{j=1}^{n}$ if the vectors $\boldsymbol{\lambda}_k = \{\lambda_{jk}\}_{j=1}^{n}$, $k = 1, \ldots, m$, are linearly independent.

- Example: Fall of a stone, $(g_1 = \mathrm{L},\ g_2 = \mathrm{T},\ g_3 = \mathrm{M})$

$$\underbrace{v}_{G_1} = f(\underbrace{h}_{G_2}, \underbrace{m}_{G_3}, \underbrace{g}_{G_4}, \underbrace{\tau}_{G_5})$$

  Following are independent combinations of $\{G_1, \ldots, G_5\}$,

$$\begin{aligned} \Pi_1 &= v \cdot (\tau/h) = G_1 G_5 G_2^{-1} & \boldsymbol{\lambda}_1 &= \langle 1, -1, 0, 0, 1 \rangle^{\mathrm{T}} \\ \Pi_2 &= g \cdot (\tau/v) = G_4 G_5 G_1^{-1} & \boldsymbol{\lambda}_2 &= \langle -1, 0, 0, 1, 1 \rangle^{\mathrm{T}} \end{aligned}$$

  since $\boldsymbol{\lambda}_1$ and $\boldsymbol{\lambda}_2$ are linearly independent.

  Notice: $[\Pi_1] = 1 = [\Pi_2]$.

Buckingham Pi Theorem

Theorem (Buckingham Pi): Let base quantities $\{g_i\}_{i=1}^{r}$ and derived quantities$\{G_j\}_{j=1}^{n}$ be given with $G_j = \prod_{i=1}^{r} g_i^{\alpha_{ij}}$, where the matrix $A = \{\alpha_{ij} : 1 \leq i \leq r, 1 \leq j \leq n\}$ satisfies rank$(A) = r$. Then there are exactly $n - r$ dimensionless independent combinations $\{\Pi_k\}_{k=1}^{n-r}$ of $\{G_j\}_{j=1}^{n}$ such that the equation

$$\Phi(G_1, \ldots, G_n) = 1$$

can be written equivalently as:

$$\Psi(\Pi_1, \ldots, \Pi_{n-r}) = 1.$$

- Example: Fall of a stone, $r = 3$, $n = 5$,

  $$\Pi_1 = v \cdot (\tau / h), \quad \Pi_2 = g \cdot (\tau / v) \qquad \text{(where?)}$$

  are $n - r = 2$ dimensionless independent combinations of $\{G_1, \ldots, G_5\}$. (See above.) It holds

  $$A = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ -1 & 0 & 0 & -2 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \begin{matrix} g_1 \\ g_2 \\ g_3 \end{matrix} \quad \text{rank}(A) = 3 = r?$$

  $$\begin{matrix} G_1 & G_2 & G_3 & G_4 & G_5 \end{matrix}$$

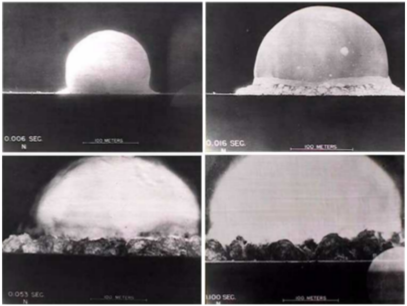
  $v = f(h, m, g, \tau) \rightarrow \Pi_1 = F(\Pi_2)$. Experiment: $\Pi_2 = 1$.
  So $\Pi_1 = F(1) = k$. Experiment: $k = 2$. Result: $v = 2h/\tau$.

Realistic Example of Dimensional Analysis

English Physicist

G.I. Taylor

determined the energy of the first Atom Bomb from a film.



- Quantities which (apparently) play a roll:

G_1	E	Energy of the explosion	ML^2T^{-2}	(K.E.$= \frac{1}{2}mv^2$)
G_2	t	Time since the explosion	T	
G_3	R	Radius of the fireball	L	
G_4	ρ_{A}	Density of the outer air	ML^{-3}	
G_5	ρ_{I}	Density of the inner air	ML^{-3}	
G_6	p_{A}	Pressure of the outer air	$ML^{-1}T^{-2}$	(F/A, kg m/s^2 / m^2)
G_7	p_{I}	Pressure of the inner air	$ML^{-1}T^{-2}$	

Realistic Example of Dimensional Analysis

- Should, e.g., the temperature be included? Then the base quantities must be supplemented with $g_4 =$temperature. With outer temperature $G_8 = T_\mathrm{A}$ and inner temperature $G_9 = T_\mathrm{I}$ there results $r = 4$, $n = 9$ and $\Pi_5 = T_\mathrm{A}/T_\mathrm{I}$. The following analysis shows that temperature is not necessary.
- $\{g_1 = \mathrm{L}, g_2 = \mathrm{T}, g_3 = \mathrm{M}\}$, $\{G_j\}_{j=1}^7 \Rightarrow r = 3$, $n = 7$.
- It holds that $\mathrm{rank}(A) = 3 = r$, (How?)

$$A = \begin{bmatrix} 2 & 0 & 1 & -3 & -3 & -1 & -1 \\ -2 & 1 & 0 & 0 & 0 & -2 & -2 \\ 1 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{matrix} g_1 \\ g_2 \\ g_3 \end{matrix}$$

$$\begin{matrix} G_1 & G_2 & G_3 & G_4 & G_5 & G_6 & G_7 \end{matrix}$$

- With Buckingham Pi one seeks $n - r = 4$ dimensionless quantities $\{\Pi_k\}_{k=1}^4$.
- Hint: Π_1 should be energy-like, so that the investigated quantity E is included.
- With the expectation of a relation $\Pi_1 = F(\Pi_2, \Pi_3, \Pi_4)$ one seeks quantities $\{\Pi_2, \Pi_3, \Pi_4\}$ which are small or constant so that $F(\Pi_2, \Pi_3, \Pi_4) \approx$ constant.

Realistic Example of Dimensional Analysis

- Take
$$\begin{aligned} \Pi_1 &= E(\rho_\mathrm{A}^{-1} R^{-5} t^2) & \Pi_2 &= p_\mathrm{A}^5 (E^{-2} \rho_\mathrm{I}^{-3} t^6) \\ \Pi_3 &= \rho_\mathrm{A}/\rho_\mathrm{I} & \Pi_4 &= p_\mathrm{A}/p_\mathrm{I} \end{aligned}$$
- It holds
$$\begin{aligned} [\Pi_1] &= \frac{\mathrm{ML}^2}{\mathrm{T}^2} \frac{\mathrm{L}^3}{\mathrm{M}} \frac{1}{\mathrm{L}^5} \mathrm{T}^2 = 1, & [\Pi_2] &= \frac{\mathrm{M}^5}{\mathrm{L}^5 \mathrm{T}^{10}} \frac{\mathrm{T}^4}{\mathrm{M}^2 \mathrm{L}^4} \frac{\mathrm{L}^9}{\mathrm{M}^3} \mathrm{T}^6 = 1, \\ [\Pi_3] &= 1, & [\Pi_4] &= 1 \end{aligned}$$
- It should be shown that $\Pi_k = \prod_{j=1}^{7} G_j^{\lambda_{kj}}$ are independent combinations of $\{G_j\}_{j=1}^{7}$:
$$\begin{aligned} \boldsymbol{\lambda}_1 &= \langle\ 1, & 2, & -5, & -1, & 0, & 0, & 0\rangle^\mathrm{T} \\ \boldsymbol{\lambda}_2 &= \langle -2, & 6, & 0, & 0, & -3, & 5, & 0\rangle^\mathrm{T} \\ \boldsymbol{\lambda}_3 &= \langle\ 0, & 0, & 0, & 1, & -1, & 0, & 0\rangle^\mathrm{T} \\ \boldsymbol{\lambda}_4 &= \langle\ 0, & 0, & 0, & 0, & 0, & 1, & -1\rangle^\mathrm{T} \end{aligned}$$
These are linearly independent. (How?)
- Buckingham Pi:
$$\Phi(E, t, R, \rho_\mathrm{A}, \rho_\mathrm{I}, p_\mathrm{A}, p_\mathrm{I}) = 1 \to \Pi_1 = F(\Pi_2, \Pi_3, \Pi_4).$$

Realistic Example of Dimensional Analysis

- In the equation $\Pi_1 = F(\Pi_2, \Pi_3, \Pi_4)$ it holds $\Pi_2, \Pi_3, \Pi_4 \approx 0$.
- With $k = F(0, 0, 0)$ the following model can be applied to the film:

$$E \rho_{\mathrm{A}}^{-1} R^{-5} t^2 = k$$

- From the film one can measure: $R = R(t)$.
- From the model: $R^5 = \left(\frac{E}{\rho_{\mathrm{A}} k}\right) t^2$ or

$$R(t) = \gamma t^{2/5} \quad \text{where} \quad \gamma = \left(\frac{E}{\rho_{\mathrm{A}} k}\right)^{\frac{1}{5}} = \text{constant}$$

- With the film data $\{(t_n, R_n)\}_{n=1}^{N}$ one estimates γ so:

$$\gamma \approx \frac{1}{N} \sum_{n=1}^{N} R_n t_n^{-\frac{2}{5}}$$

- With γ and ρ_{A} known, it follows

$$E = k(\rho_{\mathrm{A}} \gamma^5)$$

  but $k = ?$

Realistic Example of Dimensional Analysis

- One makes a smaller explosion, for which (Π_2, Π_3, Π_4) are small enough that $F(\Pi_2, \Pi_3, \Pi_4) \approx F(0,0,0) = k$ holds.
- Let E_0 be the known energy of the smaller explosion.
- It holds for the smaller experiment,
$$k \approx F(\Pi_2, \Pi_3, \Pi_4) = \Pi_1 = E_0 (\rho_\mathrm{A})_0^{-1} R_0^{-5} t_0^2.$$
or
$$R_0 = \gamma_0 t_0^{\frac{2}{5}} \quad \text{where} \quad \gamma_0 = \left(\frac{E_0}{\rho_\mathrm{A} k}\right)^{\frac{1}{5}} = \text{constant}$$
since $(\rho_\mathrm{A})_0 = \rho_\mathrm{A}$ holds.
- Similarly with data $\{(t_0, R_0)_n\}_{n=1}^N$ one estimates γ_0 so:
$$\gamma_0 = \frac{1}{N} \sum_{n=1}^{N} (R_0 t_0^{-\frac{2}{5}})_n$$
- With γ_0 and ρ_A known, it follows
$$E_0 = k(\rho_\mathrm{A} \gamma_0^5)$$
- With $k = E/(\rho_\mathrm{A}\gamma^5) = E_0/(\rho_\mathrm{A}\gamma_0^5)$ it follows
$$E = E_0(\gamma/\gamma_0)^5.$$

Regular Perturbation Analysis

- For *perturbation theory of algebraic equations* consider

$$x^2 - 1 = \epsilon x, \quad \epsilon \in (0,1)$$

with roots

$$x_1 = \epsilon/2 + \sqrt{1+\epsilon^2/4}, \quad x_2 = \epsilon/2 - \sqrt{1+\epsilon^2/4}$$

- For $0 < \epsilon \ll 1$ these are approximated by Taylor series,

$$x_1 = 1+\epsilon/2+\epsilon^2/8+\mathcal{O}(\epsilon^3), \quad x_2 = -1+\epsilon/2-\epsilon^2/8+\mathcal{O}(\epsilon^3)$$

obtained as follows without direct knowledge of x_1 and x_2.
- For undetermined $\{X_i\}$ write solutions as

$$x = X_0 + \epsilon X_1 + \epsilon^2 X_2 + \mathcal{O}(\epsilon^3)$$

- Substitute these into the algebraic equation and expand into like powers of ϵ,

$$x^2 = X_0^2 + 2\epsilon X_0 X_1 + \epsilon^2(X_1^2 + 2X_0X_2) + \mathcal{O}(\epsilon^3),$$
$$\epsilon x = \epsilon X_0 + \epsilon^2 X_1 + \mathcal{O}(\epsilon^3) \quad \Rightarrow$$
$$X_0^2 - 1 + \epsilon(2X_0X_1 - X_0) + \epsilon^2(X_1^2 + 2X_0X_2 - X_1) + \mathcal{O}(\epsilon^3) = 0$$

Regular Perturbation Analysis

- Equate the successive coefficients of powers of ϵ to zero:

$$
\begin{aligned}
\mathcal{O}(\epsilon^0): &\quad X_0^2 - 1 = 0 \\
\mathcal{O}(\epsilon^1): &\quad 2X_0X_1 - X_0 = 0 \\
\mathcal{O}(\epsilon^2): &\quad X_1^2 + 2X_0X_2 - X_1 = 0 \quad \ldots
\end{aligned}
$$

- Solve this system for $\{X_i\}$,

$$
\begin{aligned}
&\text{solution 1:} \quad X_0 = +1, \quad X_1 = 1/2, \quad X_2 = +1/8 \\
&\text{solution 2:} \quad X_0 = -1, \quad X_1 = 1/2, \quad X_2 = -1/8
\end{aligned}
$$

- For a more interesting example, consider the roots of

$$x^2 - 1 = \epsilon e^x$$

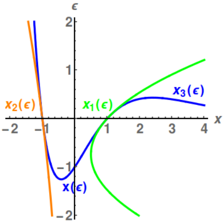
for which an expansion $x = \sum_{i=0}^{2} \epsilon^i X_i + \mathcal{O}(\epsilon^3)$ gives

$$
\begin{aligned}
\epsilon e^x = \epsilon e^{\sum_{i=0}^{2} \epsilon^i X_i + \mathcal{O}(\epsilon^3)} = \epsilon[e^{X_0} e^{\epsilon X_1} e^{\mathcal{O}(\epsilon^2)}] \\
= \epsilon e^{X_0}[1 + \epsilon X_1 + \mathcal{O}(\epsilon^2)][1 + \mathcal{O}(\epsilon^2)] = \epsilon e^{X_0} + \epsilon^2 e^{X_0} X_1 + \mathcal{O}(\epsilon^3)
\end{aligned}
$$

and substitution

$$X_0^2 - 1 + \epsilon(2X_0X_1 - e^{X_0}) + \epsilon^2(X_1^2 + 2X_0X_2 - X_1 e^{X_0}) + \mathcal{O}(\epsilon^3) = 0$$

Regular Perturbation Analysis



leads to the system

$$\begin{aligned} \mathcal{O}(\epsilon^0): &\quad X_0^2 - 1 = 0 \\ \mathcal{O}(\epsilon^1): &\quad 2X_0X_1 - e^{X_0} = 0 \\ \mathcal{O}(\epsilon^2): &\quad X_1^2 + 2X_0X_2 - X_1e^{X_0} = 0 \quad \ldots \end{aligned}$$

and solutions

$$\begin{aligned} &\text{solution 1:} \quad X_0 = 1, \quad X_1 = e/2, \quad X_2 = e^2/8 \\ &\text{solution 2:} \quad X_0 = -1, \quad X_1 = -1/(2e), \quad X_2 = -1/(8e^2) \end{aligned}$$

Yet there are 3 solutions for $0 < \epsilon < \hat{\epsilon} \approx 0.43$ and only one for $\epsilon > \hat{\epsilon}$:

- x_2 exists $\forall \epsilon > 0$,
- x_1 exists only for $\epsilon \in (0, \hat{\epsilon})$ and
- a solution x_3 cannot be obtained by regular perturbation.

- For *perturbation theory of differential equations* consider

$$y''(t) + \epsilon y'(t) + 1 = 0, \quad y(0) = 0, \quad y'(0) = 1, \quad \epsilon > 0$$

with solution

$$y(t) = (1 - e^{-\epsilon t})(1 + \epsilon)/\epsilon^2 - t/\epsilon.$$

Regular Perturbation Analysis

- The equation models the dynamics of a projectile thrown vertically into the air with friction, i.e.,
  - $\epsilon = kV/(mg)$, where
  - V is the initial velocity,
  - m is the mass,
  - k is a friction constant and
  - g is gravitational acceleration.

  Also,
  - length is measured in units of $\tilde{y} = V^2/g$ and
  - time in units of $\tilde{t} = V/g$.
- For $0 < \epsilon \ll 1$ the friction is small and $y(t)$ is approximated using $1 - e^{-z} = z - z^2/2 + z^3/3! + \mathcal{O}(z^4)$ by

  $$y(t) = t - t^2/2 + \epsilon(-t^2/2 + t^3/6) + \epsilon^2(t^3/6 - t^4/24) + \mathcal{O}(\epsilon^3)$$

  which is uniformly valid for $0 < t \ll \epsilon$.
- Without direct knowledge of the solution assume

  $$y(t) = y_0(t) + \epsilon y_1(t) + \epsilon^2 y_2(t) + \mathcal{O}(\epsilon^3)$$

- Substitute these into the differential equation and expand

Regular Perturbation Analysis

into like powers of ϵ,

$$\begin{gathered} y_0'' + 1 + \epsilon(y_1'' + y_0') + \epsilon^2(y_2'' + y_1') + \mathcal{O}(\epsilon^3) = 0, \\ y_0(0) + \epsilon y_1(0) + \epsilon^2 y_2(0) + \mathcal{O}(\epsilon^3) = 0, \\ y_0'(0) - 1 + \epsilon y_1'(0) + \epsilon^2 y_2'(0) + \mathcal{O}(\epsilon^3) = 0. \end{gathered}$$

- Equate the successive coefficients of powers of ϵ to zero:

$$\begin{array}{llll} \mathcal{O}(\epsilon^0): & y_0'' + 1 = 0, & y_0(0) = 0, & y_0'(0) - 1 = 0 \\ \mathcal{O}(\epsilon^1): & y_1'' + y_0' = 0, & y_1(0) = 0, & y_1'(0) = 0 \\ \mathcal{O}(\epsilon^2): & y_2'' + y_1' = 0, & y_2(0) = 0, & y_2'(0) = 0 \quad \ldots \end{array}$$

- Solve this system for $\{y_i\}$,

$$y_0(t) = t - t^2/2, \quad y_1(t) = -t^2/2 + t^3/6, \quad y_2(t) = t^3/6 - t^4/24$$

- Proceeding inductively gives

$$y_n(t) = (-1)^n t^{n+1}/(n+1)! - (-1)^n t^{n+2}/(n+2)!$$

Exercise: Show that the maximum height is $y^\star = y(t^\star)$ where $y'(t^\star) = 0$, $t^\star = \ln(1+\epsilon)/\epsilon$ and $y^\star = 1/\epsilon - \ln(1+\epsilon)/\epsilon^2$. Show that this result can also be obtained using dimensional analysis.

Regular Perturbation Analysis

Exericise: A model for the dynamics of a projectile in the high friction limit is

$$z'' + z' + \delta = 0, \quad z(0) = 0, \quad z'(0) = 1$$

where

- $\delta = 1/\epsilon = mg/(kV)$,
- altitude is given in units $\tilde{z} = Vm/k$ and
- time is given in units $\tilde{t} = m/k$.

Solve this equation by regular perturbation when $0 < \delta \ll 1$.

- What is the maximum altitude reached?
- What is the time of flight?
- What is the ratio between ascent and descent times?

Exercise: The dimensionless form of the pendulum equation is

$$\theta'' + \sin(\theta), \quad \theta(0) = \phi, \quad \theta'(0) = 0$$

where time is given in units $\tilde{t} = \sqrt{\ell/g}$, where ℓ is the length of the pendulum. Solve this equation by regular perturbation when $0 < \phi \ll 1$.

Exponential Growth and Decay

- The specific rate of change, or the temporal rate of change per individual, is $x'(t)/x(t)$, e.g., exponential

$$\text{growth: } x'/x = \beta > 0, \quad \text{decay: } x'/x = -\mu < 0$$

- Example: pollution in a lake, mass conservation gives

$$m' = z - a, \quad VS' = 0 - rS, \quad S(t) = S_0 e^{-rt/V}$$

where $VS = m$, $z = 0$, $a = rS$, $S(0) = S_0$, $\quad \rightarrow \square \rightarrow$

$m =$	mass of pollutant,	$S =$	pollutant concentration
$z =$	inflow,	$V =$	lake volume
$a =$	outflow,	$r =$	flow rate through the lake

specific rate of change: $S'/S = -r/V < 0$.

- Radioactive decay: $x(t) =$ number of atoms in excited state,

$$\text{specific rate of change: } x'/x = -\lambda < 0$$

$$\text{solution with } x(0) = x_0\text{: } x(t) = x_0 e^{-\lambda t}$$

half-life $= \tau$: $\quad x(\tau)/x_0 = e^{-\lambda\tau} = 1/2$

$$-\lambda\tau = -\ln(2) \quad \Rightarrow \quad \lambda = \ln(2)/\tau$$

$$x(t) = x_0 e^{-\ln(2)t/\tau} = x_0 e^{\ln 2^{-t/\tau}} = x_0 2^{-t/\tau}$$

Logistic Growth

- Specific rate of change: $P'/P = \beta - \mu$.
- $\beta = \beta_0 > 0$, $\mu = \mu_0 > 0$ constant $\Rightarrow P(t) = P_0 e^{(\beta_0 - \mu_0)t}$.
- The simplest generalization: linear dependence on the state,
  $$\beta(P) = \beta_0 - \beta_1 P, \quad \mu(P) = \mu_0 + \mu_1 P$$
  With over-population there emerge mechanisms which slow growth, e.g., less incentive to have children ($\beta_1 > 0$) or higher risk of death ($\mu_1 > 0$).
- Defining the parameters $\tau = (\beta_0 - \mu_0)^{-1}$ (time scale) and $K = [\tau(\beta_1 + \mu_1)]^{-1}$ (capacity),
  $$\frac{P'}{P} = \beta(P) - \mu(P) = \frac{1}{\tau}\left(1 - \frac{P}{K}\right)$$
- Under the condition $P(t_0) = P_0$, (Easter Island?)
  $$P(t) = \frac{K}{1 + (\frac{K}{P_0} - 1)e^{-\frac{t-t_0}{\tau}}}$$

Exercise: Solve this initial value problem.

Properties of Equilibria

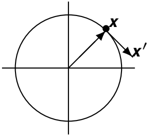
- A dynamical system $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$ is *autonomous* when $\boldsymbol{f}$ does not depend explicity on time t.
- If $\boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0}$ holds, then $\boldsymbol{x}^\star$ is an equilibrium.
- Simple example: $\boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x}$, $\boldsymbol{x}^\star = \boldsymbol{0}$ is an equilibrium.
- Simple example: $\boldsymbol{x} = \langle x, y\rangle^{\mathrm{T}}$, $\boldsymbol{x}' = A\boldsymbol{x}$,

  $$A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{Solution:} \quad \begin{cases} x(t) &= \alpha\cos(t) + \beta\sin(t) \\ y(t) &= \beta\cos(t) - \alpha\sin(t) \end{cases}$$

  Tangent to the solution curve $\boldsymbol{x}' = \langle x', y'\rangle^{\mathrm{T}}$, i.e., in this example $x' = y, y' = -x$ hold and therefore, $\|\boldsymbol{x}\|_{\ell_p} = [\sum_{i=1}^{N} |x_i|^p]^{\frac{1}{p}}$

  $$\frac{1}{2}\frac{d}{dt}\|\boldsymbol{x}(t)\|_{\ell_2}^2 = \frac{1}{2}\frac{d}{dt}\boldsymbol{x}(t)\cdot\boldsymbol{x}(t) = \boldsymbol{x}'\cdot\boldsymbol{x} = \langle y, -x\rangle\cdot\langle x, y\rangle = 0.$$

  The equilibrium $\boldsymbol{x}^\star = \boldsymbol{0}$ is *stable*, because with a perturbation the solution remains nearby.

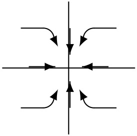
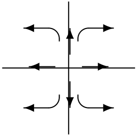
  

- A variation: $B = SAS^{-1}$, $\boldsymbol{x}' = B\boldsymbol{x}$, $\boldsymbol{x}^\star = \boldsymbol{0}$.

  $$\boldsymbol{y} = S^{-1}\boldsymbol{x}, \boldsymbol{y}' = A\boldsymbol{y} \quad \Rightarrow \quad \frac{d}{dt}\|S^{-1}\boldsymbol{x}\|_{\ell_2}^2 = \frac{d}{dt}\|\boldsymbol{y}\|_{\ell_2}^2 = 0.$$

Stability of an Equilibrium

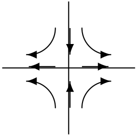
- Example: $\boldsymbol{x}' = A\boldsymbol{x}$, $A = S\Lambda S^{-1}$, $\Lambda = \text{diag}\{\lambda_1, \lambda_2\}$, $\lambda_1, \lambda_2 \in \mathbb{R}$.

  $\lambda_1, \lambda_2 < 0$  $\lambda_1, \lambda_2 > 0$ 

  For the case $\lambda_1, \lambda_2 < 0$ the equilibrium $\boldsymbol{x}^\star = \mathbf{0}$ is *asmptotically stable*, because with a perturbation with solution returns.
  For the case $\lambda_1, \lambda_2 > 0$ the equilibrium is *unstable*.

- Example: $A = S\Lambda S^{-1}$ mit $\Lambda = \text{diag}\{\lambda_1, \lambda_2\}$ and $\lambda_1 \cdot \lambda_2 < 0$, e.g., $\lambda_1 = 1 = -\lambda_2$ and $S = I$.

  Here the equilibrium $\boldsymbol{x}^\star = \mathbf{0}$ is unstable, as with a perturbation the solution *can* fly away.
  Saddle Point:

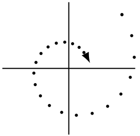
  $$A\boldsymbol{x} = -\nabla P(\boldsymbol{x}), \quad P(x, y) = (y^2 - x^2)/2$$

Stability of an Equilibrium

- Example: $\boldsymbol{x}' = A\boldsymbol{x}$, $\boldsymbol{x} = \langle x, y\rangle^{\mathrm{T}}$

$$A = \begin{bmatrix} -\epsilon & 1 \\ -1 & -\epsilon \end{bmatrix} \quad \text{Eigenvalues: } \begin{cases} 0 = \det(\lambda I - A) = \\ \lambda^2 + 2\epsilon\lambda + \epsilon^2 + 1 \\ \lambda_{1,2} = -\epsilon \pm \imath \end{cases}$$

$$\text{Solution: } \begin{cases} x(t) &= e^{-\epsilon t}[\alpha\cos(t) + \beta\sin(t)] \\ y(t) &= e^{-\epsilon t}[\beta\cos(t) - \alpha\sin(t)] \end{cases}$$



- In general:

$$\begin{aligned} \boldsymbol{x}' &= \boldsymbol{f}(\boldsymbol{x}), \quad \boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0} \\ &= \boldsymbol{f}(\boldsymbol{x}^\star)|_{=\boldsymbol{0}} + \boldsymbol{f}'(\boldsymbol{x}^\star)|_{=A}(\boldsymbol{x} - \boldsymbol{x}^\star) + \boldsymbol{g}(\boldsymbol{x}) \end{aligned}$$

where $\boldsymbol{g}(\boldsymbol{x}) = o(\|\boldsymbol{x} - \boldsymbol{x}^\star\|)$. Für $t \to t_0, g(t) = \begin{cases} \mathcal{O}(f(t)) \Leftrightarrow \lim_{t\to t_0} \frac{g(t)}{f(t)} < \infty \\ o(f(t)) \Leftrightarrow \lim_{t\to t_0} \frac{g(t)}{f(t)} = 0 \end{cases}$

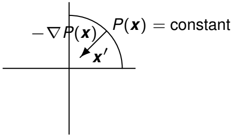
$$(\boldsymbol{x} - \boldsymbol{x}^\star)' = \boldsymbol{x}' = A(\boldsymbol{x} - \boldsymbol{x}^\star) + \boldsymbol{g}(\boldsymbol{x})$$

$\hookrightarrow$ determines the stability of $\boldsymbol{x}^\star$

$$\frac{1}{2}\frac{d}{dt}\|\boldsymbol{x} - \boldsymbol{x}^\star\|_{\ell_2}^2 = (\boldsymbol{x} - \boldsymbol{x}^\star)\cdot(\boldsymbol{x} - \boldsymbol{x}^\star)' \approx (\boldsymbol{x} - \boldsymbol{x}^\star)^{\mathrm{T}} A(\boldsymbol{x} - \boldsymbol{x}^\star) \overset{?}{\leq} 0$$

Potential Landscape

- Saddle point: $\boldsymbol{x}' = A\boldsymbol{x}$, $A = \text{diag}\{1, -1\}$,
$$A\boldsymbol{x} = -\nabla P(\boldsymbol{x}),\ P(x, y) = (y^2 - x^2)/2.$$
- In general: $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}) = -\nabla P(\boldsymbol{x})$, $\exists P$?
To be able to find a *potential* P for a given $\boldsymbol{f}$, it must be that: (P smooth enough)
$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = -\nabla^2 P = -\nabla^2 P^{\mathrm{T}} = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}^{\mathrm{T}}$$
- Meaning of a potential landscape:
Sometimes the state of a dynamical system evolves to minimize a physical potential.



- Example: $\boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x}$,
$$A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = A \neq A^{\mathrm{T}} = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}^{\mathrm{T}}$$
- A rotation develops when $\sigma(A)$ is complex.

Lyapunov Function

- If A is not necessarily symmetric, but $\sigma(A) \subset \mathbb{R}$ and $A = S\Lambda S^{-1}$, $\Lambda = \text{diag}\{\lambda_i\}$, then nevertheless the matrix $S^{-\mathrm{T}}S^{-1}A = S^{-\mathrm{T}}S^{-1}S\Lambda S^{-1} = S^{-\mathrm{T}}\Lambda S^{-1}$ is symmetric! So $\exists P$ with $S^{-\mathrm{T}}S^{-1}A\boldsymbol{x} = -\nabla P(\boldsymbol{x})$ or
$$\boldsymbol{x}' = A\boldsymbol{x} = -SS^{\mathrm{T}}\nabla P(\boldsymbol{x})$$
Then it holds
$$\nabla P(\boldsymbol{x}) \cdot \boldsymbol{x}' = -\nabla P(\boldsymbol{x})SS^{\mathrm{T}}\nabla P(\boldsymbol{x}) = -\|S^{\mathrm{T}}\nabla P(\boldsymbol{x})\|^2 \leq 0$$
and the solution does not increase P.

Def: For $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0}$, a function $F \in C^1(B(\boldsymbol{x}^\star, \epsilon))$ is a *Lyapunov Function* if:

1. F has a single minimum in $\boldsymbol{x}^\star$,
2. $\nabla F(\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x}) \leq 0$, $\forall \boldsymbol{x} \in B(\boldsymbol{x}^\star, \epsilon)$.

If $<$ (for $\boldsymbol{x} \neq \boldsymbol{x}^\star$) holds, then F is a *strict Lyapunov function*.

- A locally convex potential is a Lyapunov function.
- A Lyapunov function is nearly a potential.

Stability for Continuous Dynamical Systems

Def: For $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0}$, the equilibrium $\boldsymbol{x}^\star$ is

- *globally asymptotically stable* if $\forall \boldsymbol{x}_0$
$$\boldsymbol{x}(t) \stackrel{t\to\infty}{\longrightarrow} \boldsymbol{x}^\star,$$
- *locally asymptotically stable* if $\exists \delta > 0$ s.t.
$$|\boldsymbol{x}_0 - \boldsymbol{x}^\star| \leq \delta \Rightarrow \boldsymbol{x}(t) \stackrel{t\to\infty}{\longrightarrow} \boldsymbol{x}^\star,$$
- *locally stable* if $\forall \epsilon > 0$, $\exists \delta > 0$ s.t.
$$|\boldsymbol{x}_0 - \boldsymbol{x}^\star| \leq \delta \Rightarrow |\boldsymbol{x}(t) - \boldsymbol{x}^\star| \leq \epsilon, \forall t \geq 0,$$
- *unstable* if not locally stable.

Theorem (linearized stability): For $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0}$, let $J = \partial \boldsymbol{f} / \partial \boldsymbol{x}(\boldsymbol{x}^\star)$ with spectrum $\sigma(J)$ and $\mu = \max \Re\{\sigma(J)\}$. The equilibrium $\boldsymbol{x}^\star$

- is locally asymptotically stable if $\mu < 0$,
- is unstable if $\mu > 0$,
- could be stable or unstable if $\mu = 0$.

Exercise: Apply the theory to models above.

Stability for Continuous Dynamical Systems

- Example: $\boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x}$,

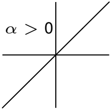
$$A = \begin{bmatrix} -\epsilon & 1 \\ -1 & -\epsilon \end{bmatrix}, \quad \sigma(A) = \{-\epsilon \pm \imath\}, \quad \mu = -\epsilon$$

  - $\epsilon > 0 \Rightarrow \boldsymbol{x}^\star = \boldsymbol{0}$ is locally (globally!) asymptotically stable.
  - $\epsilon < 0 \Rightarrow \boldsymbol{x}^\star = \boldsymbol{0}$ is unstable.
  - $\epsilon = 0$? Stability must be shown directly:

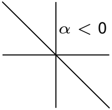
$$\frac{1}{2}\frac{d}{dt}\|\boldsymbol{x}\|_{\ell_2}^2 = \boldsymbol{x} \cdot \boldsymbol{x}' = \boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = 0$$

$$\|\boldsymbol{x}(0)\|_{\ell_2} < \delta = \epsilon \quad \Rightarrow \quad \|\boldsymbol{x}(t) - \boldsymbol{x}^\star\|_{\ell_2} = \|\boldsymbol{x}(t)\|_{\ell_2} = \|\boldsymbol{x}(0)\|_{\ell_2} < \epsilon$$

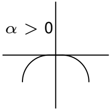
- Example: $f(x) = \alpha x$, $x^\star = 0$, $\mu = f'(0) = \alpha$



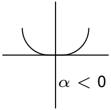
uphill in $x^\star \Rightarrow$ unstable
downhill in $x^\star \Rightarrow$ stable



$$-p'(x) = f(x) \Rightarrow p(x) = -\alpha x^2/2$$



concave in $x^\star \Rightarrow$ unstable
convex in $x^\star \Rightarrow$ stable

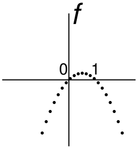


Stability for Continuous Dynamical Systems

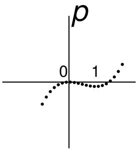
- Example: $f(x) = x(1-x)$, $x^\star \in \{0,1\}$, $f'(x) = 1-2x$

$$\begin{aligned} f'(0) &= \quad 1 > 0 \quad \Rightarrow \text{ unstable} \\ f'(1) &= -1 < 0 \quad \Rightarrow \text{ locally asymptotically stable.} \end{aligned}$$

$$-p'(x) = f(x) \Rightarrow p(x) = (2x-3)x^2/6$$



f uphill, p concave in 0 $\Rightarrow$ unstable
f downhill, p convex in 1 $\Rightarrow$ stable



- Example: $f(x) = -x^2$, $x^\star = 0$, $\mu = f'(0) = -2x|_{x=0} = 0$.

$$x_0 > 0 \Rightarrow f(x_0) < 0 \Rightarrow x(t) \to 0$$
$$x_0 < 0 \Rightarrow f(x_0) < 0 \Rightarrow x(t) \to -\infty$$

$x^\star$ is unstable.

- Example: $f(x) = -x^3$, $x^\star = 0$, $\mu = f'(0) = -3x^2|_{x=0} = 0$.

$$x_0 > 0 \Rightarrow f(x_0) < 0 \Rightarrow x(t) \to 0$$
$$x_0 < 0 \Rightarrow f(x_0) > 0 \Rightarrow x(t) \to 0$$

$x^\star$ is globally asymptotically stable.

Stability for Continuous Dynamical Systems

- Example: $s'' + s = 0$. First order form: $x = s$, $y = s'$,
$$x' = s' = y, \quad y' = s'' = -s = -x$$
$$\boldsymbol{x} = \langle x, y \rangle^{\mathrm{T}}, \quad A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x}, \quad \boldsymbol{x}^\star = \boldsymbol{0}$$
$$\mu = \max \Re\sigma\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}^\star)\right) = \max \Re\sigma(A) = 0.$$
Shown directly above: $\boldsymbol{x}^\star$ is stable.
- Example: $s^{(4)} + 2s^{(2)} + s = 0$. $\langle x, y, u, v \rangle = \langle s, s^{(1)}, s^{(2)}, s^{(3)} \rangle$,
$$x' = y, y' = u, u' = v, v' = -2u - x, \quad \boldsymbol{x} = \langle x, y \rangle^{\mathrm{T}}$$
$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & -2 & 0 \end{bmatrix}, \quad \boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x}, \quad \boldsymbol{x}^\star = \boldsymbol{0}$$
$$\mu = \max \Re\sigma\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}^\star)\right) = \max \Re\sigma(A) = \max \Re\{\lambda : (\lambda^2 + 1)^2 = 0\} = 0.$$
General solution: $s(t) = (\alpha + \beta t)\cos(t) + (\gamma + \delta t)\sin(t)$
$\beta, \delta \neq 0 \quad \Rightarrow \quad \boldsymbol{x}^\star$ unstable.

Stability for Continuous Dynamical Systems

Theorem (Gerschgorin): For $A = \{a_{ij}\}_{i,j=1}^n$ it holds

$$\sigma(A) \subset \bigcup_{i=1}^n R_i \quad \text{where} \quad R_i = \left\{ z \in \mathbb{C} : |z - a_{ii}| \le \sum_{i \ne j=1}^n |a_{ij}| \right\}$$

Furthermore, there are exactly k eigenvalues in $\cup_{j=1}^k R_{i_j}$ if this set has an empty intersection with the other discs.

- Example: $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{f}(\boldsymbol{x}) = A\boldsymbol{x} - \boldsymbol{b}$ where

$$\{a_{ij}\} = A = \text{tridiag}\{\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\alpha}\} \in \mathbb{R}^n$$

$$\boldsymbol{b} = \boldsymbol{\beta} = -\langle 2, \dots, 2 \rangle^{\mathrm{T}} \in \mathbb{R}^n, \quad \boldsymbol{\alpha} = \langle 1, \dots, 1 \rangle^{\mathrm{T}} \in \mathbb{R}^{n-1}$$

$\hat{x}_1 = \hat{x}_k - \hat{x}_{k-1} = \Delta x$
$= \hat{x}_{k+1} - \hat{x}_k = -\hat{x}_n$
$\tilde{x}_k = k\Delta x \overset{k=n}{\rightarrow} -\Delta\tilde{x}$

  - For $A\hat{\boldsymbol{x}} = \boldsymbol{0}$, a direct calculation shows that $\hat{\boldsymbol{x}} = \boldsymbol{0}$ holds. Thus $0 \notin \sigma(A)$. The only equilbrium is $\boldsymbol{x}^\star = A^{-1}\boldsymbol{b}$.
  - Since A is weakly diagonally dominant and $a_{ii} < 0$, it follows from the Gerschgorin Theorem that $\max \Re\{\sigma(A)\} < 0$.
  - Thus for $J = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}^\star) = A$, $\mu = \max \Re\{\sigma(J)\} < 0$, and the equilibrium $\boldsymbol{x}^\star$ is locally asymptotically stable.

With $\lambda_{\max} = \max\{\sigma(A)\}$ and $\theta(t) = \|\boldsymbol{x}(t) - \boldsymbol{x}^\star\|_{\ell_2}^2$ it holds too

$$\tfrac{1}{2}\theta'(t) = (\boldsymbol{x} - \boldsymbol{x}^\star)^{\mathrm{T}} A (\boldsymbol{x} - \boldsymbol{x}^\star) \le \lambda_{\max}\theta(t) \Rightarrow \theta(t) \le \theta(0)e^{\lambda_{\max} t} \Rightarrow \boldsymbol{x}(t) \overset{t\to\infty}{\longrightarrow} \boldsymbol{x}^\star$$

and therefore $\boldsymbol{x}^\star$ is globally asymptotically stable.

Stability of a Dynamic Solution

- Example: $x' = 1$. The solution $\xi(t) = t$ satisfies $\xi(0) = 0$. Let x be a perturbed solution with $x(0) = \epsilon$. The difference $\phi(t) = x(t) - \xi(t)$ satisfies
$$\phi' = x' - \xi' = 0, \quad \phi(0) = \epsilon$$
or $\phi(t) = \epsilon$. It holds $|x(t) - \xi(t)| = |\phi(t)| \overset{t\to\infty}{\longrightarrow} \mathcal{O}(\epsilon)$, and thus the solution $\xi(t)$ is stable.
- Example: A given solution $\boldsymbol{\xi}(t) = \langle \cos(t), \sin(t) \rangle^{\mathrm{T}}$ to
$$\boldsymbol{x}' = (1 - r^2)\boldsymbol{x} + A\boldsymbol{x}, \quad r = \|\boldsymbol{x}\|_{\ell_2}, \quad A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$
Let $\boldsymbol{x}(t)$ be a perturbed solution with $\|\boldsymbol{x}(0)\|_{\ell_2} = r_0 = 1 + \epsilon$. The difference $\boldsymbol{\phi}(t) = \boldsymbol{x}(t) - \boldsymbol{\xi}(t)$ satisfies $\|\boldsymbol{\phi}(0)\|_{\ell_2} = \epsilon$ and
$$(\boldsymbol{\phi} \cdot \boldsymbol{\phi})' = 2(1 - r^2)\boldsymbol{x} \cdot \boldsymbol{\phi} = (1 - r^2)(r^2 - 1 + \boldsymbol{\phi} \cdot \boldsymbol{\phi})$$
or with $\theta = \boldsymbol{\phi} \cdot \boldsymbol{\phi}$ and $r' = (1 - r^2)r$, (where $r \overset{t\to\infty}{\longrightarrow} 1$)
$$\theta' - (r'/r)\theta = -(1 - r^2)^2 \quad \Rightarrow \quad (\theta/r)' = -(1 - r^2)^2/r = (1 - r^{-2})r'$$
$$\theta \overset{t\to\infty}{\longleftarrow} \frac{\theta}{r} = \frac{\epsilon^2}{r_0} + (r - r_0) + (r^{-1} - r_0^{-1}) \overset{t\to\infty}{\longrightarrow} \frac{\epsilon^2}{r_0} - \frac{(1-r_0)^2}{r_0} = \mathcal{O}(\epsilon^2)$$
It holds $\|\boldsymbol{x}(t) - \boldsymbol{\xi}(t)\|_{\ell_2} = \|\boldsymbol{\phi}(t)\|_{\ell_2} = \sqrt{\theta(t)} \overset{t\to\infty}{\longrightarrow} \mathcal{O}(\epsilon)$, and thus the solution $\boldsymbol{\xi}(t)$ is stable.

Chemical Kinetics

- Generic Example:

$$aA + bB \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} cC + dD$$

i.e., a moles of A react with b moles of B, and there result c moles of C and d moles of D.

(1 mole contains $6.022 \cdot 10^{23}$ units.)

- (a, b, c, d) are the *stoichiometric* coefficients.
- A, B are reactants. C, D are Products.
- The reaction can run forwards with $\kappa_1 \gg \kappa_2$ (toward more products) or backwards (toward more reactants) with $\kappa_1 \ll \kappa_2$.
- The *reaction constants* κ_1 and κ_2 depend, e.g., on the surrounding temperature.
- $[A] =$ concentration of A in moles per liter.
- The *reaction extent* is $x(t)$, $x'(t)$ is the *reaction rate*, and the following hold accordingly,

$$\begin{aligned} [A](t) &= [A](0) - a \cdot x(t), & [C](t) &= [C](0) + c \cdot x(t) \\ [B](t) &= [B](0) - b \cdot x(t), & [D](t) &= [D](0) + d \cdot x(t) \end{aligned}$$

Chemische Kinetik

- As a result,

$$\frac{dx}{dt} = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt} = \frac{1}{d}\frac{d[D]}{dt}$$

($a, b, c, d = 1$ is clear, and e.g., $a = 2, b = 0$ is like $A + B \rightsquigarrow A + A$ and $AB \rightsquigarrow A^2$)

$$\begin{aligned} &= \kappa_1 [A]^a [B]^b - \kappa_2 [C]^c [D]^d \\ &= \kappa_1 ([A](0) - a \cdot x)^a ([B](0) - b \cdot x)^b \\ &- \kappa_2 ([C](0) + c \cdot x)^c ([D](0) + d \cdot x)^d \end{aligned}$$

- Simple case:

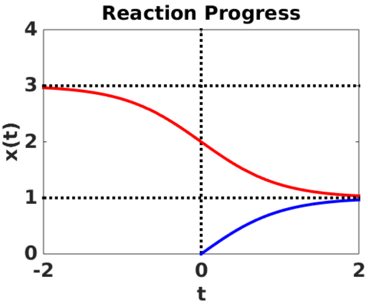
$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} C + D$$

$$\begin{aligned} x' &= \kappa_1(\alpha - x)(\beta - x) - \kappa_2(\gamma + x)(\delta + x) \\ &= \cdots = (\kappa_1 - \kappa_2)(x - x_1)(x - x_2) \end{aligned}$$

$$x_1 = 1, \quad x_2 = 3, \quad \kappa_1 > \kappa_2 \Rightarrow$$

$$f'(x_1) = (\kappa_1 - \kappa_2)(x_1 - x_2) = -f'(x_2) < 0$$

x_1 asymptotically stable, x_2 unstabil



Chemical Bifurcations

- Example: For the chemical reaction,

$$
\begin{aligned}
2A + B \quad &\underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} \quad 2C + D \\
& \kappa_i = \kappa_i(T), \quad i = 1, 2 \\
x' \quad &= \quad \kappa_1 (a - 2x)^2 (b - x) - \kappa_2 (c + 2x)^2 (d + x) \\
&= \quad \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3
\end{aligned}
$$

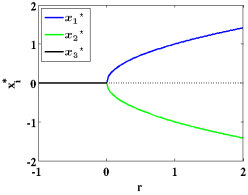
- For $\alpha_0 = 0$, $\alpha_1 = r$, $\alpha_2 = 0$, $\alpha_3 = -1$,

$$x' = f(x), \quad f(x) = x(r - x^2), \quad f'(x) = r - 3x^2$$

Equilibria:

$$
\begin{cases}
x_1^\star = \sqrt{r}, & f'(\sqrt{r}) = -2r < 0, \quad \text{asymptotically stable} \\
x_2^\star = -\sqrt{r}, & f'(-\sqrt{r}) = -2r < 0, \quad \text{same} \\
x_3^\star = 0, & f'(0) = r \begin{cases} r < 0, & \text{same} \\ r = 0, & \text{same} \\ r > 0, & \text{unstable} \end{cases}
\end{cases}
$$

Bifurcation diagram for equilibria:

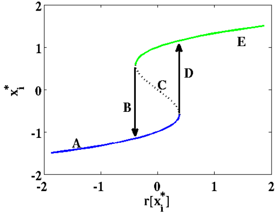


Chemical Hysteresis

- For $\alpha_0 = r$, $\alpha_1 = 1$, $\alpha_2 = 0$, $\alpha_3 = -1$, $\qquad x' = f(x)$

  $f(x) = r + x(1 - x^2), \quad f'(x) = 1 - 3x^2 > 0, -\frac{1}{\sqrt{3}} < x < \frac{1}{\sqrt{3}}$

  Equilbria: $r[x_i^\star] = x_i^\star[x_i^{\star 2} - 1]$, $i = 1, 2, 3$, $-\frac{1}{\sqrt{3}} < x_2^\star < \frac{1}{\sqrt{3}}$



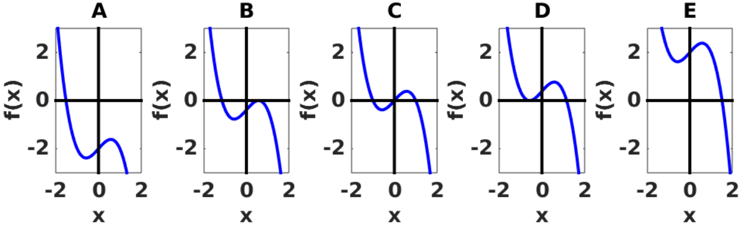
A: $r < -\frac{2}{3\sqrt{3}} \; = r[x_{2,3}^\star(\mathrm{B})] \Rightarrow$ only $x_1^\star$

B: $r = -\frac{2}{3\sqrt{3}} \Rightarrow x_1^\star < x_2^\star = x_3^\star \quad f'(x_{2,3}^\star) = 0$

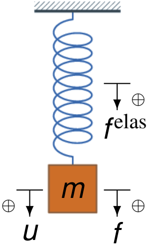
C: $-\frac{2}{3\sqrt{3}} < r < \frac{2}{3\sqrt{3}} \Rightarrow x_1^\star < x_2^\star < x_3^\star$

D: $r = \frac{2}{3\sqrt{3}} \Rightarrow x_1^\star = x_2^\star < x_3^\star \quad f'(x_{1,2}^\star) = 0$

E: $r > \frac{2}{3\sqrt{3}} \; = r[x_{1,2}^\star(\mathrm{D})] \Rightarrow$ only $x_3^\star$



Mass Spring System



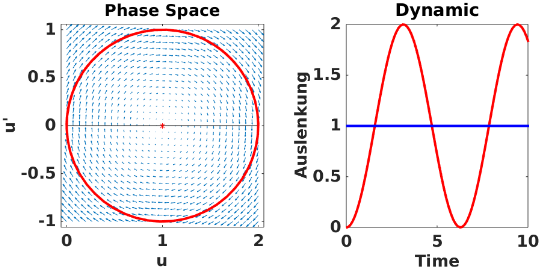
- Let m be a mass and u the downward displacement from the rest state.
- Let f^{elas} be an inner elastic force which works against displacement from the rest state. With
$$f^{\text{elas}} = -ku, \quad k > 0$$
this force is modeled to depend linearly upon u, and k is the *spring constant*.
- Let f be an external downward force on the mass.
- The motion can be modeled acccording to Newtons Law
$$mu'' = -ku + f$$
where u'' is the acceleration and $F(u) = -ku + f$ is the sum of forces acting on the mass m.
- The forces $F(u) = -P'(u)$ can also be represented in terms of a potential minimized by the system
$$P(u) = ku^2/2 - fu$$
where $ku^2/2$ is the elastic energy in the spring and fu represents the opposing work performed by external force.

Harmonic Oscillations

- The ODE $mu'' = -P'(u)$ can be rewritten in first-order form,

$$\underbrace{\begin{bmatrix} 1 & 0 \\ 0 & m \end{bmatrix}}_{=:M} \begin{bmatrix} u \\ u' \end{bmatrix}' = \underbrace{\begin{bmatrix} 0 & 1 \\ -k & 0 \end{bmatrix}}_{=:K} \begin{bmatrix} u \\ u' \end{bmatrix} + \begin{bmatrix} 0 \\ f \end{bmatrix}$$

  The system matrix $A = M^{-1}K$ satisfies $\sigma(A) = \{\pm\imath\sqrt{k/m}\}$.
- A simulation with $m = 1$, $k = 1$ and $f = 1$ gives:



  - The path of the state in phase space is a circle.
  - The mass undergoes *harmonic oscillations* about the rest state $u^\star = f/k = 1$.

Friction Forces

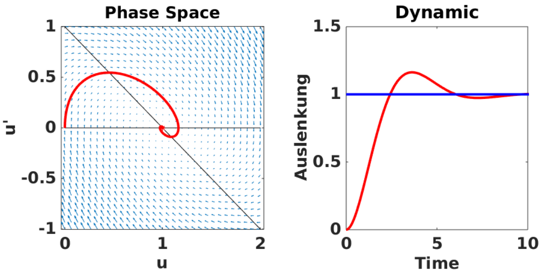
- Such motion is not realistic, because there is internal friction which brings the mass to the rest state.
- The faster the motion, the higher the friction, i.e., a frictional force f^{fric} works against u'.
- This is modeled to depend linearly upon u',
$$f^{\text{fric}} = -cu', \quad c > 0$$
- The ODE $mu'' = -ku + f - cu'$ can be rewritten in first-order form,

$$\underbrace{\begin{bmatrix} 1 & 0 \\ 0 & m \end{bmatrix}}_{=:M} \begin{bmatrix} u \\ u' \end{bmatrix}' = \underbrace{\begin{bmatrix} 0 & 1 \\ -k & -c \end{bmatrix}}_{=:K} \begin{bmatrix} u \\ u' \end{bmatrix} + \begin{bmatrix} 0 \\ f \end{bmatrix}$$

- As the eigenvalues of the system matrix $A = M^{-1}K$ satisfy,
$$\lambda(m\lambda + c) + k = 0, \quad \lambda \in \{(-c \pm \sqrt{c^2 - 4k})/(2m)\}$$
it holds that $\max \Re\{\sigma(A)\} < 0$, and the equilibrium $u^\star = f/k$ ($u' = 0$) is (even globally!) asymptotically stable.
- If $c^2 < 4k$ holds, there are damped oscillations. If $c^2 > 4k$ holds, the rest state is achieved monotonically.

Damped Oscillations

- A simulation with $m = 1$, $k = 1$, $f = 1$ and $c = 1$ gives:



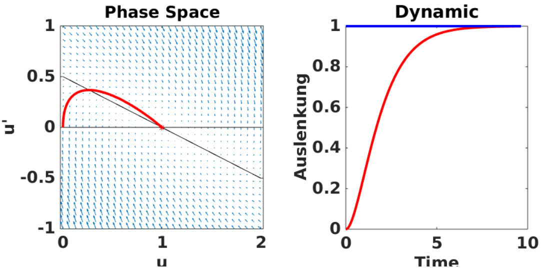
  - The path of the state in phase space is a spiral.
  - On the lines in phase space the direction field is either horizontal (tangent $(u, u')' \propto (u, 0)$, $u' = 0$) or vertical (tangent $(u, u')' \propto (0, u')$, $u = 0$):

$$\begin{array}{rcl} u' = 0 & \Leftarrow & 0 = \\ u' = (f - ku)/c & \Leftarrow & 0 = \end{array} \begin{bmatrix} u \\ u' \end{bmatrix}' = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix} \begin{bmatrix} u \\ u' \end{bmatrix} + \begin{bmatrix} 0 \\ f/m \end{bmatrix}$$

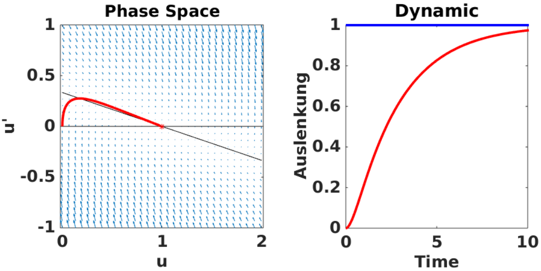
  - The mass undergoes *damped oscillations* around the rest state $u^\star = f/k = 1$. The state is *under damped*.

Damped Oscillations

- With $m = 1$, $k = 1$, $f = 1$ and $c = 2$, i.e., $\sigma(A) = \{-c/(2m)\}$ the state is critically damped:



- With $m = 1$, $k = 1$, $f = 1$ and $c = 3$, i.e., $\sigma(A) = \{(-c \pm \sqrt{c^2 - 4k})/(2m)\} \subset \mathbb{R}$ the state is over damped:



Exercise: Für $A = [0, 1; -1, -3]$ construct P with $A = S\Lambda S^{-1}$, $S^{-\top} S^{-1} A\boldsymbol{x} = -\nabla P(\boldsymbol{x})$ and $\nabla P(\boldsymbol{x}) \cdot \boldsymbol{x}' \leq 0$.

Competing Species

- Size of 2 companies at time t: $x(t)$ and $y(t)$.
- Construction of a specific rate of change for x:

$$\text{without } y: \frac{x'}{x} = a_1, \quad \text{with } y: \frac{x'}{x} = a_1 - b_1 y$$

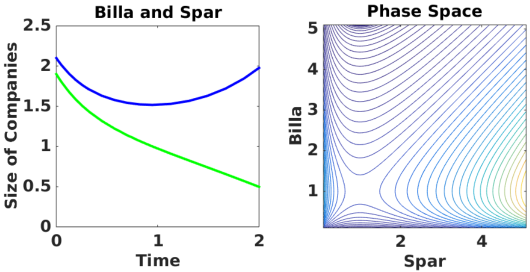
- Construction of a specific rate of change for y:

$$\text{without } x: \frac{y'}{y} = a_2, \quad \text{with } x: \frac{y'}{y} = a_2 - b_2 x$$

- Gause equations: $x^\star = a_2/b_2,\ y^\star = a_1/b_1$

$$x' = (a_1 - b_1 y)x, \quad y' = (a_2 - b_2 x)y$$

simulations: $(a_1 = a_2 = b_1 = b_2 = 1;\ x_0 = 2.1,\ y_0 = 1.9)$



equilibrium

Competing Species

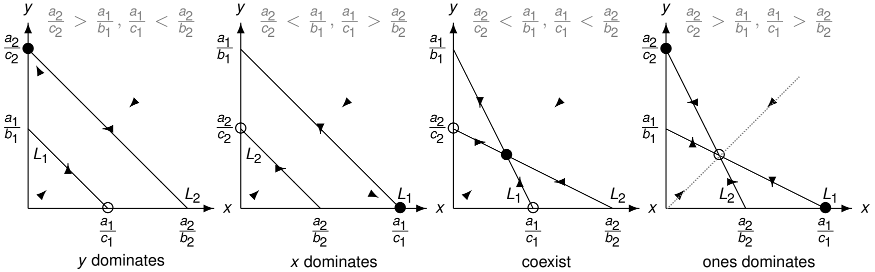
- Logistic change to the above system:

$$x' = (a_1 - c_1 x - b_1 y)x, \quad y' = (a_2 - c_2 y - b_2 x)y$$

i.e., without y, $x' = (a_1 - c_1 x)x$, without x, $y' = (a_2 - c_2 y)y$.

- Phase space with respect to the lines:

$$L_1 : c_1 x + b_1 y = a_1, \quad L_2 : b_2 x + c_2 y = a_2$$



- Companies (and species) coexist in fact.

Predator-Prey Models

- An ecossytem:

$$\begin{aligned} x(t) &= \text{number of herbivores at time } t \\ y(t) &= \text{number of carnivores at time } t \end{aligned}$$

- Construction of a specific rate of change for x:

$$\text{without } y: \frac{x'}{x} = a_1, \quad \text{with } y: \frac{x'}{x} = a_1 - b_1 y$$

- Construction of a specific rate of change for y:

$$\text{without } x: \frac{y'}{y} = -a_2, \quad \text{with } x: \frac{y'}{y} = -a_2 + b_2 x$$

- Lotka-Volterra, predator-prey equations,

$$\begin{aligned} x' &= (a_1 - b_1 y)x \\ y' &= (b_2 x - a_2)y \end{aligned}$$

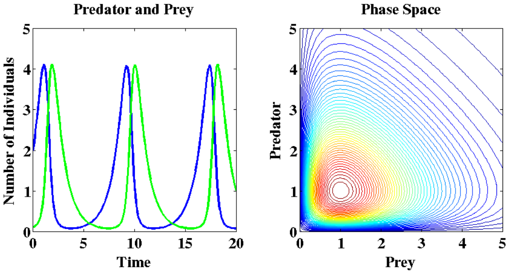
- Equilibrium:

$$x^\star = a_2/b_2, \quad y^\star = a_1/b_1$$

- Yet most solutions are periodic. Realistically?

Predator-Prey

- Simulation: $(a_1 = a_2 = b_1 = 1, b_2 = \frac{1}{2}; x_0 = 2, y_0 = \frac{1}{10})$



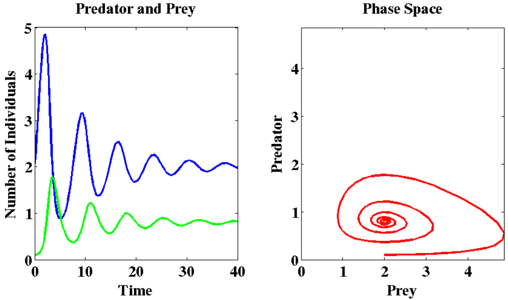
- *Structural Stability*:
  - When nature makes a small perturbation, the system behavior should not change radically.
  - Otherwise the system would adapt to such perturbations until it were more robust.
  - If small perturbations ($\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\tilde{\boldsymbol{x}}' = \tilde{\boldsymbol{f}}(\tilde{\boldsymbol{x}})$, $\boldsymbol{f} - \tilde{\boldsymbol{f}} \in C^1$) are made in a model and the topology of the solutions does not change, the model is *structurally stable*.

Predator-Prey

- Claim: classical predator-prey is not structurally stable.
- When the model is changed as follows,

$$\begin{aligned} x' &= a_1 x(1-\epsilon x) - b_1 xy \\ y' &= (b_2 x - a_2)y \end{aligned}$$

  i.e., the herbivors grow logistically and not exponentially, then the topology of the solutions changes.
- Simulation: $(a_1 = a_2 = b_1 = 1, b_2 = \frac{1}{2}, \epsilon = \frac{1}{10}; x_0 = 2, y_0 = \frac{1}{10})$



- A model with a stable but not asymptotically stable equilibrium is expected not to be structurally stable.

Attractors and Repellers

- Is there a modification of classical predator-prey which leads to a structurally stable model with periodic solutions?
- Yes, in fact, with a stable *limit cycle*:
$$x' = a_1 x\left(1 - \frac{x}{K}\right) - \frac{b_1 xy}{1 + c_1 x}, \quad y' = a_2 y\left(1 - \frac{y}{b_2 x}\right)$$
with prey capacity K, limit b_1/c_1 for the predator effect and predator capacity $b_2 x$.

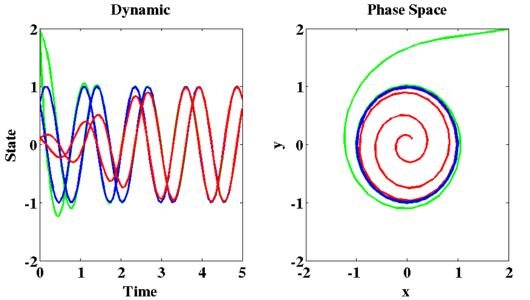
Def: For $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, the set M is an *attractor* if $\exists \delta > 0$ such that $\forall \boldsymbol{x}_0$ with $\text{dist}(\boldsymbol{x}_0, M) < \delta$, the convergence $\text{dist}(\boldsymbol{x}(t), M) \overset{t\to\infty}{\longrightarrow} 0$ holds. If the convergence $\text{dist}(\boldsymbol{x}(t), M) \overset{t\to-\infty}{\longrightarrow} 0$ holds, then M is a *repeller*.

Def: For $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, the set G is a *limit cycle* if a periodic solution $\boldsymbol{x}_G$ lies in G and there exists at least one other solution $\tilde{\boldsymbol{x}}$, which satisfies $\text{dist}(\tilde{\boldsymbol{x}}(t), G) \overset{t\to\infty}{\longrightarrow} 0$ or $\text{dist}(\tilde{\boldsymbol{x}}(t), G) \overset{t\to-\infty}{\longrightarrow} 0$. G is a *stable limit cycle* if it is an attractor, and G is an *unstable limit cycle* if it is a repeller.

Limit Cycles

- Explicit example of a stable *limit cycle*:

$$\begin{cases} x' = (1-r^2)x - 5y \\ y' = (1-r^2)y + 5x \end{cases} \qquad r^2 = x^2 + y^2$$



$$\begin{aligned} xx' &= (1-r^2)x^2 - 5xy \\ yy' &= (1-r^2)y^2 + 5xy \\ \hline rr' = xx' + yy' &= (1-r^2)r^2 \quad \Rightarrow \quad r' = r(1-r^2) \end{aligned}$$

$$\begin{cases} r \in (0,1) \Rightarrow r' > 0 \\ r \in (1,\infty) \Rightarrow r' < 0 \end{cases} \quad \Rightarrow \quad r = 1 \text{ is (asymptotically) stable.}$$

Limit Cycles

- Decomposition into a potential and a rotation:

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} (1-r^2)x \\ (1-r^2)y \end{bmatrix} + A\boldsymbol{x}, \quad A = \begin{bmatrix} 0 & -5 \\ 5 & 0 \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} x \\ y \end{bmatrix}$$

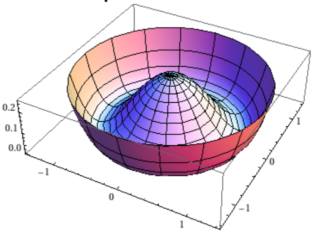
$$\begin{aligned} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} &= \begin{bmatrix} 1-3x^2-y^2 & -5-2xy \\ 5-2xy & 1-x^2-3y^2 \end{bmatrix} \\ &= \begin{bmatrix} 1-2x^2-r^2 & -2xy \\ -2xy & 1-2y^2-r^2 \end{bmatrix} + A \\ &= \text{symmetric} + \text{skew-symmetric} \end{aligned}$$

- It holds

$$\boldsymbol{f}(\boldsymbol{x}) = \underbrace{A\boldsymbol{x}}_{\text{rotation}} - \underbrace{\nabla P(\boldsymbol{x})}_{\text{potential}}$$

with $P(\boldsymbol{x}) = \frac{1}{4}(1-x^2-y^2)^2$

landscape:



Stability for Continuous Systems

- Stability of the equilibrium for classical predator-prey?

$$\boldsymbol{x} = \begin{bmatrix} x \\ y \end{bmatrix}, \quad \boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} (a_1 - b_1 y)x \\ (b_2 x - a_2)y \end{bmatrix}, \quad \boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}), \quad \boldsymbol{x}^\star = \begin{bmatrix} a_2/b_2 \\ a_1/b_1 \end{bmatrix}$$

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} a_1 - b_1 y & -b_1 x \\ b_2 y & b_2 x - a_2 \end{bmatrix}$$

$$J = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}^\star) = \begin{bmatrix} 0 & -b_1 a_2/b_2 \\ b_2 a_1/b_1 & 0 \end{bmatrix}$$

$$\sigma(J) = \{\lambda : \lambda^2 + a_1 a_2 = 0\}, \quad \mu = \max \Re\sigma(J) = 0...?$$

Theorem: If there exists a Lyapunov Function F for $\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$, with $\boldsymbol{f}(\boldsymbol{x}^\star) = \boldsymbol{0}$, then $\boldsymbol{x}^\star$ is a locally stable equilibrium. If F is strict, then $\boldsymbol{x}^\star$ is locally asyptotically stable.

Exercise: Construct a Lyapunov Function to show that the equilibrium for classical predator-prey is stable (although not asymptotically stable).

Chaos

Def: A dynamical system evolving within the phase space set Ω is *chaotic* if

(a) $\forall x_0 \in \Omega$, $\forall \epsilon > 0$, $\exists$ periodic solution π and time t with $|\pi(t) - x_0| < \epsilon$. (periodic solutions are dense)

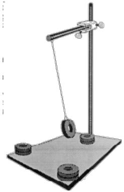
(b) $\forall x_1, x_2 \in \Omega$, $\forall \epsilon > 0$, $\exists$ solution x and times t_1, t_2 with $|x(t_1) - x_1| < \epsilon$, $|x(t_2) - x_2| < \epsilon$. (topologically mixing)

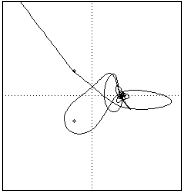
(c) $\exists M > 0$ where for every solution x and $\forall \epsilon > 0$, $\exists$ solution $\tilde{x}$ and time t with $|x(t) - \tilde{x}(t)| > M$ although $|x(0) - \tilde{x}(0)| < \epsilon$. (sensitive dependence - follows from others!)

- Chaos is possible for Systems in $\Omega \subset \mathbb{R}^n$
  - with $n \geq 1$ for discrete Systems, e.g., logistic, but
  - only with $n \geq 3$ for continuous systems, e.g., Lorenz.
- Continuous in $\mathbb{R}^2$: Let $D = \cup\{x \in \pi : \pi \text{ a periodic orbit}\}$. Fix $x \in \overline{D} \backslash D$ and $\{x_n\} \subset D$ with $x_n \in \pi_n$ and $x_n \to x$. System is autonomous and regular, so (Jordan) π_n divides $\mathbb{R}^2$ into an interior I_n and an exterior E_n. Thus π_n separates $x_k \in I_n$ from $x_m \in E_n$ for some $k, m \neq n$ and prevents topological mixing.

Strange Attractors for Chaotic Systems

- Continuous chaotic system: pendulum and magnets





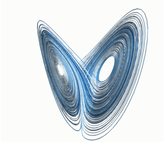
- Degrees of freedom $x_1(t), x_2(t)$, positions in $\mathbb{R}^2$, $v_1(t), v_2(t)$ velocities in $\mathbb{R}^2$.
- State $\langle x_1(t), x_2(t), v_1(t), v_2(t)\rangle \in \mathbb{R}^4$.

- Continuous chaotic system: Lorenz, simplified atmosphere

$$\begin{aligned} \dot{X} &= \sigma(Y - X) \\ \dot{Y} &= (\rho - Z)X - Y \\ \dot{Z} &= XY - \beta Z \end{aligned}$$

$\sigma =$ Prandtl #
$\rho =$ Rayleigh #
$\sigma = 10, \beta = 8/3$,
$\rho = 28 \Rightarrow$ chaos

Strange Attractor
$D \approx 2.06 \pm 0.01$



Def: Let E be a subset of $\mathbb{R}^n$ with diameter $L = \sup\{\|\boldsymbol{x} - \boldsymbol{y}\|_{\ell_2} : \boldsymbol{x}, \boldsymbol{y} \in E\}$ and let $N(\ell)$ be the minimum number of sets with diameter ℓ, which are necessary to cover E. Then the dimension of E is defined as $D(E) = \lim_{l\downarrow 0} \ln(N(\ell))/\ln(L/\ell)$.

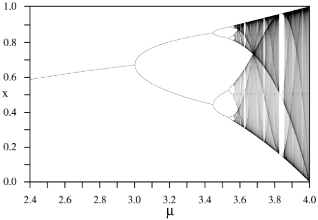
Exercise: Show that the Cantor set has dimension $\ln(2)/\ln(3)$.

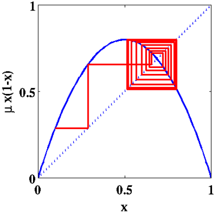
Discrete Models

- Example: logistic evolution,

$$x_{n+1} = \mu x_n(1 - x_n)$$

x_n = population after the n-th time unit or after the n-th transition.





  - $\mu \in [0, 1)$, die off.
  - $\mu \in [1, 3)$, $x_n \to (\mu - 1)/\mu$.
  - $\mu \in [3, 1 + \sqrt{6})$, $x_n \to \{x^\star_{1,0}(\mu), x^\star_{1,1}(\mu)\}$.
  - $\mu \in [\mu_k, \mu_{k+1})$, $x_n \to \{x^\star_{k,j}(\mu)\}_{j=0}^{2^k-1}$ (period doubling).
  - $\mu \approx 3.56995$ and larger, *chaos*.
- Hybrid: continuous model embedded in a discrete model,

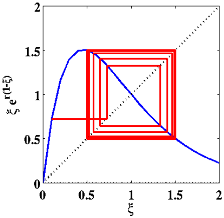
$$y(t_n) = A(x_n), \quad y' = g(y), \quad x_{n+1} = B(y(t_{n+1}))$$

Salmon Dynamics

- State variables:
  - x_n = number of 10^8 salmon (adult) at the end of the n-th spawning cycle, also at the beginning of the $(n+1)$-st.
  - $y(t)$ = number of 10^8 larva at time $t \in [t_n, t_{n+1}]$, i.e., during the $(n+1)$-st spawning cycle.
- Relation between $y(t_n)$ and x_n?
  - $x_n \uparrow \quad \Rightarrow \quad$ females $\uparrow \quad \Rightarrow \quad$ eggs $\uparrow \quad \Rightarrow \quad$ larva $\uparrow$
  - As simple as possible,
$$y(t_n) = \alpha x_n$$
- Relation between $y(t_n)$, i.e., x_n, and $y(t_{n+1})$?
  - Adults eat the larva!
  - $x_n \uparrow \quad \Rightarrow \quad$ number of eaten larva $\uparrow$.
  - As simple as possible,
$$y' = -\beta x_n y, \quad y(t_{n+1}) = y(t_n) e^{-\beta x_n (t_{n+1} - t_n)} = \alpha x_n e^{-\beta x_n (t_{n+1} - t_n)}$$
- Relation between $y(t_{n+1})$ and x_{n+1}?
  - Fraction γ of $y(t_{n+1})$ surviving.
  - Fraction δ of surviving x_n? Pacific: $\delta = 0$. Atlantic: $\delta > 0$. Take Pacific, so $\delta = 0$.
  - As simple as possible,
$$x_{n+1} = \gamma y(t_{n+1}) + \delta x_n$$

Salmon Dynamics

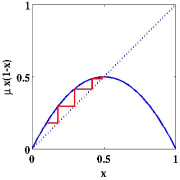
- Everything together
$$x_{n+1} = a x_n e^{-b x_n}$$
where $a = \gamma\alpha$, $b = \beta(t_{n+1} - t_n)$.
- Further,
$$x_{n+1} = x_n e^{\ln a - b x_n} = x_n e^{\ln a [1 - \frac{b}{\ln a} x_n]}$$
- Dimensionless, $r = \ln a$, $\xi_n = \frac{b}{r} x_n$,
$$\xi_{n+1} = \frac{b}{r} x_{n+1} = \frac{b}{r} x_n e^{r(1 - \frac{b}{r} x_n)} = \xi_n e^{r(1-\xi_n)} = F(\xi_n)$$



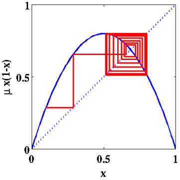
- $r \in (r_0, r_1)$, $\xi_n \to \xi^\star_{0,0} = F(\xi^\star_{0,0})$.
- $r \in (r_1, r_2)$, $\xi_n \to \{\xi^\star_{1,0}, \xi^\star_{1,1}\}$.
$\xi^\star_{1,0} = F(F(\xi^\star_{1,0}))$, $\quad \xi^\star_{1,1} = F(F(\xi^\star_{1,1}))$
- $r \in (r_k, r_{k+1})$, $\xi_n \to \{\xi^\star_{k,j}\}_{j=0}^{2^k - 1}$
e.g., $\xi^\star_{2,i} = F(F(F(F(\xi^\star_{2,i}))))$
(period doubling).
- $r^\star \approx 2.6924$, chaos.

Stability for Discrete Dynamical Systems

- The logistic model: $x_{n+1} = f(x_n), \quad f(x) = \mu x(1-x)$

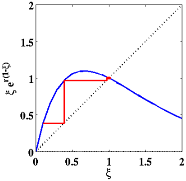


$\mu = 2, \quad x^\star = \frac{\mu-1}{\mu} = \frac{1}{2}$
$f'(x^\star) = 0,$

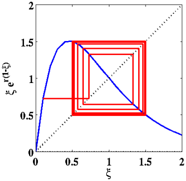


$\mu = \frac{16}{5}, \quad x^\star = \frac{\mu-1}{\mu} = \frac{11}{16}$
$f'(x^\star) = -6/5$

- The salmon model: $\xi_{n+1} = F(\xi_n), \quad F(\xi) = \xi e^{r(1-\xi)}$



$r = \frac{3}{2}, \quad \xi^\star = 1$
$F'(\xi^\star) = -1/2,$



$r = \frac{11}{5}, \quad \xi^\star = 1$
$F'(\xi^\star) = -6/5$

Stability for Discrete Dynamical Systems

Def: For $\boldsymbol{x}^{k+1} = \boldsymbol{f}(\boldsymbol{x}^k)$, where $\boldsymbol{x}^\star = \boldsymbol{f}(\boldsymbol{x}^\star)$, the equilibrium $\boldsymbol{x}^\star$ is

- *globally asymptotically stable* if $\forall \boldsymbol{x}^0$
$$\boldsymbol{x}^k \stackrel{k\to\infty}{\longrightarrow} \boldsymbol{x}^\star,$$
- *locally asymptotically stable* if $\exists \delta > 0$ s.t.
$$|\boldsymbol{x}^0 - \boldsymbol{x}^\star| \leq \delta \Rightarrow \boldsymbol{x}^k \stackrel{k\to\infty}{\longrightarrow} \boldsymbol{x}^\star,$$
- *locally stable* if $\forall \epsilon > 0$, $\exists \delta > 0$ s.t.
$$|\boldsymbol{x}^0 - \boldsymbol{x}^\star| \leq \delta \Rightarrow |\boldsymbol{x}^k - \boldsymbol{x}^\star| \leq \epsilon,\ \forall k \geq 0,$$
- *unstable* if not locally stable.

Theorem (linearized stability): For $\boldsymbol{x}^{k+1} = \boldsymbol{f}(\boldsymbol{x}^k)$, where $\boldsymbol{x}^\star = \boldsymbol{f}(\boldsymbol{x}^\star)$, let $J = \partial \boldsymbol{f}/\partial \boldsymbol{x}(\boldsymbol{x}^\star)$ with spectral radius $\rho(J)$. The equilibrium $\boldsymbol{x}^\star$

- is locally asymptotically stable if $\rho(J) < 1$,
- is unstable if $\rho(J) > 1$,
- could be stable or unstable if $\rho(J) = 1$.

Exercise: Derive a stable periodic orbit for the salmon model.

Stochastic Processes

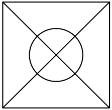
- Previous deterministic models have had the property,
$$\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}), \quad \boldsymbol{x}(t+s) = \ell(t; \boldsymbol{x}(s))$$
that the solution formula ℓ holds independently of s.
- Analogously in probability theory there is the *Markov* property, where the conditional probability
$$P(X(t+s) = j \,|\, X(s) = i)$$
is independent of s. Here $X(t)$ is a random variable and $\{X(t)\}_{t \geq 0}$ is a *stochastic process*.
- In particular it holds that
$$P(X(t+s) = j \,|\, X(s) = i) = P(X(t) = j \,|\, X(0) = i)$$
- Analogous to the model $x' = \text{(birth rate)} - \text{(death rate)}$ or
$$x(t+dt) - x(t) = \underbrace{b(x)dt + o(dt)}_{\text{births in } [t, t+dt]} - \underbrace{d(x)dt + o(dt)}_{\text{deaths in } [t, t+dt]}$$
probabilistically,

$$\begin{aligned} P(X(t+dt) = i+1 \,|\, X(t) = i) &= b_i dt + o(dt) \\ P(X(t+dt) = i-1 \,|\, X(t) = i) &= d_i dt + o(dt) \\ P(X(t+dt) = i \,|\, X(t) = i) &= 1 - \oplus - \ominus = 1 - b_i dt - d_i dt + o(dt) \end{aligned}$$

(constrained transitions)

Markov Property and Bayes Rule

- Let $p_i(t) = P(X(t) = i)$. If the possible states are $X(t) \in \{0, 1, \ldots, N\}$, then



$$
\begin{aligned}
& p_i(t + dt) \\
= \quad & P(X(t + dt) = i) \\
= \quad & \textstyle\sum_{j=0}^{N} P(X(t + dt) = i \,|\, X(t) = j) \cdot P(X(t) = j) && \text{(Bayes)} \\
= \quad & \textstyle\sum_{j=0}^{N} P(X(dt) = i \,|\, X(0) = j) \cdot p_j(t) && \text{(Markov)} \\
= \quad & \textstyle\sum_{|i-j|\le 1} P(X(dt) = i \,|\, X(0) = j) \cdot p_j(t) + o(dt) && \text{(transitions)} \\
= \quad & \underbrace{b_{i-1}\,dt}_{i\ge 1}\, p_{i-1}(t) + (1 - \underbrace{b_i\,dt}_{i\le N-1} - \underbrace{d_i\,dt}_{i\ge 1})p_i(t) + \underbrace{d_{i+1}\,dt}_{i\le N-1}\, p_{i+1}(t) + o(dt)
\end{aligned}
$$

- It follows for $1 \le i \le N$,

$$
p_i'(t) \overset{0\leftarrow dt}{\longleftarrow} \frac{p_i(t + dt) - p_i(t)}{dt} = \overbrace{b_{i-1}}^{i\ge 1} p_{i-1}(t) - (\overbrace{b_i}^{i\le N-1} + \overbrace{d_i}^{i\ge 1})p_i(t) + \overbrace{d_{i+1}}^{i\le N-1} p_{i+1}(t)
$$

or

$$
\boldsymbol{p}' = A\boldsymbol{p}, \quad A = \text{tridiag}\{\underbrace{b_{i-1}}_{i\ge 1}, -(\underbrace{b_i}_{i\le N-1} + \underbrace{d_i}_{i\ge 1}), \underbrace{d_{i+1}}_{i\le N-1}\} \in \mathbb{R}^{(N+1)\times(N+1)}
$$

Population Dynamics

- Example: Population is 1 individual, $N = 1$.

$$\begin{aligned} 0 = P(X(dt) = 1 \,|\, X(0) = 0) &= b_0 dt + o(dt) \Rightarrow b_0 = 0 \\ P(X(dt) = 0 \,|\, X(0) = 1) &= d_1 dt + o(dt) \end{aligned}$$

The system of ODEs $\boldsymbol{p}' = A\boldsymbol{p}$ is

$$\begin{aligned} p_0' &= -b_0|_{=0} p_0 + d_1 p_1 & & \text{with solution,} \\ p_1' &= \qquad\qquad -d_1 p_1 & \Rightarrow \quad & p_1(t) = e^{-d_1 t} p_1(0) \\ & \quad p_0(t) + p_1(t) = 1 & \Rightarrow \quad & p_0(t) = 1 - e^{-d_1 t} p_1(0) \end{aligned}$$

- Example: Population consists of N men, i.e., no births.

$$\begin{aligned} 0 = P(X(dt) = i+1 \,|\, X(0) = i) &= b_i dt + o(dt) \Rightarrow b_i = 0 \\ P(X(dt) = i-1 \,|\, X(0) = i) &= d_i dt + o(dt) \quad d_i = D \end{aligned}$$

For the system of ODEs $\boldsymbol{p}' = A\boldsymbol{p}$,

$$A = \text{tridiag}\{0, -d_i \delta_{i>0}, d_{i+1}\} = \text{tridiag}\{0, -D\delta_{i>0}, D\}$$

Death Process

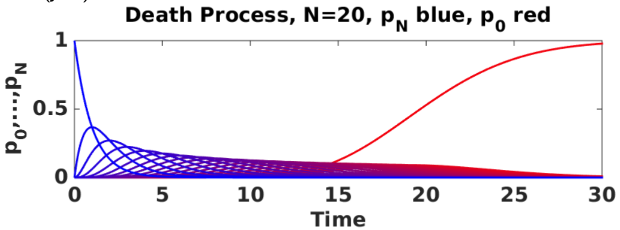
Solution to the system,

$$
\begin{aligned}
p'_N &= -Dp_N \quad\Rightarrow\quad p_N(t) = e^{-Dt}p_N(0)\\
p'_{N-1} &= -Dp_{N-1} + Dp_N = -Dp_{N-1} + De^{-Dt}p_N(0)\\
&\Rightarrow\ (e^{Dt}p_{N-1})' = Dp_N(0) \quad \Big| \quad \int_0^t dt\\
&\Rightarrow\ e^{Dt}p_{N-1}(t) - p_{N-1}(0) = p_N(0)Dt\\
&\Rightarrow\ p_{N-1}(t) = e^{-Dt}[p_{N-1}(0) + p_N(0)Dt]\\
p'_{N-2} &= -Dp_{N-2} + Dp_{N-1} = -Dp_{N-2} + De^{-Dt}[p_{N-1}(0) + p_N(0)Dt]\\
&\Rightarrow\ (e^{Dt}p_{N-2})' = D[p_{N-1}(0) + p_N(0)Dt] \quad \cdots\\
&\Rightarrow\ p_{N-2}(t) = e^{-Dt}[p_{N-2}(0) + p_{N-1}(0)Dt + p_N(0)\tfrac{1}{2}(Dt)^2]
\end{aligned}
$$

usw.

$$p_i(t) = e^{-Dt}\sum_{j=i}^{N} p_j(0)\frac{(Dt)^{j-i}}{(j-i)!}, \quad 1 \le i \le N, \quad p_0(t) = 1 - \sum_{i=1}^{N} p_i(t)$$

With initial conditions $p_i(0) = \delta_{i,N}$:



Death Process

- Confirmation of the formula $p_0(t) = 1 - \sum_{i=1}^{N} p_i(t)$:

$$p_0' = -\sum_{i=1}^{N} p_i' \quad = \quad D\sum_{i=1}^{N} p_i - D\sum_{i=1}^{N-1} p_{i+1}$$
$$= \quad D\sum_{i=1}^{N} p_i - D\sum_{i=2}^{N} p_i = Dp_1 \checkmark$$

- The expected value $E[X(t)]$ satisfies

$$\begin{aligned} E[X(t)] &= \sum_{n=0}^{N} np_n(t) \quad \Rightarrow \\ E[X(t)]' &= \sum_{n=0}^{N} np_n'(t) \\ &= -D\sum_{n=1}^{N} np_n(t) + D\sum_{n=0}^{N-1} np_{n+1}(t) \\ &= -D\sum_{n=1}^{N} np_n(t) + D\sum_{n=1}^{N}(n-1)p_n(t) \\ &= -D\sum_{n=1}^{N} p_n(t) = -D[1 - p_0(t)] \end{aligned}$$

While $p_0(t)$ is small, it holds that

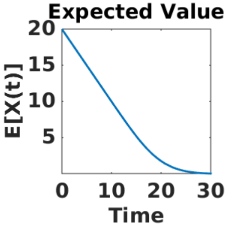
$$E[X(t)]' \approx -D$$

or

$$E[X(t)] \approx E[X(0)] - Dt$$

Finally it holds that

$$E[X(t)] \stackrel{t\to\infty}{\longrightarrow} 0.$$



Birth Process

- Example: A discovery process,
  - $X(t) =$ Number of discoveries until time t.
  - $X(t) \in \{0, \ldots, N\}$
  - It holds that

$$\begin{aligned} P(X(dt) = i+1 \mid X(0) = i) &= b_i dt + o(dt) \quad b_i = B \\ 0 = P(X(dt) = i-1 \mid X(0) = i) &= d_i dt + o(dt) \Rightarrow d_i = 0 \end{aligned}$$

  For the system of ODEs $\boldsymbol{p}' = A\boldsymbol{p}$,

$$A = \text{tridiag}\{b_i, -b_i\delta_{i<N}, 0\} = \text{tridiag}\{B, -B\delta_{i<N}, 0\}$$

- Analogous to a death process,

$$\begin{aligned} p_0' &= -Bp_0 & \Rightarrow \quad & p_0(t) = e^{-Bt}p_0(0) \\ p_1' &= Bp_0 - Bp_1 & \cdots \quad & p_1(t) = e^{-Bt}[p_1(0) + p_0(0)Bt] \\ p_2' &= Bp_1 - Bp_2 & \cdots \quad & p_2(t) = e^{-Bt}[p_2(0) + p_1(0)Bt + p_0(0)\tfrac{1}{2}(Bt)^2] \end{aligned}$$

etc.

$$p_i(t) = e^{-Bt}\sum_{j=0}^{i} p_j(0)\frac{(Bt)^{i-j}}{(i-j)!}, \quad 0 \le i \le N-1, \quad p_N(t) = 1 - \sum_{i=0}^{N-1} p_i(t)$$

Poisson Distribution

- Now an infinite number of states are allowed for a birth process, i.e., $N \to \infty$.
- Sample birth process: Treasures are discovered and not forgotten, so there is no simultaneous death process.
- Let
  - $X(t) =$ number of discovered treasures by time t.
  - $A(t) =$ number of treasures discovered in the time interval $[0, t]$.
- It holds that

$$
\begin{aligned}
P(X(dt) = i+1 \mid X(0) = i) &= b_i dt + o(dt) \quad b_i = B \\
0 = P(X(dt) = i-1 \mid X(0) = i) &= d_i dt + o(dt) \Rightarrow d_i = 0 \\
P(A(t) = k) &= P(X(t) = k \mid X(0) = 0)
\end{aligned}
$$

- For $A(t)$ the initial conditions for $p_n(t)$ are given through $p_n(0) = \delta_{n,0}$, and the *Poisson Distribution* results,

$$P(A(t) = k) = e^{-Bt} \sum_{j=0}^{k} p_j(0) \frac{(Bt)^{k-j}}{(k-j)!} = e^{-Bt} \frac{(Bt)^k}{k!}$$

Poisson Distribution

- The expected value is

$$E[A(t)] = \sum_{n=0}^{\infty} np_n(t) = e^{-Bt}\sum_{n=0}^{\infty} n\frac{(Bt)^n}{n!} = (Bt)e^{-Bt}\sum_{n=1}^{\infty}\frac{(Bt)^{n-1}}{(n-1)!} = Bt$$

- Let G be the time until the next discovery. It holds for $t > 0$

$$\begin{array}{rcl} P(G > t) & = & P(X(t+s) = i \,|\, X(s) = i) \\ \forall i & = & P(X(t+s) = 0 \,|\, X(s) = 0) \\ \forall s & = & P(X(t) = 0 \,|\, X(0) = 0) \\ \text{(with initial conditions)} & = & p_0(t) = e^{-Bt} \end{array}$$

- Let g be the probability density for G, i.e.,

  $$P(G \in M) = \int_M g(s)ds$$

  With the above formula the *Exponential Distribution* results

  $$e^{-Bt} = P(G > t) = \int_t^{\infty} g(s)ds \quad (t > 0)$$

  i.e., $g(t) = Be^{-Bt}$ for $t \geq 0$ and $g(t) = 0$ for $t < 0$.

- The expected value is

$$E[G] = \int_0^{\infty} sg(s)ds = \int_0^{\infty} sBe^{-Bs}ds = 1/B$$

Length of a Queue

- Customers arrive at a single cashier.
  - Let $X(t)$ be number of customers in the queue with
    $$X(t) \in \{0, \ldots, N\}$$
  - Birth: A new customer arrives.
  - Death: A waiting customer is served.
- As seen above, the following hold with corresponding initial conditions.
  - Pure birth process:
    $G =$ time until the next customer arrives.
    $$P(G > t) = e^{-Bt}, \quad E(G) = 1/B =: c$$
    where $c =$ average time between customer arrivals.
  - Pure death process:
    $T =$ time until the next customer is served.
    $$P(T > t) = e^{-Dt}, \quad E(T) = 1/D =: s$$
    where $s =$ average service time for a customer.
- With $b_j = 1/c$ and $d_j = 1/s$ the system $\boldsymbol{p}' = A\boldsymbol{p}$ is

$$\begin{cases} p_0' &= -b_0 p_0 + d_1 p_1 \\ p_j' &= b_{j-1} p_{j-1} - (b_j + d_j) p_j + d_{j+1} p_{j+1}, \quad 0 < j < N \\ p_N' &= b_{N-1} p_{N-1} - d_N p_N \end{cases}$$

Length of a Queue

- Analogous to the previous examples the system matrix is

$$A = \text{tridiag}\{\tfrac{1}{c}, -\tfrac{1}{c}\delta_{i<N}, 0\} + \text{tridiag}\{0, -\tfrac{1}{s}\delta_{i>0}, \tfrac{1}{s}\}$$

$$= \begin{bmatrix} -\frac{1}{c} & \frac{1}{s} & & & 0 \\ \frac{1}{c} & -(\frac{1}{c}+\frac{1}{s}) & \frac{1}{s} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{c} & -(\frac{1}{c}+\frac{1}{s}) & \frac{1}{s} \\ 0 & & & \frac{1}{c} & -\frac{1}{s} \end{bmatrix}$$

- A *stationary* state $\boldsymbol{p}^\star$ ($\boldsymbol{p}' = A\boldsymbol{p} \to 0$) satisfies $A\boldsymbol{p}^\star = 0$.
  - 1. equation:
  $$\frac{p_0^\star}{c} = \frac{p_1^\star}{s}, \quad p_1^\star = \rho p_0^\star, \quad \rho = s/c.$$
  - 2. equation:
  $$0 = \left(\frac{p_0^\star}{c} - \frac{p_1^\star}{s}\right) - \frac{p_1^\star}{c} + \frac{p_2^\star}{s}, \quad p_2^\star = \rho p_1^\star = \rho^2 p_0^\star$$
  - Further,
  $$p_i^\star = \rho^i p_0^\star, \quad 1 \le i \le N$$

Length of a Queue

- $p_0^\star$ is given through

$$1 = \sum_{i=0}^{N} p_i^\star = \sum_{i=0}^{N} \rho^i p_0^\star \quad \text{or} \quad p_0^\star = 1 \Big/ \sum_{i=0}^{N} \rho^i = \frac{1-\rho}{1-\rho^{N+1}}$$

- The expected value is

$$\begin{aligned} E[X^\star] = \sum_{i=0}^{N} i p_i^\star &= p_0^\star \sum_{i=0}^{N} i \rho^i = \rho p_0^\star \frac{d}{d\rho} \sum_{i=1}^{N} \rho^i \\ &= \left[\frac{\rho(1-\rho)}{1-\rho^{N+1}}\right] \frac{d}{d\rho} \left[-1 + \frac{1-\rho^{N+1}}{1-\rho}\right] \\ &= \frac{\rho(1-(N+1)\rho^N + N\rho^{N+1})}{(1-\rho)(1-\rho^{N+1})} \end{aligned}$$

$$E[X^*] \xrightarrow{\rho \to 1} \frac{N}{2}, \qquad E[X^*] \xrightarrow{N \to \infty} \frac{\rho}{1-\rho} =: L_1$$

Waiting Time in a Queue

- I arrive at the queue for a single cashier at time $t = 0$. Let $X(t) =$ number of waiting customers in front of me at time t.
- Let $Y =$ my total waiting time, i.e., the sum of service times for the customers in front of me *plus* my own service time. Distribution? Expected value?
- $c, s =$ average times between customer arrivals and for customer servicing, $\rho = s/c \leq 1$.
- For simplicity it is assumed that the number of customers who can wait in the queue is not bounded or that $N \to \infty$,

$$p_0^\star = \frac{1-\rho}{1-\rho^{N+1}} \overset{N\to\infty}{\longrightarrow} 1-\rho, \quad p_i^\star = \rho^i p_0^\star \overset{N\to\infty}{\longrightarrow} \rho^i(1-\rho)$$

- For the distribution of Y,

$$P(Y \leq t) = \sum_{i=0}^{\infty} P(Y \leq t \,|\, X(0) = i) P(X(0) = i)$$

  - Take $P(X(0) = i) = p_i^\star = \rho^i(1-\rho)$.
  - $P(Y \leq t \,|\, X(0) = i)$ corresponds to the probability $p_0(t)$ that all among a maximum of $i+1$ individuals in a pure death process with initial conditions $p_j(0) = \delta_{i+1,j}$ have expired:

Waiting Time in a Queue

- For the pure death process with initial conditions $p_j(0) = \delta_{i+1,j}$ there holds for $j = 1, \dots, i+1$,

$$p_j(t) = e^{-t/s} \sum_{k=j}^{\infty} \underbrace{p_k(0)}_{=\delta_{i+1,k}} \frac{(t/s)^{k-j}}{(k-j)!} = e^{-t/s} \frac{(t/s)^{i+1-j}}{(i+1-j)!} \quad p_0(t) = 1 - \sum_{j=1}^{i+1} p_j(t)$$

and with $p_0(0) = 0$,

$$p_0'(t) = -\frac{d}{dt} \sum_{j=1}^{i+1} p_j(t) = \frac{e^{-t/s}}{s} \frac{(t/s)^i}{i!}, \quad p_0(t) = \int_0^t \frac{(\tau/s)^i}{i!} \frac{e^{-\tau/s}}{s} d\tau$$

- Summarized,

$$P(Y \le t) = \sum_{i=0}^{\infty} \rho^i (1-\rho) \int_0^t \frac{(\tau/s)^i}{i!} \frac{e^{-\tau/s}}{s} d\tau$$

$$= \frac{1-\rho}{s} \int_0^t e^{-\tau/s} \underbrace{\sum_{i=0}^{\infty} \frac{(\rho\tau/s)^i}{i!}}_{=e^{\rho\tau/s}} d\tau = \frac{1-\rho}{s} \left. \frac{e^{(\rho-1)\tau/s}}{(\rho-1)/s} \right|_0^t = 1 - e^{-(1/s-1/c)t}$$

or $P(Y > t) = 1 - P(Y \le t) = e^{-(1/s-1/c)t}$.

Waiting Time in a Queue

- Let y be the probability density of Y, i.e.,
$$P(Y \in M) = \int_M y(\tau) d\tau$$
With the formula above it follows
$$e^{-(1/s-1/c)t} = P(Y > t) = \int_t^\infty y(\tau) d\tau \quad (t > 0)$$
i.e., the exponential distribution results,
$$y(t) = (1/s - 1/c) e^{-(1/s-1/c)t}$$
- The expected value is
$$E[Y] = \int_0^\infty \tau y(\tau) d\tau = \int_0^\infty \tau (1/s - 1/c) e^{-(1/s-1/c)t}$$
$$= \underbrace{- \tau e^{-(1/s-1/c)\tau} \Big|_0^\infty}_{=0} + \int_0^\infty e^{-(1/s-1/c)\tau} d\tau = \frac{e^{-(1/s-1/c)\tau}}{-(1/s - 1/c)} \Bigg|_0^\infty$$
$$= \frac{1}{1/s - 1/c} = \frac{s}{1-\rho} =: W = cL_1 \quad L_1 = \frac{\rho}{1-\rho}, \quad \rho = \frac{s}{c}$$
- At the stationary state: (expected) waiting time $=$ (average) time between customer arrivals $\times$ (expected) length of the queue at a *single* cashier. Open more cashiers?

Discrete Probabilistic Models

- Example: State of an elevator.
- First the continuous case:
  - Possible states: $X(t) \in \{0\ (\mathrm{G})\ , \ldots, N\}$, i.e., $N+1$ floors.
  - $X(t) = i$ at time t if at the i-th floor or
    on the way to the i-th floor.
  - Birth: $X(t) = i \quad \rightarrow \quad X(t+dt) = i+1$.
  - Death: $X(t) = i \quad \rightarrow \quad X(t+dt) = i-1$.

e.g., $N = 2$, $\boldsymbol{p}' = A\boldsymbol{p}$, where

$$A = \begin{bmatrix} -b_0 & d_1 & 0 \\ b_0 & -(b_1+d_1) & d_2 \\ 0 & b_1 & -d_2 \end{bmatrix}, \quad \text{i.e.} \quad \begin{matrix} d_0 = 0 \\ \\ b_2 = 0 \end{matrix}$$

Solution: With $A = S\Lambda S^{-1}$, $\boldsymbol{p}(t) = e^{At}\boldsymbol{p}_0 = Se^{\Lambda t}S^{-1}\boldsymbol{p}(0)$

$$b_0 = b_1 = d_1 = d_2 \quad \Rightarrow \quad \boldsymbol{p}(t) \xrightarrow{t\to\infty} \langle \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \rangle^{\mathrm{T}}$$

i.e., all floors are equally likely in the long run.

Markov Chains

- Now the discrete case:
  - $X(n) = i$ if at the i-th floor after the n-th transition.
  - $n =$ transition index, non-linear time.
  - $p_i(n) = P(X(n) = i)$
- The distribution for a transition is given through

$$p_j(1) = \sum_{i=0}^{N} \underbrace{P(X(1) = j \mid X(0) = i)}_{P_{i,j}} p_i(0)$$

  $P = \{P_{i,j}\}$ is the transition probability matrix. $\sum_{j=0}^{N} P_{i,j} = 1$

Def: A *Markov Chain* (linear with contant transition probabilities) is a discrete time dynamic model consisting of states $\{S_i\}$ and probabilities $\{P_{i,j}\}$, where the transition $S_i|_n \to S_j|_{n+1}$ takes place with probability $P_{i,j}$.

- One step of the above Markov chain is represented through

$$\boldsymbol{p}^{\mathrm{T}}(1) = \boldsymbol{p}^{\mathrm{T}}(0)P$$

  and n steps through

$$\boldsymbol{p}^{\mathrm{T}}(n) = \boldsymbol{p}^{\mathrm{T}}(n-1)P = \cdots = \boldsymbol{p}^{\mathrm{T}}(0)P^n$$

State of an Elevator

- Take $N = 2$. One never travels through the transitions $0 \to 2$ or $2 \to 0$. Hence,
$$P_{2,0} = P_{0,2} = 0$$
- One never makes a transition $i \to i$. Hence,
$$P_{0,0} = P_{1,1} = P_{2,2} = 0$$
- Since the row sum of the transition matrix is always 1, it follows for some $\theta \in [0, 1]$
$$P = \begin{bmatrix} 0 & 1 & 0 \\ \theta & 0 & 1-\theta \\ 0 & 1 & 0 \end{bmatrix} \quad \text{and} \quad P^{2k} = \begin{bmatrix} \theta & 0 & 1-\theta \\ 0 & 1 & 0 \\ \theta & 0 & 1-\theta \end{bmatrix}, \quad P^{2k+1} = P$$
- Therefore,
$$\boldsymbol{p}(0) = \langle 1, 0, 0 \rangle^{\mathrm{T}} \quad \Rightarrow \quad \boldsymbol{p}(2k+1) = \langle 0, 1, 0 \rangle^{\mathrm{T}}, \quad \boldsymbol{p}(2k) = \langle \theta, 0, 1-\theta \rangle^{\mathrm{T}}$$
- Starting from G the elevator will certainly be in the middle floor after odd transitions, but this is not possible after even transitions.
- The difference between the continuous and the discrete result has to do with the time variables t vs. n.

Weather Transitions

- Example: Assume the weather on a given day is in one of the states: S (sunny), W (cloudy) or R (rainy).
- Estimated transition probabilities are summarized in the table,

	S	W	R
S	$\frac{1}{2}$	$\frac{1}{2}$	0
W	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
R	0	$\frac{1}{2}$	$\frac{1}{2}$

$$P = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$(P^n > 0, n > 1)$
(mixing)

- $P \in \mathbb{S}$ (*stochastic matrices*): $(\mathbf{1})_i = 1, \forall i \Rightarrow P\mathbf{1} = \mathbf{1}$.
- $\boldsymbol{s} \in \mathbb{W}$ (*probability vectors*): $(\boldsymbol{s})_i \in [0, 1]$ and $\boldsymbol{s} \cdot \mathbf{1} = 1$.
- With starting state $\boldsymbol{s}^n \in \mathbb{W}$, the transition state is $\boldsymbol{s}^{n+1} = P^{\mathrm{T}}\boldsymbol{s}^n \in \mathbb{W}$.
- With starting state $\boldsymbol{s}^0 \in \mathbb{W}$, the n-th state is $\boldsymbol{s}^n = (P^{\mathrm{T}})^n\boldsymbol{s}^0 \in \mathbb{W}$.
- For the example $\boldsymbol{s}^n \overset{n\to\infty}{\longrightarrow} \hat{\boldsymbol{s}} = \langle \frac{2}{5}, \frac{2}{5}, \frac{1}{5} \rangle^{\mathrm{T}}$ (equilibrium).

Theorem: For $P \in \mathbb{S}$ with $P^n > 0, n > 1$, $\exists! \hat{\boldsymbol{s}} \in \mathbb{W}$, where $P^{\mathrm{T}}\hat{\boldsymbol{s}} = \hat{\boldsymbol{s}}$, and $(P^{\mathrm{T}})^n\boldsymbol{e}_i \overset{n\to\infty}{\longrightarrow} \hat{\boldsymbol{s}}, \forall \boldsymbol{e}_i$ with $(\boldsymbol{e}_i)_j = \delta_{i,j}$.

Compartment Models

- A *compartment* in a model is a homogeneous unit, in which the state of like system elements depends at most upon time.
- A compartment can be spatially connected or not. See the SIR model below.
- Example: For the heating problem
  - the house is one compartment and the outside environment is one compartment.
  - The temperature is spatially constant inside each compartment.
  - The parameters are constant within and at the boundary of each compartment.
- Example: For a pharmacokinetic problem
  - the compartments are different volumes in the body, in which the concentration of a medicine is constant.
  - The parameters are constant within and on the boundary of each compartment.
- A compartment model is a lumped parameter model.

Infection Models

- The goal of this modeling is to understand and possibly to control the spread of a disease.
- Goal questions:
  - Does the disease die out?
  - Does the disease become endemic?
  - Does the disease always come back after apparently disappearing?
  - How can one control the disease?
- The disease can be thought of as existing among living beings (at risk of an epidemic) or, e.g., among firms (at risk of a financial crisis).
- For the so-called SIR model 3 compartments are identified:
  - S = *susceptible*
  - I = *infected*
  - R = *recovered*
- Assumed effects:

$$S \xrightarrow{+} I, \quad I \xrightarrow{-} S, \quad I \xrightarrow{+} R$$

SIR Model

- Set balance:

$$\begin{array}{c}\text{internal rate}\\ \text{of change}\end{array} = \begin{array}{c}\text{immigration}\\ -\text{emigration}\end{array} + \begin{array}{c}\text{birth}-\\ \text{death}\end{array} \pm \text{infection} \pm \text{healing}$$

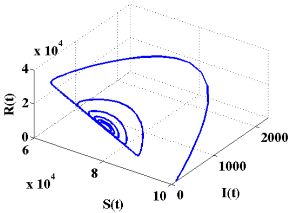
- It is assumed:
  - Emigration is negligible, and the immigrants are susceptible, i.e.,
    $$S' = \beta + \cdots \quad , \text{immigration rate} = \beta > 0$$
  - In each group the fertility (birth rate) is smaller than the mortality (death rate), i.e.,
    $$S' = \beta - \mu S + \cdots \quad , \text{(net) mortality} = \mu > 0$$
    $$I' = -\mu I + \cdots \quad R' = -\mu R + \cdots$$
  - Because of the effect $I \xrightarrow{-} S$, the reduction in S depends upon the infection from I. The simplest relationship is linear:
    $$S' = \beta - (\mu + \lambda I)S, \quad \text{susceptibility} = \lambda > 0$$
  - Because of the effect $S \xrightarrow{+} I$, the increase in I depends upon the transmission to S, and the increase of I balances with the reduction of S. It follows
    $$I' = (\lambda S - \mu)I + \cdots$$

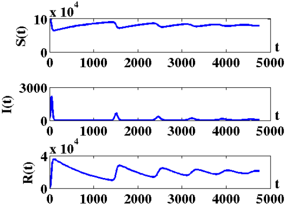
Formulation and Solution of the SIR Model

- It is assumed:
  - Because of the effect $I \xrightarrow{+} R$, the increase in R depends upon healing of I. The simplest relationship is linear:
    $$R' = -\mu R + \gamma I, \quad \text{healability} = \gamma > 0$$
  - The increase of R through healing balances with the corresponding reduction of I. Finally it follows
    $$I' = (\lambda S - \mu - \gamma) I$$
- Summarized,

$$S' = \beta - (\mu + \lambda I) S, \quad I' = (\lambda S - \mu - \gamma) I, \quad R' = -\mu R + \gamma I$$

- Solution with $\beta = 100$, $\mu = 0.001$, $\gamma = 0.4$, $\lambda = 5 \cdot 10^{-6}$,





Investigation of the SIR Model

- Equilibria:
  - Case 1 (healthy):
    $$S_1^\star = \frac{\beta}{\mu},\ I_1^\star = 0,\ R_1^\star = 0$$
  - Case 2 (endemic):
    $$S_2^\star = \frac{\mu+\gamma}{\lambda},\ I_2^\star = \frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda},\ R_2^\star = \frac{\gamma}{\mu}\left[\frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda}\right]$$
    only meaningful if $I_2^\star > 0$.
- Are these equilibria stable?
- There is no coupling from R back to the S- and I-equations, so R is determined from (S, I).
- Let
  $$\boldsymbol{x} = \begin{bmatrix} S \\ I \end{bmatrix}, \quad \boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} \beta - \mu S - \lambda S I \\ -(\gamma+\mu)I + \lambda S I \end{bmatrix}$$
- It holds
  $$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} -\mu - \lambda I & -\lambda S \\ \lambda I & -(\gamma+\mu) + \lambda S \end{bmatrix}$$
- For $\boldsymbol{x}_1^\star = \langle S_1^\star, I_1^\star \rangle^{\mathrm{T}}$, $(S_1^\star = \beta/\mu,\ I_1^\star = 0 = R_1^\star)$
  $$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}_1^\star) = \begin{bmatrix} -\mu & -\lambda\beta/\mu \\ 0 & -(\gamma+\mu) + \lambda\beta/\mu \end{bmatrix}, \quad \left.\frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda}\right|_{=I_2^\star} \overset{?}{<} 0$$

Investigation of the SIR Model

- When $I_2^\star < 0$, $(S_1^\star, I_1^\star, R_1^\star)$ is locally asymptotically stable.
- When $I_2^\star > 0$, $(S_1^\star, I_1^\star, R_1^\star)$ is unstable.

Exercise: Investigate the stability explicitly for the solution shown graphically above. How can one steer toward the healthy equilibrium?

General (global) result for the case $I_2^\star > 0$:

- There are 2 equilibria: healthy and endemic.
- When $I(0) > 0$, $(S, I, R) \overset{t\to\infty}{\longrightarrow} (S_2^\star, I_2^\star, R_2^\star)$ (endemic).
- When $I(0) = 0$, $(S, I, R) \overset{t\to\infty}{\longrightarrow} (S_1^\star, I_1^\star, R_1^\star)$ (healthy).

General (global) result for the case $I_2^\star < 0$:

- It holds $(S, I, R) \overset{t\to\infty}{\longrightarrow} (S_1^\star, I_1^\star, R_1^\star)$ (healthy).

Given these results:

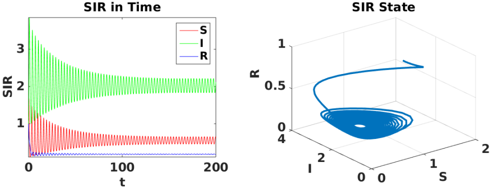
- There is no periodic solution.

Exercise: Develop a variant of this model for which there is a periodic solution. (attractor? R-coupling?)

SIR Models with Periodic Solutions

- Classic predator-prey model with backward R-coupling:

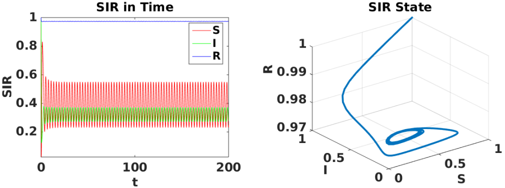
$$
\begin{aligned}
S' &= S(a_1 - a_2 I) + a_5 R \\
I' &= I(a_2 S - a_3) - a_4 I \\
R' &= a_4 I - a_5 R - a_6 R
\end{aligned}
$$



R-coupling creates a limit cycle!

- Logistic variant of the predator-prey model:

$$
\begin{aligned}
S' &= a_1 S(1 - S/a_3) + a_7 R \\
&\quad - a_4 SI/(1 + a_6 S) \\
I' &= a_2 I(1 - I/(a_5 S)) \\
&\quad - a_8 I \\
R' &= a_8 I + a_1 R(1 - R/a_3) \\
&\quad - a_7 R
\end{aligned}
$$



has a limit cycle also with backward R-coupling.

Time Dependent Susceptability

- The modified model

$$S'(t) = \beta - \lambda(t)SI - \mu S, \quad I'(t) = \lambda(t)SI - \gamma I - \mu I, \quad R'(t) = \gamma I - \mu R$$

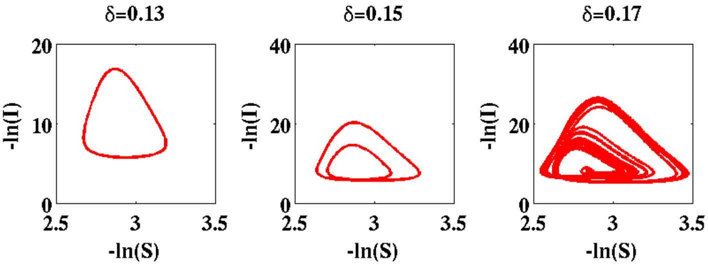
  with time dependent λ for season dependence,

$$\lambda(t) = (\delta \sin(2\pi t) + 1)\lambda_0, \quad \lambda_0 \in (0, \infty), \quad \delta \in [0, 1]$$

- No backward R-coupling.
- Simulations are carried out for the (S, I)-system with the parameters:

$$\mu = \beta = 0.04, \lambda_0 = 1800, \gamma = 100$$

- The parameter δ is increased, and period doubling (in limit cycles) and apparent transition to chaos are exhibited:



Discrete SIR Model

- The discrete SIR Model

$$
\begin{aligned}
S^{k+1} &= \beta + (1 - \mu - \lambda I^k) S^k \\
I^{k+1} &= (\lambda S^k + 1 - \mu - \gamma) I^k \\
R^{k+1} &= (1 - \mu) R^k + \gamma I^k
\end{aligned}
$$

  can also be viewed as a discretization of the system of ODEs.
- Qualitative behaviour similar?
  - Equilibria stable?
  - Periodic solutions?
- Equilibria: $S^{k+1} = S^k$, $I^{k+1} = I^k$, $R^{k+1} = R^k$,
  - Case 1 (healthy):
    $$S_1^\star = \frac{\beta}{\mu},\ I_1^\star = 0,\ R_1^\star = 0$$
  - Case 2 (endemic):
    $$S_2^\star = \frac{\mu+\gamma}{\lambda},\ I_2^\star = \frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda},\ R_2^\star = \frac{\gamma}{\mu}\left[\frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda}\right]$$
    only meaningful when $I_2^\star > 0$.

  reflect the conditions for the system of ODEs. Stability?

Discrete SIR Model

- There is no backward coupling from R to the S- and I-equations, so R is determined from (S, I).
- Let
$$\boldsymbol{x} = \begin{bmatrix} S \\ I \end{bmatrix}, \quad \boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} \beta + (1 - \mu - \lambda I)S \\ (\lambda S + 1 - \mu - \gamma)I \end{bmatrix}$$
- It holds
$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} 1 - \mu - \lambda I & -\lambda S \\ \lambda I & \lambda S + 1 - \gamma - \mu \end{bmatrix}$$
- For $\boldsymbol{x}_1^\star = \langle S_1^\star, I_1^\star \rangle^{\mathrm{T}}$, $(S_1^\star = \beta/\mu,\ I_1^\star = 0 = R_1^\star)$
$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}_1^\star) = \begin{bmatrix} 1 - \mu & -\lambda\beta/\mu \\ 0 & \lambda\beta/\mu + 1 - \mu - \gamma \end{bmatrix}$$
- Stability conditions: $\left(I_2^\star = \frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda}\right)$
$$\begin{aligned} |1 - \mu| < 1 \quad &\Leftrightarrow \quad \mu \in (0, 2) \\ |\lambda\beta/\mu + 1 - \mu - \gamma| < 1 \quad &\Leftrightarrow \quad \lambda(1 + \gamma/\mu)(-I_2^\star) \in (0, 2) \end{aligned}$$
  reflect the conditions for the system of ODEs.
- Periodic solutions? $\boldsymbol{f}(\boldsymbol{f}(\boldsymbol{x}^\star)) = \boldsymbol{x}^\star \neq \boldsymbol{f}(\boldsymbol{x}^\star)$

Exercise: Implement the model and investigate.

Discrete SIR Model

- With $\beta = 1$, $\mu = 3$, $\gamma = 3$, $\lambda = 30$, solutions to $\boldsymbol{f}(\boldsymbol{f}(\boldsymbol{x}^\star)) = \boldsymbol{x}^\star$ are given by

$$
\begin{aligned}
S_1 &= \tfrac{1}{3}, & I_1 &= 0 \\
S_2 &= \tfrac{1}{5}, & I_2 &= \tfrac{1}{15} \\
S_3 &= \tfrac{1}{15}(4+\sqrt{2}), & I_3 &= \tfrac{1}{60}(2-\sqrt{2}) \\
S_4 &= \tfrac{1}{15}(4-\sqrt{2}), & I_4 &= \tfrac{1}{60}(2+\sqrt{2})
\end{aligned}
$$

  which are 1- and 2-periodic but unstable solutions.

Exercise: Consider

$$
\begin{cases}
S_{k+1} = S_k + S_k(1 - S_k/100) - \lambda S_k I_k/(1 + S_k/10) \\
I_{k+1} = I_k + I_k(1/10 - I_k/S_k)
\end{cases}
$$

for a suitable parameter $\lambda \in (\frac{1}{2}, \frac{3}{2})$ to determine whether there are stable or unstable equilibria, limit cycles or even period doubling and transition to chaos.

Stochastic SIR Model

- Let the dynamic number of susceptible, infected and recovered individuals be represented by stochastic processes:
$$S, I, R : [0, \infty) \to \mathbb{N}_0$$
- At time t the random variables $S(t)$, $I(t)$ and $R(t)$ have the respective distributions,

$$s_n(t) = P(S(t) = n), \quad i_n(t) = P(I(t) = n), \quad r_n(t) = P(R(t) = n)$$

- Let $\overline{S}(t)$, $\overline{I}(t)$ and $\overline{R}(t)$ be the expected values of $S(t)$, $I(t)$ and $R(t)$ at time t.
- Conditional probabilities are modeled for S as follows:

$$P(S(t + dt) = n + 1 \mid S(t) = n) = \beta dt$$

$$P(S(t + dt) = n - 1 \mid S(t) = n)$$

$$= \sum_{m=0}^{\infty} P(S(t + dt) = n - 1 \mid S(t) = n, I(t) = m) i_m(t)$$

$$P(I(t) = m \mid S(t) = n) \to i_m(t)$$

$$= \sum_{m=0}^{\infty} ndt(\mu + m\lambda) i_m(t) = ndt[\mu + \lambda \overline{I}(t)]$$

Stochastic SIR Model

- Conditional probabilities are modeled for I as follows:

$$P(I(t+dt)=n-1 \mid I(t)=n)=(\mu+\gamma)ndt$$

$$P(I(t+dt)=n+1 \mid I(t)=n)$$
$$=\sum_{m=0}^{\infty} P(I(t+dt)=n+1 \mid I(t)=n, S(t)=m)s_m(t)$$

$$P(S(t)=m \,|I(t)=n) \rightarrow s_m(t)$$

$$=\sum_{m=0}^{\infty} nm\lambda s_m(t)dt=\lambda n\overline{S}(t)dt$$

- Conditional probabilities are modeled for R as follows:

$$P(R(t+dt)=n-1 \mid R(t)=n)=\mu ndt$$

$$P(R(t+dt)=n+1 \mid R(t)=n)$$
$$=\sum_{m=0}^{\infty} P(R(t+dt)=n+1 \mid R(t)=n, I(t)=m)i_m(t)$$

$$P(I(t)=m \,|R(t)=n) \rightarrow i_m(t)$$

$$=\sum_{m=0}^{\infty} \gamma m i_m(t)dt=\gamma\bar{I}(t)dt$$

Stochastic SIR Model

- The dynamics for $\{s_n(t)\}_{n=0}^{\infty}$ are modeled as follows:

$$\begin{aligned}
s_n(t+dt) &= P(S(t+dt)=n \mid S(t)=n-1)s_{n-1}(t) \\
&+ P(S(t+dt)=n \mid S(t)=n+1)s_{n+1}(t) \\
&+ P(S(t+dt)=n \mid S(t)=n)s_n(t) \\
&= \beta s_{n-1}(t)dt \\
&+ (n+1)dt[\mu+\lambda\bar{I}(t)]s_{n+1}(t) \\
&+ \{1-\beta dt - ndt[\mu+\lambda\bar{I}(t)]\}s_n(t)
\end{aligned}$$

or

$$s_n'(t) = \beta s_{n-1}(t) - \{\beta + n[\mu+\lambda\bar{I}(t)]\}s_n(t) + (n+1)[\mu+\lambda\bar{I}(t)]s_{n+1}(t)$$

- and similarly for $\{i_n(t)\}_{n=0}^{\infty}$,

$$i_n'(t) = (n-1)\lambda\overline{S}(t)i_{n-1}(t) - [n\lambda\overline{S}(t)+n(\mu+\gamma)]i_n(t) + (n+1)(\mu+\gamma)i_{n+1}(t)$$

- and for $\{r_n(t)\}_{n=0}^{\infty}$,

$$r_n'(t) = \gamma\bar{I}(t)r_{n-1}(t) - [\gamma\bar{I}(t)+n\mu]r_n(t) + (n+1)\mu r_{n+1}(t)$$

Exercise: Derive a system of ODEs for $(\overline{S}, \overline{I}, \overline{R})$.

Equilibria for the Stochastic Model

- Assume there are only $N < \infty$ positions in the living space.
- For $N = 2$ the above stochastic system is:

$$\begin{bmatrix} s_0 \\ s_1 \\ s_2 \end{bmatrix}'(t) = \begin{bmatrix} -\beta & [\mu + \lambda \bar{I}(t)] & 0 \\ \beta & -\{\beta + [\mu + \lambda \bar{I}(t)]\} & 2[\mu + \lambda \bar{I}(t)] \\ 0 & \beta & -2[\mu + \lambda \bar{I}(t)] \end{bmatrix} \begin{bmatrix} s_0 \\ s_1 \\ s_2 \end{bmatrix}(t)$$

$$\begin{bmatrix} i_0 \\ i_1 \\ i_2 \end{bmatrix}'(t) = \begin{bmatrix} 0 & (\mu + \gamma) & 0 \\ 0 & -[\lambda \overline{S}(t) + (\mu + \gamma)] & 2(\mu + \gamma) \\ 0 & \lambda \overline{S}(t) & -2(\mu + \gamma) \end{bmatrix} \begin{bmatrix} i_0 \\ i_1 \\ i_2 \end{bmatrix}(t)$$

$$\begin{bmatrix} r_0 \\ r_1 \\ r_2 \end{bmatrix}'(t) = \begin{bmatrix} -\gamma \bar{I}(t) & \mu & 0 \\ \gamma \bar{I}(t) & -[\gamma \bar{I}(t) + \mu] & 2\mu \\ 0 & \gamma \bar{I}(t) & -2\mu \end{bmatrix} \begin{bmatrix} r_0 \\ r_1 \\ r_2 \end{bmatrix}(t)$$

Exercise: Show that the only equilibrium is

$$s_0 = 1/(1 + \tfrac{\beta}{\mu} + \tfrac{\beta^2}{2\mu^2}), \quad s_1 = \tfrac{\beta}{\mu} s_0, \quad s_2 = \tfrac{\beta^2}{2\mu^2} s_0, \quad i_0 = 1, \quad r_0 = 1$$

with $(\overline{S}, \bar{I}, \overline{R}) = (\tfrac{\beta}{\mu}(1 + \tfrac{\beta}{\mu})/(1 + \tfrac{\beta}{\mu} + \tfrac{\beta^2}{2\mu^2}), 0, 0) \approx (S_1^\star, I_1^\star, R_1^\star)$.

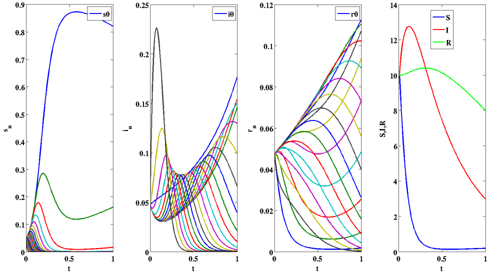
- What about $(S_2^\star, I_2^\star, R_2^\star)$ for $N \to \infty$?

Implementation of the Stochastic SIR Model

$N = 20$

$\beta = \mu = \lambda = \gamma = 1$

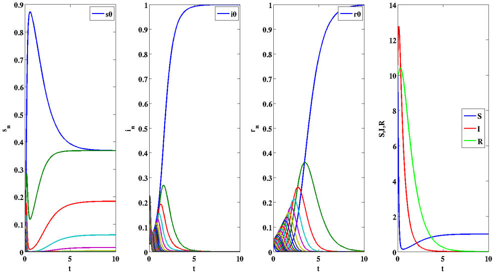
$s_n(0) = i_n(0) = r_n(0) = 1/(N+1)$



$t_{\max} = 1$ (above)

$t_{\max} = 10$ (below)

Equilibrium:
$\bar{S}^\star \approx 1$, $\bar{I}^\star = 0$, $\bar{R}^\star = 0$.



Implementation of the Stochastic SIR Model

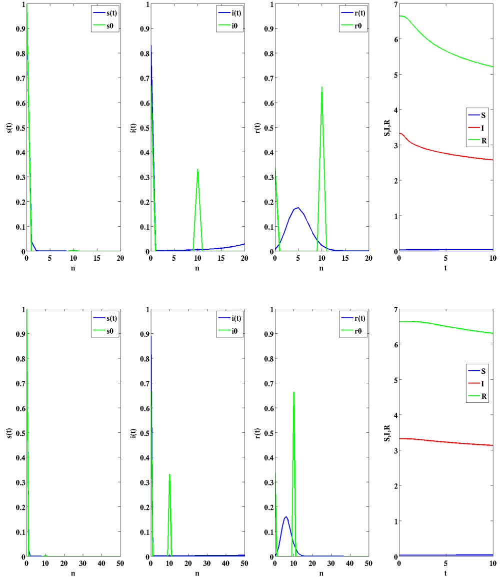
$\beta = 10,\ \mu = 1$

$\gamma = 2,\ \lambda = 100$

$s_{10}(0) = \frac{S_2^\star}{10} = 1 - s_0(0)$

$i_{10}(0) = \frac{I_2^\star}{10} = 1 - i_0(0)$

$r_{10}(0) = \frac{R_2^\star}{10} = 1 - r_0(0)$



$$\begin{aligned} \bar{S}(0) &= S_2^\star \\ \bar{I}(0) &= I_2^\star \\ \bar{R}(0) &= R_2^\star \end{aligned}$$

$N = 20$ (above)

$N = 50$ (below)

$N \to \infty \Rightarrow (\bar{S}, \bar{I}, \bar{R})(t)$
$\quad \to (S_2^\star, I_2^\star, R_2^\star)$

Exercise: Show for $N = \infty$, $\forall n \geq 1$, $i_n(t) \stackrel{t\to\infty}{\longrightarrow} 0$ although $\bar{I}(t) = I_2^\star$.

SIR Model with Spontaneous Infection

- New conditional probabilities:

$$
\begin{aligned}
P(S(t+dt) = n-1 \mid S(t) = n) &= ndt[\mu + \lambda \bar{I}(t)] + \epsilon ndt \\
P(I(t+dt) = n+1 \mid I(t) = n) &= \lambda n \bar{S}(t)dt + \epsilon \bar{S}(t)dt
\end{aligned}
$$

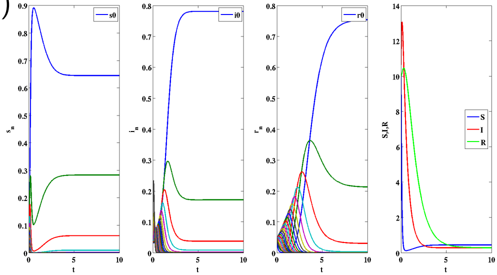
- New System:

$$
\begin{aligned}
s_n'(t) &= \beta s_{n-1}(t) \\
&- \{\beta + n[\mu + \epsilon + \lambda \bar{I}(t)]\} s_n(t) \\
&+ (n+1)[\mu + \epsilon + \lambda \bar{I}(t)] s_{n+1}(t) \\
i_n'(t) &= [(n-1)\lambda + \epsilon] \bar{S}(t) i_{n-1}(t) \\
&- [(n\lambda + \epsilon)\bar{S}(t) + n(\mu + \gamma)] i_n(t) \\
&+ (n+1)(\mu + \gamma) i_{n+1}(t) \\
r_n'(t) &= \gamma \bar{I}(t) r_{n-1}(t) \\
&- [\gamma \bar{I}(t) + n\mu] r_n(t) \\
&+ (n+1)\mu r_{n+1}(t)
\end{aligned}
$$

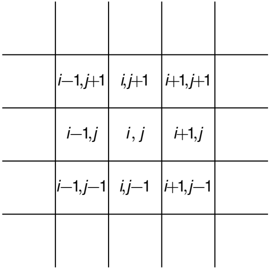
$$
\begin{aligned}
s_n(0) = i_n(0) = r_n(0) \\
= 1/(N+1)
\end{aligned}
$$

New Equilibria solve:

$$
\begin{aligned}
0 &= \beta - (\lambda \bar{I}^\star + \mu + \epsilon)\bar{S}^\star \\
0 &= (\lambda \bar{S}^\star - \mu - \gamma)\bar{I}^\star + \epsilon \bar{S}^\star \\
0 &= -\mu \bar{R}^\star + \gamma \bar{I}^\star
\end{aligned}
$$



Stochastic SIR Cellular Automaton



- Let the living space be partitioned into a grid.
- At a discrete time point n the cell $Z_{i,j}$ is in exactly one of the states:
  - susceptible (S),
  - infected (I),
  - recovered (R) or
  - empty (E).
- The state of a cell can change, depending upon the states in the neighborhood

$$U_{i,j} = \{Z_{i+p,j+q}\}_{\|(p,\,q)\|_\infty=1}.$$

- For the total SIR cellular automaton with $N \times M$ cells there are 4^{NM} possible states.
- Torus boundary conditions are assumed.
- The evolution of the states is modeled as a *Markov chain*.

Transition Probabilities for the SIR Model

- From the starting state E:
  $P(Z_{i,j}^{n+1} = S \mid Z_{i,j}^n = E) = \beta, \quad P(Z_{i,j}^{n+1} = E \mid Z_{i,j}^n = E) = 1 - \beta$
  $P(Z_{i,j}^{n+1} = I \mid Z_{i,j}^n = E) = 0 = P(Z_{i,j}^{n+1} = R \mid Z_{i,j}^n = E)$
  where $\beta \in (0,1)$,
- From the starting state S:
  $P(Z_{i,j}^{n+1} = E \mid Z_{i,j}^n = S) = \mu, \quad P(Z_{i,j}^{n+1} = R \mid Z_{i,j}^n = S) = 0$
  $P(Z_{i,j}^{n+1} = S \mid Z_{i,j}^n = S) = 1 - \mu - \lambda \bar{I}_{i,j}$
  $P(Z_{i,j}^{n+1} = I \mid Z_{i,j}^n = S) = \lambda \bar{I}_{i,j}, \quad \bar{I}_{i,j} = \underset{\|(p,q)\|_\infty = 1}{\text{mean}} (Z_{i+p,j+q} = I)$
  where $\mu, \lambda, \mu + \lambda \in (0,1)$.
- From the starting state I:
  $P(Z_{i,j}^{n+1} = S \mid Z_{i,j}^n = I) = 0, \quad P(Z_{i,j}^{n+1} = I \mid Z_{i,j}^n = I) = 1 - \mu - \gamma$
  $P(Z_{i,j}^{n+1} = R \mid Z_{i,j}^n = I) = \gamma, \quad P(Z_{i,j}^{n+1} = E \mid Z_{i,j}^n = I) = \mu$
  where $\mu, \gamma, \mu + \gamma \in (0,1)$.
- From the starting state R:
  $P(Z_{i,j}^{n+1} = E \mid Z_{i,j}^n = R) = \mu, \quad P(Z_{i,j}^{n+1} = R \mid Z_{i,j}^n = R) = 1 - \mu$
  $P(Z_{i,j}^{n+1} = S \mid Z_{i,j}^n = R) = 0 = P(Z_{i,j}^{n+1} = I \mid Z_{i,j}^n = R)$

Transition Probabilities for the SIR Model

Exercise: For $N = 2$, $M = 1$ and given β, γ, λ, μ, write the transition probabilities of the cellular automaton as a stochastic matrix and find the equilibrium. Compare with the following!

Monte-Carlo simulation:

- Initialize with a random state for each cell.
- For each time step generate a uniformly distributed random value z for each cell.
- With starting state E, the transition state becomes
$$S, z \in [0, \beta), \quad E, z \in [\beta, 1].$$
- With starting state S, the transition state becomes
$$E, z \in [0, \mu), \quad I, z \in [\mu, \mu + \lambda\bar{I}), \quad S, z \in [\mu + \lambda\bar{I}, 1].$$
- With starting state I, the transition state becomes
$$E, z \in [0, \mu), \quad R, z \in [\mu, \mu + \gamma), \quad I, z \in [\mu + \gamma, 1].$$
- With starting state R, the transition state becomes
$$E, z \in [0, \mu), \quad R, z \in [\mu, 1].$$
- In the course of generations notice whether the total number of S, I, R, E reaches an equilibrium, or else...?

Implementation of an SIR Cellular Automaton

- The state of the grid can be stored with arrays `C` and `Ib`:

$$\texttt{C(i,j)} = \begin{cases} 0, & Z_{i,j} = E \\ 1, & Z_{i,j} = S \\ 2, & Z_{i,j} = I \\ 3, & Z_{i,j} = R \end{cases}$$

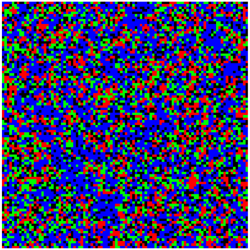
```
Ib = -double(C==2);
for i=-1:1; for j=-1:1;
 Ib = Ib + circshift(C==2,[i,j]);
end; end; Ib=Ib/8;
```

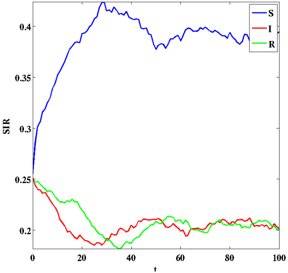
where $\texttt{Ib(i,j)} = \text{mean}_{U_{i,j}}(Z_{p,q} = I)$

- Transitions can be implemented with the array `C` as follows:

```
Z = rand(N,M);
C = 1* ((C==0) & (Z < beta)) ...
  + 2* ((C==1) & (Z ≥ mu) & (Z < mu + lambda*Ib))...
  + 1* ((C==1) & (Z ≥ mu + lambda*Ib))...
  + 3* ((C==2) & (Z ≥ mu) & (Z < mu + gamma))...
  + 2* ((C==2) & (Z ≥ gamma + mu))...
  + 3* ((C==3) & (Z ≥ mu));
```

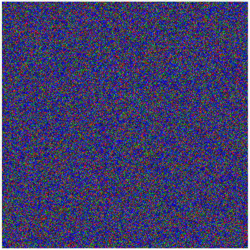
Implementation of an SIR Cellular Automaton

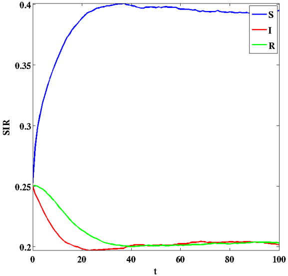




$\beta = 0.4$, $\mu = 0.1$
$\lambda = 0.7$, $\gamma = 0.1$

$N = M = 100$
(above)
$N = M = 1000$
(below)





Initially:

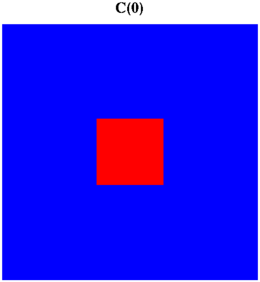
```
C = randi(4,N,M)-1;
```

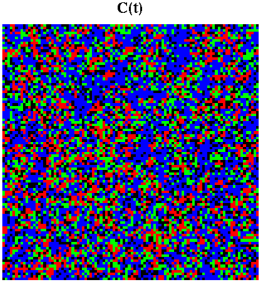
$\bar{S}(t), \bar{I}(t), \bar{R}(t)$
smoother when N, M
larger.

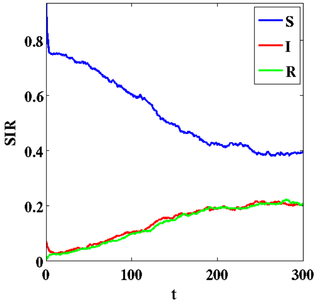
Equilibrium endemic?

Implementation of an SIR Cellular Automaton

- Here the parameters are the same as above,
  $\beta = 0.4$, $\mu = 0.1$, $\lambda = 0.7$, $\gamma = 0.1$, $N = M = 100$
  but initially there are only infected within a square and only susceptibles outside.



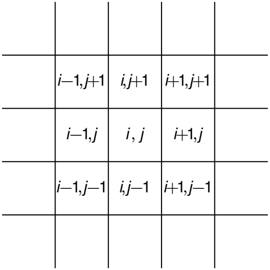




- Yet there develops the same equilibrium.
- The same result is obtained for larger N, M, but it takes longer until the equilibrium develops.
- Why is the case $N = 2$, $M = 1$ so different?

Lotka-Volterra Equations for SIR with Motion

- Let the living space be partitioned into an $N \times M$ grid with torus boundary conditions.



- Let the number of susceptibles, infected and recovered in the cell $Z_{i,j}$ at time t be denoted respectively by $S_{i,j}(t), I_{i,j}(t), R_{i,j}(t)$.
- When there are no infected, and the susceptibles can move between $Z_{i,j}$ and $Z_{i+1,j}$, then (analogous to Newton's cooling law) this motion can be modeled as follows:

$$S'_{i,j} = \hat{\sigma}_{i+\frac{1}{2},j}(S_{i+1,j} - S_{i,j}) - \mu S_{i,j}$$

where $\hat{\sigma}_{i+\frac{1}{2},j}$ represents a motility transfer coefficient at the interface between the cells.
- When die susceptibles in $Z_{i,j}$ can move to the neighbor cells $U_{i,j} = \{Z_{i+p,j+q}\}_{\|(p,q)\|_\infty = 1}$,

$$S'_{i,j} = \sum_{\|(p,q)\|_\infty = 1} \hat{\sigma}_{i+\frac{p}{2},j+\frac{q}{2}}(S_{i+p,j+q} - S_{i,j}) - \mu S_{i,j}$$

Lotka-Volterra Equations for SIR with Motion

- The motion of the infected and of the recovered can be modeled analogously with transfer coefficients $\hat{\iota}$ and $\hat{\rho}$.
- The SIR model with motion is then:

$$\begin{cases} S'_{i,j} = \sum_{\|(p,q)\|_\infty=1} \hat{\sigma}_{i+\frac{p}{2},j+\frac{q}{2}}(S_{i+p,j+q} - S_{i,j}) + \beta - (\mu + \lambda I_{i,j})S_{i,j} \\ I'_{i,j} = \sum_{\|(p,q)\|_\infty=1} \hat{\iota}_{i+\frac{p}{2},j+\frac{q}{2}}(I_{i+p,j+q} - I_{i,j}) + (\lambda S_{i,j} - \mu - \gamma)I_{i,j} \\ R'_{i,j} = \sum_{\|(p,q)\|_\infty=1} \hat{\rho}_{i+\frac{p}{2},j+\frac{q}{2}}(R_{i+p,j+q} - R_{i,j}) + \gamma I_{i,j} - \mu R_{i,j} \end{cases}$$

  where $1 \leq i \leq N$ and $1 \leq j \leq M$.
- The interfaces $i = \frac{1}{2}$ and $j = \frac{1}{2}$ are indentified with the interfaces $i = N + \frac{1}{2}$ and $j = M + \frac{1}{2}$ through the torus boundary conditions.
- Also through torus boundary conditions, the cell values in $Z_{i,0}$ and $Z_{0,j}$ are identified respectively with those in $Z_{i,M}$ and $Z_{N,j}$, and the cell values $Z_{i,M+1}$ and $Z_{N+1,j}$ are identified respectively with those in $Z_{i,1}$ and $Z_{1,j}$.

Lotka-Volterra Equations for SIR with Motion

Exercise: For $N = 2$, $M = 1$ and spatially independent $\hat{\sigma}, \hat{\iota}, \hat{\rho}$ show for $I_2^\star = \frac{\beta}{\mu+\gamma} - \frac{\mu}{\lambda} < 0$ that the equilibrium $(S_{i,j}, I_{i,j}, R_{i,j}) = (S_1^\star, I_1^\star, R_1^\star) = (\beta/\mu, 0, 0)$ is locally asymptotically stable.

Distributed Model

- Now let the *density* of susceptibles, infected and recovered be denoted respectively by $s = s(t, \boldsymbol{x})$, $i = i(t, \boldsymbol{x})$ and $r = r(t, \boldsymbol{x})$.
- With Fick's Law the flow $\boldsymbol{F}_s$ of susceptibles over an interface can be modeled by $\boldsymbol{F}_s = -\sigma \nabla s$, where σ is a diffusion coefficient.
- By conservation (and $\mu = \lambda = 0$ for now),

$$S'_{i,j} = \partial_t \int_{Z_{i,j}} s = -\int_{\partial Z_{i,j}} \boldsymbol{F}_s \cdot \hat{\boldsymbol{n}} = \int_{\partial Z_{i,j}} \sigma \frac{\partial s}{\partial n}$$

and

$$\int_{\partial Z_{i,j}} \sigma \frac{\partial s}{\partial n} \approx \sum_{\|(p,q)\|_\infty = 1} \delta \cdot \hat{\sigma}_{i+\frac{p}{2}, j+\frac{q}{2}} \frac{S_{i+p,j+q} - S_{i,j}}{\delta}$$

where

$\delta =$ wall thickness (cell center separation)

$$\hat{\sigma}_{i+\frac{p}{2}, j+\frac{q}{2}} = \frac{1}{\delta} \int_{\overline{Z}_{i,j} \cap \overline{Z}_{i+p,j+q}} \sigma$$

Lotka-Volterra Equations for SIR with Motion

- With the Gauß Theorem,
$$0 = \partial_t \int_{Z_{i,j}} s - \int_{\partial Z_{i,j}} \sigma \nabla s \cdot \hat{\boldsymbol{n}} = \int_{Z_{i,j}} [\partial_t s - \nabla \cdot (\sigma \nabla s)]$$
- Taking $Z_{i,j}$ arbitrarily small, it must hold pointwise that,
$$\partial_t s = \nabla \cdot (\sigma \nabla s) \qquad \text{(for } \mu = \lambda = 0\text{)}$$
- Similarly with Fick's Law the flows $\boldsymbol{F}_i$ and $\boldsymbol{F}_r$ of the infected and of the recovered over an interface can be modeled respectively by $\boldsymbol{F}_i = -\iota \nabla i$ and $\boldsymbol{F}_r = -\rho \nabla r$, where ι and ρ are diffusion coefficients.
- The SIR model with diffusion is given by the Lotka-Volterra system of equations: $t > 0$, $\boldsymbol{x} \in \Omega = (0,1)^2$
$$\left\{ \begin{array}{rcll} \partial_t s &=& \nabla \cdot (\sigma \nabla s) + \beta - (\mu + \lambda i)s, & s(0,\boldsymbol{x}) = s_0(\boldsymbol{x}) \\ \partial_t i &=& \nabla \cdot (\iota \nabla i) + (\lambda s - \mu - \gamma) i, & i(0,\boldsymbol{x}) = i_0(\boldsymbol{x}) \\ \partial_t r &=& \nabla \cdot (\rho \nabla r) + \gamma i - \mu r, & r(0,\boldsymbol{x}) = r_0(\boldsymbol{x}) \end{array} \right.$$
with periodic boundary conditions
$$s(t,0,y) = s(t,1,y), \quad s(t,x,0) = s(t,x,1), \quad \text{etc.}$$

Lotka-Volterra Equations for SIR with Motion

- Classical predator-prey model with backward R-coupling:

$$\begin{cases} \partial_t s = \nabla\cdot(\sigma\nabla s) + s(a_1 - a_2 i) + a_5 r, & s(0,\boldsymbol{x}) = s_0(\boldsymbol{x}) \\ \partial_t i = \nabla\cdot(\iota\nabla i) + i(a_2 s - a_3) - a_4 i, & i(0,\boldsymbol{x}) = i_0(\boldsymbol{x}) \\ \partial_t r = \nabla\cdot(\rho\nabla r) + a_4 i - a_5 r - a_6 r, & r(0,\boldsymbol{x}) = r_0(\boldsymbol{x}) \end{cases}$$

- Logistic variant of the predator-prey model:

$$\begin{cases} \partial_t s = \nabla\cdot(\sigma\nabla s) + a_1 s(1 - s/a_3) & \\ \qquad + a_7 r - a_4 si/(1 + a_6 s), & s(0,\boldsymbol{x}) = s_0(\boldsymbol{x}) \\ \partial_t i = \nabla\cdot(\iota\nabla i) - a_8 i & \\ \qquad + a_2 i(1 - i/(a_5 s)), & i(0,\boldsymbol{x}) = i_0(\boldsymbol{x}) \\ \partial_t r = \nabla\cdot(\rho\nabla r) + a_8 i & \\ \qquad + a_1 r(1 - r/a_3) - a_7 r, & r(0,\boldsymbol{x}) = r_0(\boldsymbol{x}) \end{cases}$$

- Both with periodic boundary conditions

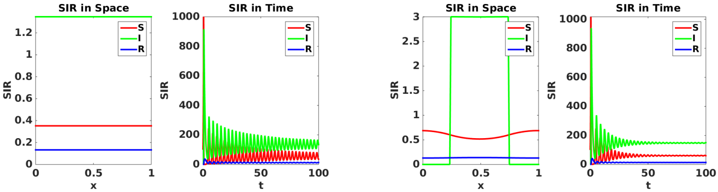
$$s(t,0,y) = s(t,1,y), \quad s(t,x,0) = s(t,x,1), \quad \text{etc.}$$

- Quarantine is implemented with $\iota = 0$ at the boundary of an interior region.

Lotka-Volterra Equations for SIR with Motion

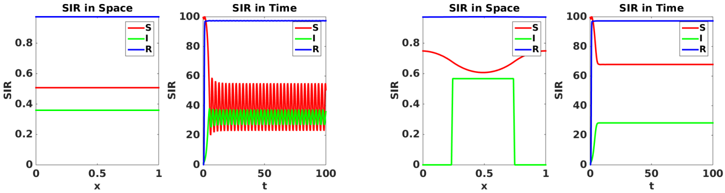
Left pair without quarantine, right pair with quarantine.
The infected begin for both at one point in the middle.

- Classical predator-prey model with backward *R*-coupling:



R-coupling creates a limit cycle! Quarantine stabilizing.

- Logistic variant of the predator-prey model:

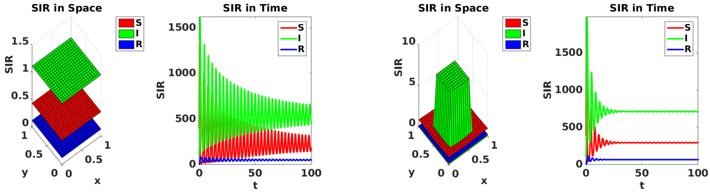


Limit cycle also with *R*-coupling. Quarantine stabilizing.

Lotka-Volterra Equations for SIR with Motion

Left pair without quarantine, right pair with quarantine.
The infected begin for both at one point in the middle.

- Classical predator-prey model with backward R-coupling:



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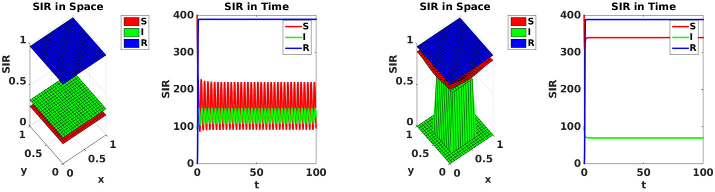


Limit cycle also with R-coupling. Quarantine stabilizing.

Pattern Formation

- With $\Omega = (0, \pi)$ consider the reaction diffusion equation,

$$\begin{cases} w_t = w_{xx} + w, & x \in \Omega \quad t > 0 \\ w = 0, & x \in \partial\Omega \quad t > 0 \\ w = w_0, & x \in \Omega \quad t = 0 \end{cases}$$

- With $n \in \mathbb{N}$ and eigenvalue $\lambda_n = -n^2$, let $\phi_n(x) = \sin(nx)$ be the nth eigenfunction of ∂_x^2 with Dirichlet BCs,

$$\phi_n''(x) = \lambda_n \phi_n(x), \quad x \in \Omega, \quad \phi_n(x) = 0, \quad x \in \partial\Omega$$

- Using separation of variables, w is expressed as

$$w(x,t) = \sum_{n=1}^{\infty} s_n(t)\phi_n(x), \quad w_0(x) = \sum_{n=1}^{\infty} w_n \phi_n(x)$$

and the expansion of $w_t - w_{xx} - w$ gives

$$\sum_{n=1}^{\infty} \phi_n(x)[s_n'(t) - (\lambda_n + 1)s_n(t)] = 0 \quad \text{or} \quad \begin{cases} s_n'(t) = (1 - n^2)s_n(t) \\ s_n(0) = w_n \end{cases}$$

- For $n \geq 2$, $s_n(t) = w_n e^{(1-n^2)t} \stackrel{t\to\infty}{\longrightarrow} 0$ but $s_1(t) = w_1$, $t \geq 0$.

Pattern Formation

- If the initial condition $w_0(x)$ has a ϕ_1-component $w_1 > 0$, then the pattern emerges $w(x,t) \stackrel{t\to\infty}{\longrightarrow} w_1 \sin(x)$.
- Thus the dissipative and accretive mechanisms in $Aw = w_{xx} + w$ in the reaction diffusion equation compete with each other to produce the pattern.

Exercise: Show that a similar result is obtained for $\Omega = (0, L)$ and $Aw = \delta w_{xx} + \kappa w$ if $\delta(\pi/L)^2 = \kappa$. Further, given that $f(w^*) = 0$, show that if $Aw = \delta w_{xx} + f(w)$ and $f(w) = f(w^*) + \kappa(w - w^*) + \mathcal{O}(w - w^*)$ a similar result is obtained for $z = w - w^*$ sufficiently small.

- For $\Omega = (0, \pi)$ consider the reaction diffusion system,

$$\left\{ \begin{array}{rcllll} u_t & = & \frac{1}{4}u_{xx} + u + v, & x \in \Omega & t > 0 \\ v_t & = & 2v_{xx} - 3u - 2v, & x \in \Omega & t > 0 \\ u_x = v_x & = & 0, & x \in \partial\Omega & t > 0 \\ (u, v) & = & (u_0, v_0), & x \in \Omega & t = 0 \end{array} \right.$$

Pattern Formation

- With $n \in \mathbb{N}_0$ and eigenvalue $\lambda_n = -n^2$, let $\psi_n(x) = \cos(nx)$ be the nth eigenfunction of ∂_x^2 with Neumann BCs,

$$\psi_n''(x) = \lambda_n \psi_n(x), \quad x \in \Omega, \quad \psi_n'(x) = 0, \quad x \in \partial\Omega$$

- Using separation of variables, (u, v) are expressed as

$$\begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix} = \sum_{n=0}^{\infty} \begin{bmatrix} s_n(t) \\ r_n(t) \end{bmatrix} \psi_n(x), \quad \begin{bmatrix} u_0(x) \\ v_0(x) \end{bmatrix} = \sum_{n=0}^{\infty} \begin{bmatrix} u_n \\ v_n \end{bmatrix} \psi_n(x)$$

  and the expansion of the reaction diffusion equation gives

$$\sum_{n=0}^{\infty} \psi_n(x) \left\{ \begin{bmatrix} s_n'(t) \\ r_n'(t) \end{bmatrix} - \begin{bmatrix} 1 + \frac{1}{4}\lambda_n & 1 \\ -3 & -2 + 2\lambda_n \end{bmatrix} \begin{bmatrix} s_n(t) \\ r_n(t) \end{bmatrix} \right\} = 0$$

- For $n = 0$ the eigenvalues $\{-\frac{1}{2} \pm \imath\frac{\sqrt{3}}{2}\}$ give

$$\begin{bmatrix} s_0'(t) \\ r_0'(t) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ -3 & -2 \end{bmatrix} \begin{bmatrix} s_0(t) \\ r_0(t) \end{bmatrix}, \quad \begin{bmatrix} s_0(t) \\ r_0(t) \end{bmatrix} \xrightarrow{t\to\infty} 0$$

- $\mathrm{tr}(n) = -(1 + \frac{9}{4}n^2)$ and $\det(n) = \frac{1}{2}(n^2 - 1)(n^2 - 2)$ give the same decay for $n \geq 2$.

Pattern Formation

- For $n = 1$ the eigenpairs $-\frac{13}{4}$, $[-\frac{1}{4}, 1]^\top$ and 0, $[-\frac{4}{3}, 1]^\top$ give

$$\begin{bmatrix} s_1'(t) \\ r_1'(t) \end{bmatrix} = \begin{bmatrix} \frac{3}{4} & 1 \\ -3 & -4 \end{bmatrix} \begin{bmatrix} s_1(t) \\ r_1(t) \end{bmatrix}, \quad \begin{bmatrix} s_1(t) \\ r_1(t) \end{bmatrix} \overset{t\to\infty}{\longrightarrow} \alpha \begin{bmatrix} -\frac{4}{3} \\ 1 \end{bmatrix}$$

  where $\alpha = -\frac{3}{13}(4u_1 + v_1)$. **Exercise**: Show this.
- If (u_0, v_0) have a ψ_1-component $(u_1, v_1) \neq 0$, then the pattern emerges $(u(x,t), v(x,t)) \overset{t\to\infty}{\longrightarrow} \alpha \cos(x)(-\frac{4}{3}, 1)$.

Exercise: Repeat for other (linearized) model parameters.

- While both the reaction and diffusion mechanisms are dissipative, the combination cooperates to form a pattern.
- *Turing instability* emerges when the sum of two stable system yields an unstable equilibrium.

Exercise: Investigate Turing instability for the morphogenesis,

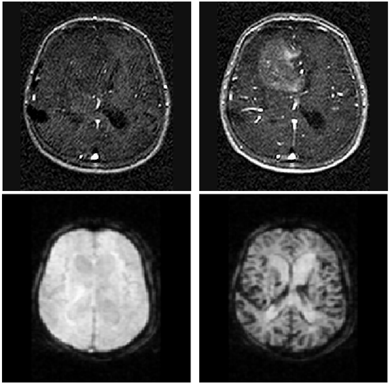
$$u_t = d_1 u_{xx} + p - uv^2, \quad v_t = d_2 v_{xx} + q - v + uv^2$$

where $p > q > 0$, $(p+q)^3 > (p-q)$ and $0 < d_2 \ll d_1$.

Exercise: Investigate Turing instability for the SIR models.

Material Transport

- For DCE-MRI contrast agent is introduced to increase image contrast dynamically.



- As in the last chapter, conservation of mass is used here to model the distribution of contrast agent.
- Goal: determine transport parameters.

DCE-MRI

- Let $C(\boldsymbol{x}, t)$ be the concentration of contrast agent at the tissue point $\boldsymbol{x} \in \Omega$ (body) and at time $t > 0$.
- The convective flux $\boldsymbol{F}_\mathrm{k}$ of contrast agent can be modeled with $\boldsymbol{F}_\mathrm{k} = \boldsymbol{v}C$, where $\boldsymbol{v}$ is the velocity.
- With Fick's Law the diffusive flux $\boldsymbol{F}_\mathrm{d}$ can be modeled with $\boldsymbol{F}_\mathrm{d} = -D\nabla C$, where D is the diffusivity.
- It is assumed that the diffusivity depends upon $\boldsymbol{v}$,
$$D(\boldsymbol{v}) = d\hat{\boldsymbol{v}}\hat{\boldsymbol{v}}^\mathrm{T} + p[I - \hat{\boldsymbol{v}}\hat{\boldsymbol{v}}^\mathrm{T}], \quad \hat{\boldsymbol{v}} = \boldsymbol{v}/\|\boldsymbol{v}\|_{\ell_2}.$$
Here d applies along $\boldsymbol{v}$ and p orthogonal to $\boldsymbol{v}$.
- Through conservation of mass, $\forall V \subseteq \Omega$

$$\partial_t \int_V C = -\int_{\partial V} (\boldsymbol{F}_\mathrm{d} + \boldsymbol{F}_\mathrm{k}) \cdot \hat{\boldsymbol{n}} = \underbrace{\int_{\partial V} D(\boldsymbol{v})\nabla C \cdot \hat{\boldsymbol{n}}}_{\text{diffusion}} - \underbrace{\int_{\partial V} C\boldsymbol{v} \cdot \hat{\boldsymbol{n}}}_{\text{convection}}$$

a convection-diffusion equation results for C,

$$\partial_t C + \nabla \cdot [\boldsymbol{v}C] = \nabla \cdot [D(\boldsymbol{v})\nabla C], \quad \boldsymbol{x} \in \Omega, \quad t > 0$$

DCE-MRI

- Let $V \subseteq \Omega$ be a subdomain in which the following holds,

$$\begin{cases} \partial_t C &= -\nabla \cdot [\boldsymbol{v} C] + \nabla \cdot [D(\boldsymbol{v}) \nabla C] \\ & \quad + (C - C_{\mathrm{AIF}}) \boldsymbol{v} \cdot \hat{\boldsymbol{n}} \delta_{\partial V^{\mathrm{in}}}, \quad \boldsymbol{x} \in V, \quad t > 0 \\ 0 &= D(\boldsymbol{v}) \nabla C \cdot \hat{\boldsymbol{n}}, \quad \boldsymbol{x} \in \partial V, \quad t > 0 \\ C &= C_0, \quad \boldsymbol{x} \in V, \quad t = 0 \end{cases}$$

  where
  - $C_{\mathrm{AIF}} = C_{\mathrm{AIF}}(t)$ is the *arterial input function*
  - $\partial V^{\mathrm{in}} = \{\boldsymbol{x} \in \partial V : \boldsymbol{v} \cdot \hat{\boldsymbol{n}} < 0\}$, $\partial V^{\mathrm{out}} = \{\boldsymbol{x} \in \partial V : \boldsymbol{v} \cdot \hat{\boldsymbol{n}} > 0\}$
  - The Dirac delta-function $\delta_{\partial V^{\mathrm{in}}}$ satisfies

$$\int_V C \delta_{\partial V^{\mathrm{in}}} = \int_{\partial V^{\mathrm{in}}} C, \quad \forall C \text{ smooth enough}$$

  - On ∂V there is no diffusive flux!
- Let the differential operator A be formally so defined:

$$AC = -\nabla \cdot [\boldsymbol{v} C] + \nabla \cdot [D(\boldsymbol{v}) \nabla C] + C \boldsymbol{v} \cdot \hat{\boldsymbol{n}} \delta_{\partial V^{\mathrm{in}}}$$

$$\mathrm{Dom}(A) = \{C \text{ smooth enough} : D(\boldsymbol{v}) \nabla C \cdot \hat{\boldsymbol{n}} = 0 \text{ on } \partial V\}$$

Convolution Model

- After integration of the PDE the Gauß Theorem gives,

$$\int_V \partial_t C + \int_{\partial V^{\text{out}}} C\boldsymbol{v}\cdot\hat{\boldsymbol{n}} + \int_{\partial V^{\text{in}}} C_{\text{AIF}}\boldsymbol{v}\cdot\hat{\boldsymbol{n}} = \int_{\partial V} D(\boldsymbol{v})\nabla C\cdot\hat{\boldsymbol{n}} = 0.$$

  where $C|_{\partial V^{\text{out}}} = C_{\text{VOF}}$ is the *venous output function*.
- The formal solution formula for C is

$$C(t) = e^{At}C(0) + \int_0^t e^{A(t-s)}\delta_{\partial V^{\text{in}}}|\boldsymbol{v}\cdot\hat{\boldsymbol{n}}|C_{\text{AIF}}(s)ds$$

- If $C_0 = 0$ holds, the convolution follows

$$C_{\text{T}}(t) = \int_0^t K(t-s)C_{\text{AIF}}(s)ds$$

  where the *tissue concentration function* and convolution kernel are given respectively by

$$C_{\text{T}}(t) = \frac{1}{|V|}\int_V C(t), \qquad K(t) = \frac{1}{|V|}\int_V e^{At}\delta_{\partial V^{\text{in}}}|\boldsymbol{v}\cdot\hat{\boldsymbol{n}}|$$

- C_{AIF} and C_{T} are measured by imaging and K is to be determined.

Physiological Parameters from the Convolution Kernel

- Physiological parameters can be derived from the convolution kernel as follows.
- After integration of the PDE in space and time the Gauß Theorem gives,

$$|V|C_{\mathrm{T}}(t) = \int_V C = \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \int_0^t C_{\mathrm{AIF}}(s)ds - \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}>0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \int_0^t C_{\mathrm{VOF}}(s)ds$$

- With the convolution equation follows $C_{\mathrm{T}}(t) = K(t)$ with $C_{\mathrm{AIF}}(t) = \delta(t)$, where the Dirac delta function satisfies

$$\int_{t_0-\epsilon}^{t_0+\epsilon} \delta(t - t_0)dt = 1, \quad \forall \epsilon > 0$$

- With $C_{\mathrm{AIF}}(t) = \delta(t)$ and $C_{\mathrm{VOF}}(t) \stackrel{t\to 0}{\longrightarrow} 0$ letting $t \to 0$ above gives,

$$K(0) = \frac{1}{|V|} \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| = \mathcal{F}_{\mathrm{T}}$$

i.e., $K(0)$ is the volumetric flowrate per unit volume (Perfusion).

Physiological Parameters from the Convolution Kernel

- The function $R(t) = K(t)/K(0)$ is the *residue function*, and it represents the fraction of impulsively introduced contrast agent which has not yet washed out of V.
- It is assumed that fluid does not collect in V,

$$\text{flux}^{\text{in}} = \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| = \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}>0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| = \text{flux}^{\text{out}}$$

- With equations for the convolution and for $K(0)$ it follows

$$\begin{aligned}\int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \int_0^t R(t-s)C_{\text{AIF}}(s)ds &= \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \int_0^t C_{\text{AIF}}(s)ds \\ &- \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}>0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \int_0^t C_{\text{VOF}}(s)ds\end{aligned}$$

or after d/dt,

$$C_{\text{AIF}}(t) + \int_0^t R'(t-s)C_{\text{AIF}}(s)ds = C_{\text{AIF}}(t) - C_{\text{VOF}}(t)$$

- With $R(t) = \int_t^\infty h(s)ds$ follows

$$C_{\text{VOF}}(t) = \int_0^t h(t-s)C_{\text{AIF}}(s)ds$$

Physiological Parameters from the Convolution Kernel

- The function $h(t)$ is interpreted as the probability density of the transit time of a contrast agent particle.
- Then the mean transit time is given through

$$\mathcal{T}_{\mathrm{T}} = \int_0^\infty t h(t) dt = \int_0^\infty R(t) dt = \int_0^\infty K(t)/K(0) dt$$

- With $C_{\mathrm{AIF}}(t) = \delta(t)$, $C_{\mathrm{VOF}}(t) = h(t)$ and $C_{\mathrm{T}}(t) = K(t)$ in the integration of the PDE it follows

$$|V| K(t) = \int_{\boldsymbol{v}\cdot\hat{\boldsymbol{n}}<0} |\boldsymbol{v}\cdot\hat{\boldsymbol{n}}| \left[1 - \int_0^t h(s) ds\right] = |V| \mathcal{F}_{\mathrm{T}} R(t)$$

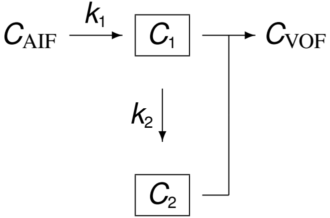
or

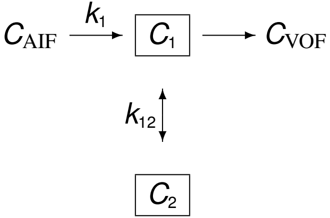
$$\int_0^\infty K(t) dt = \mathcal{F}_{\mathrm{T}} \int_0^\infty R(t) dt = \mathcal{F}_{\mathrm{T}} \mathcal{T}_{\mathrm{T}} = \mathcal{V}_{\mathrm{T}}$$

i.e., $\int_0^\infty K(t) dt$ is the effective volumetric fraction of V, in which contrast agent is distributed.

Determination of the Convolution Kernel

- Discrete Examples.
  - Assume that V consists of 2 well mixed compartments.
  - In the left example there is pure convection between compartments.
  - In the right example there is diffusion between the compartments.





- The transport in these examples are modeled as follows:

$$\begin{cases} V_1 C_1' + k_1(C_1 - C_{\mathrm{AIF}}) = 0 \\ V_2 C_2' + k_2(C_2 - C_1) = 0 \end{cases} \qquad \begin{cases} V_1 C_1' + k_1(C_1 - C_{\mathrm{AIF}}) = k_{12}(C_2 - C_1) \\ V_2 C_2' = k_{12}(C_1 - C_2) \end{cases}$$

Exercise: Determine $K(t) = \alpha_1 e^{-\lambda_1 t} + \alpha_2 e^{-\lambda_2 t}$ for these examples.

Deconvolution is Ill-Posed

- Assume that contrast agent passed through $n+1$ equivalent well mixed compartments (every mean transit time $= 1/\nu$), after it is injected impulsively and before it arrives in V.
- Model of $C_{\rm AIF}$ for V is

$$C_{\rm AIF}(t) = \delta(t) * [\nu e^{-\nu t}]_1 * \cdots * [\nu e^{-\nu t}]_{n+1} = \nu \frac{(\nu t)^n}{n!} e^{-\nu t}$$

- Let $C_{\rm T} = K_{\rm e} * C_{\rm AIF}$, where $K_{\rm e}$ is an exact convolution kernel.
- Assume that $C_{\rm T}(t) + N_\epsilon(t)$ instead of $C_{\rm T}(t)$ is measured, where $N_\epsilon(t)$ represented measurement noise. This measurement error creates an error $E_\epsilon(t)$ in the convolution kernel, which satisfies:

$$C_{\rm T}(t) + N_\epsilon(t) = \int_0^t C_{\rm AIF}(t-s)[K_{\rm e}(s) + E_\epsilon(s)]ds$$

Theorem: There exists $N_\epsilon = \mathcal{O}(\epsilon)$ for which $E_\epsilon = \mathcal{O}(\epsilon^{-n})$.

Exercise: Construct a simple example $(N_\epsilon, C_{\rm AIF}, E_\epsilon)$ with $N_\epsilon \overset{\epsilon\to 0}{\longrightarrow} 0$ and $E_\epsilon \overset{\epsilon\to 0}{\longrightarrow} \infty$.

Regularization of Convolution

- Due to discontinuous dependence on data, the determination of the convolution kernel must be regularized.
- A known approach for this regularization is based upon a singular value decomposition of the system matrix, which arises through discretization of the convolution.
- Let the convolution be discretized by the trapezoidal rule:

$$\begin{aligned} C_{\mathrm{T}}(t_i) &= \int_0^{t_i} C_{\mathrm{AIF}}(t_i - s)K(s)ds \\ &\approx \sum_{j=1}^{i-1} [C_{\mathrm{AIF}}(t_i - t_j)K(t_j) + C_{\mathrm{AIF}}(t_i - t_{j+1})K(t_{j+1})](t_{j+1} - t_j)/2 \end{aligned}$$

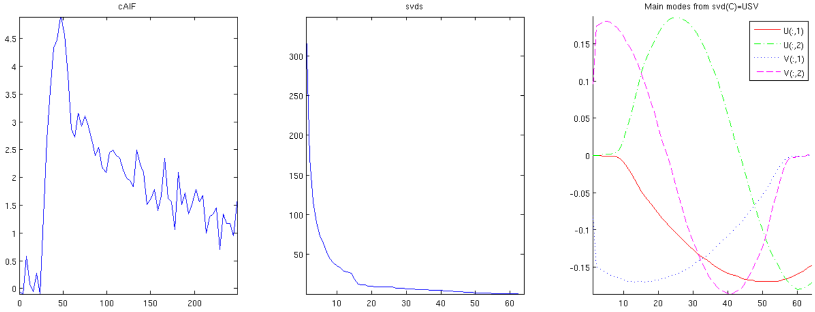
$i = 1, \ldots, n$, with $t_1 = 0$ and $t_n = T$, or

$$\boldsymbol{C}_{\mathrm{T}} = A\boldsymbol{K}, \quad \boldsymbol{C}_{\mathrm{T}} = \{C_{\mathrm{T}}(t_i)\}_{i=1}^n, \quad \boldsymbol{K} = \{K(t_j)\}_{j=1}^n$$

$$A = \frac{1}{2}\begin{bmatrix} 0 & 0 & \cdots & 0 \\ C_{\mathrm{AIF}}(t_2-t_1)(t_2-t_1) & C_{\mathrm{AIF}}(t_2-t_2)(t_2-t_1) & \ddots & \vdots \\ C_{\mathrm{AIF}}(t_3-t_1)(t_2-t_1) & C_{\mathrm{AIF}}(t_3-t_2)(t_3-t_1) & C_{\mathrm{AIF}}(t_3-t_3)(t_3-t_2) & \vdots \\ \vdots & & \ddots & 0 \\ C_{\mathrm{AIF}}(t_n-t_1)(t_2-t_1) & C_{\mathrm{AIF}}(t_n-t_2)(t_3-t_1)\cdots & C_{\mathrm{AIF}}(t_n-t_j)(t_{j+1}-t_{j-1})\cdots & C_{\mathrm{AIF}}(t_n-t_n)(t_n-t_{n-1}) \end{bmatrix}$$

Regularization of Convolution through SVD

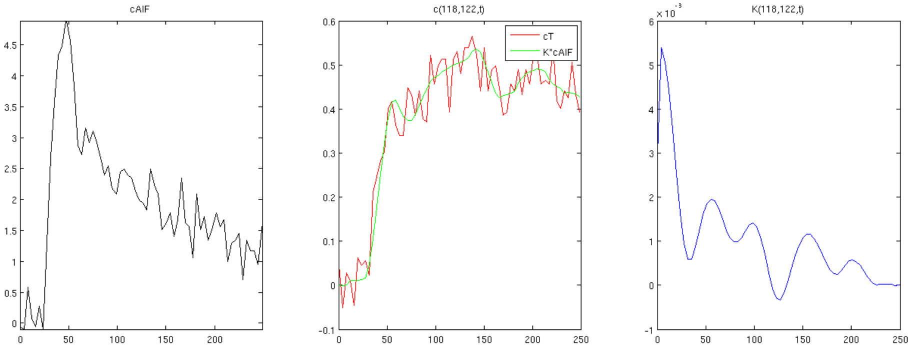
- With the singular value decomposition of the system matrix,
$$A = U\Sigma V$$
one typically obtains results as follows.



- The singular values $\{\sigma_i\}_{i=1}^n = \mathrm{diag}(\Sigma)$ are truncated, i.e., with $\sigma^\star = \frac{1}{10}\max\{\sigma_i\}_{i=1}^n$ let
$$\tilde{\Sigma}^\dagger = \mathrm{diag}\{(\sigma_i > \sigma^\star)/(\sigma_i + (\sigma_i \leq \sigma^\star))\}_{i=1}^n$$
- The regularized solution is
$$\boldsymbol{K} = V^{\mathrm{T}}\tilde{\Sigma}^\dagger U^{\mathrm{T}}\boldsymbol{C}_{\mathrm{T}}$$

Regularization of Convolution through SVD

- Typical measured and estimated time courses appear so:



- In spite of regularization the estimated kernel has many oscillations.
- In spite of oscillations the estimated tissue concentration is a smoothing of the measured tissue concentration.

Regularization of Convolution through SVD

- In spite of the above disadvantages in the estimated time courses the physiological parameters appear spatially so:

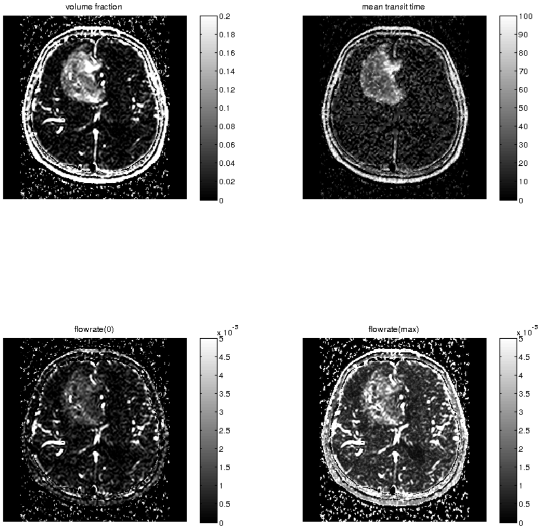
$$\mathcal{V}_\mathrm{T} = \sum_{i=1}^{n-1} [K_i + K_{i+1}] \times \frac{1}{2}(t_i - t_{i-1})$$

$$\mathcal{T}_\mathrm{T} = \mathcal{V}_\mathrm{T} / \mathcal{F}_\mathrm{T}$$

$$\mathcal{F}_\mathrm{T} = K_1$$

or

$$\mathcal{F}_\mathrm{T} = \max\{K_i\}_{i=1}^{n}$$



Regularization of Convolution through EXP

- Preferred approach: Convolution kernel is approximated with an exponential basis:
$$K(t;\boldsymbol{k}) = \sum_{m=1}^{M} k_m \exp[-\lambda_m t]$$
where $\boldsymbol{k} = \langle k_1, \ldots, k_M \rangle$ and $\boldsymbol{\lambda} = \langle \lambda_1, \ldots, \lambda_M \rangle$.
- The time scales $\{1/\lambda_m\}$ are *harmonically* distributed:
$$\lambda_m = m/T, \quad m = 1, \ldots, M$$

Theorem (Müntz): If $\lambda_m > 0$, $\lambda_m \stackrel{m\to\infty}{\longrightarrow} +\infty$ and $\sum_{m=1}^{\infty} 1/\lambda_m = +\infty$ holds, then $\{e^{-\lambda_m t}\}_{m=1}^{\infty}$ is dense in $L^p[0,\infty)$, $1 \le p < \infty$.

Theorem: The convolution kernel is monotone decreasing if
$$D_{M-1}^{-T} \cdots D_1^{-T} \Lambda \boldsymbol{k} \ge 0$$
where $\Lambda = \mathrm{diag}\{\lambda_m\}$ and with $q_i^j = 1/(\lambda_i - \lambda_j)$
$$D_m = \mathrm{tridiag}\left\{\begin{bmatrix} -q_{m+1}^1 & -q_{m+2}^2 & \cdots & -q_M^{M-m} & 0 & \cdots & 0 & - \\ +q_{m+1}^1 & +q_{m+2}^2 & \cdots & +q_M^{M-m} & 1 & \cdots & 1 & 1 \\ - & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\right\}$$

Regularization of Convolution through EXP

- To obtain a condition for monotonicity K is written as,

$$K(t) = \int_0^\infty e^{-\lambda t} d\mu(\lambda), \qquad \mu'(\lambda) = \sum_{m=1}^{M} k_m \delta(\lambda - \lambda_m)$$

- The *excessively constraining* condition

$$-K'(t) = \int_0^\infty \lambda e^{-\lambda t} \underbrace{d\mu(\lambda)}_{\geq 0} \geq 0, \quad \mu'(\lambda) = \sum_{m=1}^{M} \underbrace{k_m}_{\geq 0} \delta(\lambda - \lambda_m) \geq 0$$

  leads to the property *completely monotone*

$$(-1)^n K^{(n)}(t) = \int_0^\infty \lambda^n e^{-\lambda t} d\mu(\lambda) \geq 0$$

- The implemented condition is derived as follows:

$$-K'(t) = t^n \int_0^\infty d\ell_n \exp(-\ell_n t) \underbrace{\int_0^{\ell_n} d\ell_{n-1} \int_0^{\ell_{n-1}} d\ell_{n-2} \cdots \int_0^{\ell_1} \ell_0 d\mu(\ell_0)}_{\geq 0} \geq 0$$

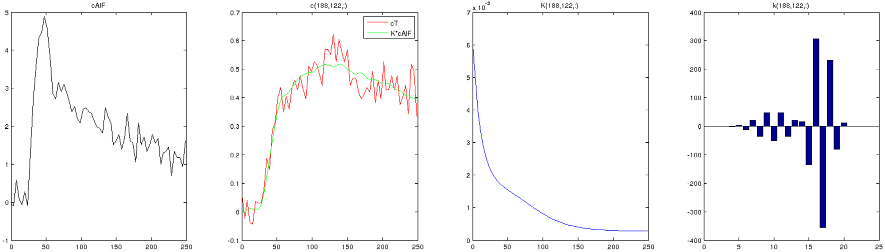
- Discrete: $D_{M-1}^{-T} \cdots D_1^{-T} \Lambda \boldsymbol{k} \geq 0 \Rightarrow$

$$-K'(t) = \boldsymbol{k}^{\mathrm{T}} [\Lambda D_1^{-1} \cdots D_{M-1}^{-1}][D_{M-1} \cdots D_1] \exp(-\boldsymbol{\lambda} t) \geq 0.$$

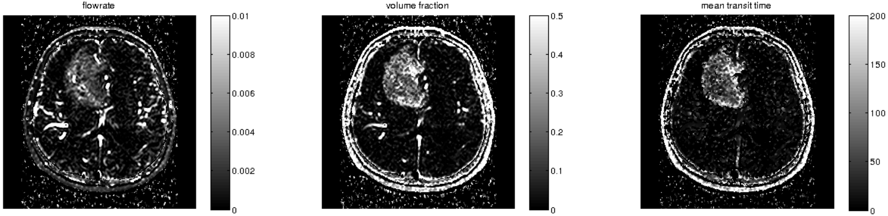
- Then $\|\boldsymbol{C}_{\mathrm{T}} - AK(\boldsymbol{t}, \boldsymbol{k})\|_{\ell_2}^2$ is minimized under this condition, where $K(\boldsymbol{t}, \boldsymbol{k}) = \{K(t_j, \boldsymbol{k})\}_{j=1}^n$. ($\boldsymbol{C}_{\mathrm{T}}, A$ as before.)

Regularization of Convolution through EXP

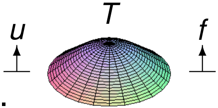
- With the exponential basis the time courses appear so:



- Notice: $K * C_{\mathrm{AIF}}$ is a smoothing of C_{T}, K is monotone decreasing and the spectrum $\boldsymbol{k}$ is well distributed.
- The parameters $\mathcal{F}_{\mathrm{T}}$, $\mathcal{V}_{\mathrm{T}}$ and $\mathcal{T}_{\mathrm{T}}$ appear so:



Modeling a Membrane



- We saw 1D mass spring systems earlier.
  Now consider displacements of a membrane.
  At the position $\boldsymbol{x} \in \Omega$ set:
  - $u(\boldsymbol{x})$ = upward directed displacement of the membrane,
  - $f(\boldsymbol{x})$ = upward directed external force and
  - $T(\boldsymbol{x})$ = tension of the membrane.
- To model the state of the membrane, we define an energy to be minimized:
  - Let a small piece of membrane $\mathcal{S}$ be perturbed from equilibrium to $\tilde{\mathcal{S}}$ through changes in area dS and volume dV, where dV lies between $\mathcal{S}$ and $\tilde{\mathcal{S}}$.
  - These perturbations increase the energy $\mathcal{F}$ according to $d\mathcal{F} = TdS - fdV$, and additional energy is then available for work to bring the membrane piece back to equilibrium. The work performed for this is
    - work $-fdV$ from the force per unit area $-f$ after the perturbation dV and
    - work TdS from the force per unit length T after the perturbation dS.

Variational Derivatives of Energy

- Let $u^\star$ be the displacement in equilibrium. According to $d\mathcal{F} = TdS - fdV$ the variational derivatives satisfy
$$\frac{\delta \mathcal{F}}{\delta u}(u^\star; v) = T\frac{\delta S}{\delta u}(u^\star; v) - f\frac{\delta V}{\delta u}(u^\star; v)$$
- With $S(u^\star) = \sqrt{1 + |\nabla u^\star|^2} d\boldsymbol{x}$ holds
$$\frac{\delta S}{\delta u}(u; v) = \frac{\nabla u \cdot \nabla v}{\sqrt{1 + |\nabla u|^2}} d\boldsymbol{x}$$
- With $V(u^\star) = u^\star d\boldsymbol{x}$ holds
$$\frac{\delta V}{\delta u}(u^\star; v) = v d\boldsymbol{x}$$
- The energy satisfies
$$\frac{\delta \mathcal{F}}{\delta u}(u^\star; v) = \left[T\frac{\nabla u^\star \cdot \nabla v}{\sqrt{1 + |\nabla u^\star|^2}} - fv\right] d\boldsymbol{x}$$
- When integrated over the whole membrane domain Ω, the energy to be minimized satisfies
$$\frac{\delta J}{\delta u}(u^\star; v) = \int_\Omega \left[T\frac{\nabla u^\star \cdot \nabla v}{\sqrt{1 + |\nabla u^\star|^2}} - fv\right]$$

Minimization of the Energy

- For T and f independent of u, let the energy be given by

$$J(u) = \int_\Omega T\sqrt{1+|\nabla u|^2} - \int_\Omega fu$$

i.e., a sum of elastic energy of the membrane and the opposing work of the external force.

- Then the variational derivative is given by,

$$\begin{aligned}
\frac{\delta J}{\delta u}(u;v) &= \lim_{\epsilon\to 0} \frac{d}{d\epsilon} J(u+\epsilon v) \\
&= \lim_{\epsilon\to 0} \frac{d}{d\epsilon} \int_\Omega T[1+|\nabla(u+\epsilon v)|^2]^{\frac{1}{2}} - \int_\Omega f(u+\epsilon v) \\
&= \lim_{\epsilon\to 0} \int_\Omega \tfrac{1}{2} T[1+|\nabla(u+\epsilon v)|^2]^{-\frac{1}{2}} 2\nabla(u+\epsilon v)\cdot\nabla v - \int_\Omega fv \\
&= \int_\Omega T[1+|\nabla u|^2]^{-\frac{1}{2}} \nabla u\cdot\nabla v - \int_\Omega fv
\end{aligned}$$

which agrees with the previously established result.

- The displacement $u^\star$ in equilibrium satisfies

$$\frac{\delta J}{\delta u}(u^\star;v) = 0, \quad \forall v \text{ smooth enough.}$$

Minimization of the Energy

- To characterize $u^\star$, this derivative must be reformulated through partial integration,

$$0 \stackrel{!}{=} \frac{\delta J}{\delta u}(u;v) = -\int_\Omega v\nabla\cdot\left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}}\right] + \int_{\partial\Omega} v\hat{\boldsymbol{n}}\cdot\left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}}\right] - \int_\Omega fv$$

- If v_ϵ with the properties

$$\hat{\boldsymbol{x}} \in \Omega^\circ, \quad v_\epsilon = 0 \text{ in } \Omega \backslash B(\hat{\boldsymbol{x}},\epsilon), \quad v_\epsilon(\hat{\boldsymbol{x}}) \stackrel{\epsilon\to 0}{\longrightarrow} \infty, \quad \int_\Omega v_\epsilon = 1$$

is chosen, there results

$$0 = \underbrace{\int_\Omega v_\epsilon}_{=1} \left\{\nabla\cdot\left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}}\right] + f\right\} \stackrel{\epsilon\to 0}{\longrightarrow} \left\{\nabla\cdot\left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}}\right] + f\right\}(\hat{\boldsymbol{x}})$$

- If v_ϵ with the properties

$$\check{\boldsymbol{x}} \in \partial\Omega, \quad v_\epsilon = 0 \text{ in } \overline{\Omega} \backslash B(\check{\boldsymbol{x}},\epsilon), \quad v_\epsilon(\check{\boldsymbol{x}}) \stackrel{\epsilon\to 0}{\longrightarrow} \infty, \quad \int_{\partial\Omega} v_\epsilon = 1$$

is chosen, there results

$$0 = \underbrace{\int_{\partial\Omega} v_\epsilon}_{=1} \hat{\boldsymbol{n}}\cdot\left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}}\right] \stackrel{\epsilon\to 0}{\longrightarrow} \left[\frac{T\partial u/\partial n}{\sqrt{1+|\nabla u|^2}}\right](\check{\boldsymbol{x}})$$

Potentielle Energie

- Since $\hat{\boldsymbol{x}}$ and $\check{\boldsymbol{x}}$ are arbitrary, $u^\star$ is characterized by the boundary value problem,

$$-\nabla \cdot \left[\frac{T\nabla u}{\sqrt{1+|\nabla u|^2}} \right] = f \text{ in } \Omega, \quad \frac{T\partial u/\partial n}{\sqrt{1+|\nabla u|^2}} = 0 \text{ auf } \partial\Omega$$

Exercise: For small κ it holds that

$$\sqrt{1+\kappa^2} - 1 = \frac{(1+\kappa^2) - 1}{\sqrt{1+\kappa^2}+1} \approx \tfrac{1}{2}\kappa^2$$

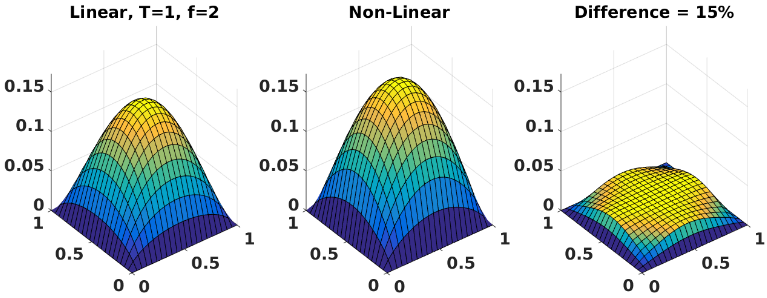
and thus for small displacements $\sqrt{1+|\nabla u|^2}$ in J can be approximated with $\frac{1}{2}|\nabla u|^2$. Show for the approximated energy functional that the minimizing displacement satisfies:

$$-\nabla \cdot [T\nabla u] = f \text{ in } \Omega, \quad T\partial u/\partial n = 0 \text{ on } \partial\Omega$$

- In case the Membrane is clamped on the boundary, the *Neumann* boundary condition $\partial u/\partial n = 0$ is replaced with the *Dirichlet* boundary condition $u = 0$.
- For the derivation of the Dirichlet boundary value problem, $v = 0$ must hold on $\partial\Omega$ to avoid a boundary perturbation.

Investigation of the Approximation

- For $T = 1$ and $f = 2$ and Dirichlet boundary conditions solutions of the linear (Poisson) and non-linear (minimal surface) problems are compared:



- For the solution to the minimal surface problem a *Picard* Iteration is used, ($f \gg T \Rightarrow$ no solution! Why?)

$$-\nabla \cdot \left[\frac{T \nabla u_{k+1}}{\sqrt{1 + |\nabla u_k|^2}} \right] = f \text{ in } \Omega, \quad \frac{T \partial u_{k+1} / \partial n}{\sqrt{1 + |\nabla u_k|^2}} = 0 \text{ on } \partial\Omega, \quad k = 0, 1, \ldots$$

where $u_0 = 0$ and u_1 solves the Poisson problem.

Membrane Dynamics

- The derivative of the energy is a force.
- With Newton's Law ($ma = F$) the membrane dynamics can be modeled so,

$$\int_\Omega \rho u_{tt} v = -\frac{\delta J}{\delta u}(u; v), \quad \forall v \text{ smooth enough}$$

  where ρ is the mass per unit area.
- By choosing v strategically with Dirichlet boundary conditions together with initial conditions, the wave equation results,

$$\begin{cases} \rho u_{tt} & = & \nabla \cdot \left[\dfrac{T \nabla u}{\sqrt{1 + |\nabla u|^2}} \right] + f, & \Omega \times (0, \infty) \\ u & = & 0, & \partial\Omega \times (0, \infty) \\ u & = & u_0, & \Omega \times \{0\} \\ u_t & = & u_1, & \Omega \times \{0\} \end{cases}$$

- This PDE is analogous to the ODE $mu'' = -P'(u)$ for the undamped mass spring system.

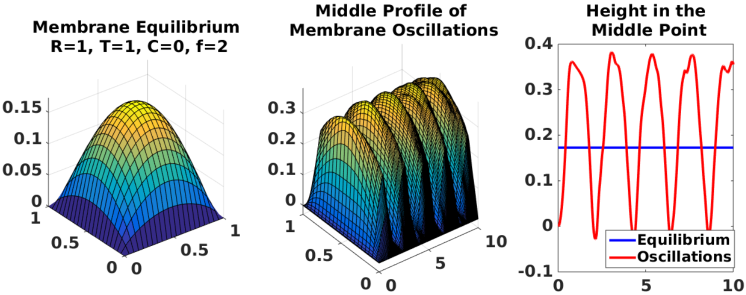
Membrane Dynamics

- Analogous to the damped mass spring system frictional forces f^{fric} can be introduced,
$$f^{\text{fric}} = -cu_t$$
which work against the velocity u_t.
- With such damping the PDE becomes
$$\rho u_{tt} + cu_t = \nabla \cdot \left[\frac{T \nabla u}{\sqrt{1 + |\nabla u|^2}} \right] + f$$
and it can be re-written in first order form so,
$$\underbrace{\begin{bmatrix} I & 0 \\ 0 & \rho \end{bmatrix}}_{=:M} \begin{bmatrix} u \\ u_t \end{bmatrix}_t = \underbrace{\begin{bmatrix} 0 & I \\ \nabla \cdot \frac{T}{\sqrt{1+|\nabla u|^2}} \nabla & -c \end{bmatrix}}_{=:K(u)} \begin{bmatrix} u \\ u_t \end{bmatrix} + \begin{bmatrix} 0 \\ f \end{bmatrix}$$
- The equilibrium $u^\star$ should solve the static minimal surface problem. $f \gg T \Rightarrow$ no solution!
- Does the system matrix $A = M^{-1} K(u^\star)$ satisfy the conditions,
$$\Re(\sigma(A)) < 0? \qquad \Im(\sigma(A)) = \emptyset?$$
- This evolution can be compared with the Picard iteration for the solution to the mimimal surface problem.

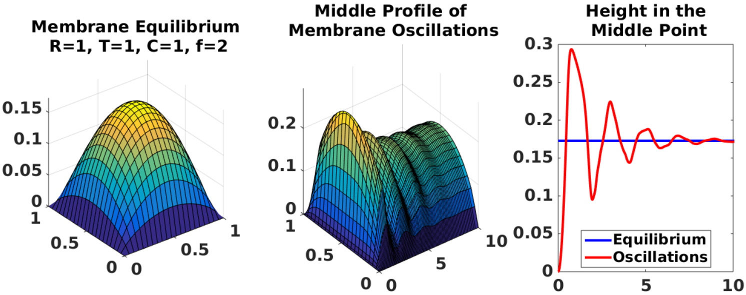
Membrane Dynamics

- With $c = 0$ there is no damping.

  $(R = \rho)$

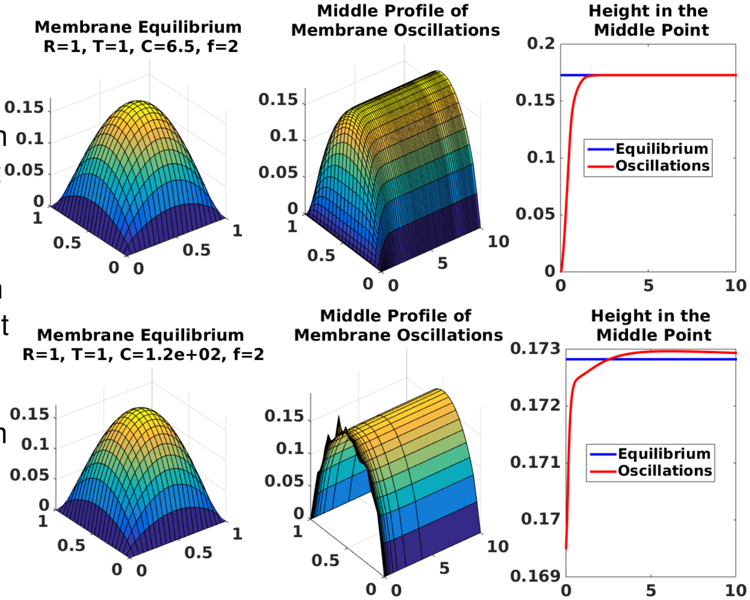


- With $c = 1$ the membrane is under damped.



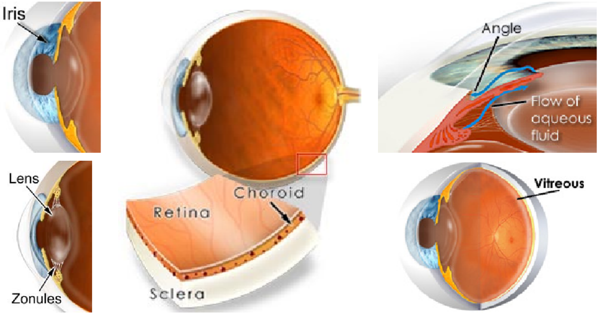
Membrane Dynamics

- Membrane *effectively* critically damped with $C = 6.5$, but $\emptyset \neq \Im\sigma(A)$.
- $\sigma(A) \subset (-\infty, 0]$ with $C = 120$, but local oscillations after random perturbations of the equilibrium.



Application: Eyeball Dynamics

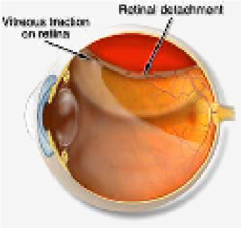
- Anatomy of the Eyeball:

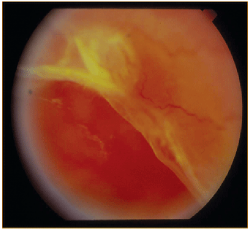


- Sclera: the white protection of the eyeball
- Choroid blood vessels, nourishment
- Retina: photo receptors
- Self regulation of flow: constant pressure

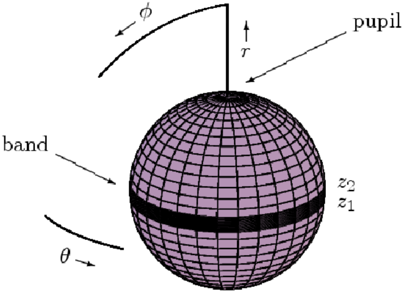
Cerclage Operation

- Diseased state: retinal tear or retinal detachment



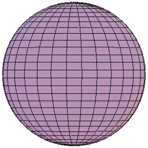


- Surgical solution:
  Apply a *Cerclage*
  (rubber band),
  to press the eyeball
  together.

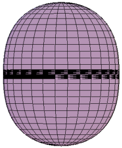


Before, During and After the Operation

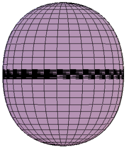
- States of the eyeball: pre-, intra- and post-operative:



approximately a sphere
volume $= V_1$
pressure $= p_1$



deformed by the band
volume $= V_1$
pressure $> p_1$



less deformed
volume $< V_1$
pressure $\approx p_1$

- Goal: predict these states to facilitate operation planning.
- Eyeball boundary is modeled as a *Membrane*:
  - Thickness neglected, (non-linear) elastic effects.
  - Intraoperative: constrained minimization of an energy under constant volume.
  - Postoperative: the same under a constant volume, which fits together with the original pressure.

Modeling the Energy

- Let a small membrane piece $\mathcal{S}$ (i.e., of the eyeball boundary) be perturbed from equilibrium to $\tilde{\mathcal{S}}$ through changes in surface area dS and volume dV, where dV lies between $\mathcal{S}$ and $\tilde{\mathcal{S}}$.
- These perturbations increase the energy $\mathcal{F}$ by
$$d\mathcal{F}(u,p) = T(u)dS - F(u,p)dV$$
where
$$\begin{aligned} u &= \text{distance from the eyeball center} \\ p &= \text{internal pressure of the eyeball} \\ T(u) &= \text{tension of the membrane} \\ F(u,p) &= \text{force from internal pressure and from rubber band} \end{aligned}$$
- The additional energy is then available for work to bring the membrane back to equilibrium. The work performed for this is:
  - work $-F(u,p)dV$ from the force per unit area $-F(u,p)$ after the perturbation dV and
  - work $T(u)dS$ from the force per unit length $T(u)$ after the perturbation dS.

Modeling the Energy

- Let $u^\star$ be the displacement from equilibrium with a currently fixed internal pressure p. According to $d\mathcal{F}(u,p) = T(u)dS - F(u,p)dV$ the variational derivatives satisfy: $$\frac{\delta \mathcal{F}}{\delta u}(u^\star, p; v) = T(u^\star)\frac{\delta S}{\delta u}(u^\star; v) - F(u^\star, p)\frac{\delta V}{\delta u}(u^\star; v)$$
- By symmetry we have $u^\star = u^\star(\phi)$. With

$$X(\phi,\theta;u) = \langle u(\phi)\cos(\theta)\sin(\phi), u(\phi)\sin(\theta)\sin(\phi), u(\phi)\cos(\phi)\rangle^{\mathrm{T}}$$

it follows that

$$S(u) = |X_\phi(\phi,\theta;u) \times X_\theta(\phi,\theta;u)|d\phi d\theta = u\sin(\phi)\sqrt{u^2 + u_\phi^2}d\phi d\theta$$

and
$$\frac{\delta S}{du}(u^\star; v) = \frac{{u_\phi^\star}^2 v + 2{u^\star}^2 v + u u_\phi v_\phi}{\sqrt{{u^\star}^2 + {u_\phi^\star}^2}}\sin(\phi)d\phi d\theta$$

- Through the sum of terms $T(u^\star)\delta S(u^\star; v)/\delta u$ over all membrane pieces $\mathcal{S}$ there results the derivative of the energy due purely to membrane-internal forces:
$$\frac{\delta J_{\mathrm{i}}}{\delta u}(u^\star; v) = 2\pi\int_0^\pi T(u^\star)\frac{{u_\phi^\star}^2 v + 2{u^\star}^2 v + u u_\phi v_\phi}{\sqrt{{u^\star}^2 + {u_\phi^\star}^2}}\sin(\phi)d\phi$$

Modeling the Energy

- With
$$V(u) = \sin(\phi)d\phi d\theta \int_0^u r^2 dr$$
follows
$$\frac{dV}{du}(u^\star; v) = vu^{\star 2}\sin(\phi)d\phi d\theta$$
- Let $\hat{\boldsymbol{e}}_R = \langle \cos(\theta), \sin(\theta), 0\rangle$ be the radial unit vector in cylindrical coordinates.
- Let $f(R,z)\hat{\boldsymbol{e}}_R$ be the radial inwardly directed force per unit area of the rubber band in cylindrical coordinates (R, z) on the surface of the eyeball.
- The sum of the outwardly directed forces per unit area in an eyeball point is
$$F(u,p) = p - f(u\cos(\phi), u\sin(\phi))\hat{\boldsymbol{e}}_R \cdot \hat{\boldsymbol{n}}$$
where the outwardly directed unit normal vector is given by
$$\hat{\boldsymbol{n}} = \frac{X_\phi(\phi,\theta;u) \times X_\theta(\phi,\theta;u)}{|X_\phi(\phi,\theta;u) \times X_\theta(\phi,\theta;u)|} = \frac{1}{\sqrt{u^2 + u_\phi^2}} \times$$
$$\langle -\cos(\phi)(u\cos(\phi))_\phi, -\sin(\phi)(u\cos(\phi))_\phi, -\cos(\phi)(u\sin(\phi))_\phi\rangle$$

Incompressibility Constraint

- Through the sum of terms $F(u^\star, p)\delta V(u^\star; v)/\delta u$ over all membrane pieces $\mathcal{S}$ there results the derivative of the energy due purely to membrane-external forces:

$$\frac{\delta J_\mathrm{e}}{\delta u}(u^\star;v) = -2\pi\int_0^\pi \left\{ f(u^\star\cos(\phi), u^\star\sin(\phi))\frac{(u^\star\cos(\phi))_\phi}{\sqrt{u^{\star 2}+u_\phi^{\star 2}}} + p \right\} v u^{\star 2}\sin(\phi)d\phi$$

- For the constraint of a constant volume let r_1 be the radius of the undeformed eyeball. With a deformation it must hold that

$$J_\mathrm{c}(u^\star) = V(u^\star) - V(r_1) = \frac{2\pi}{3}\int_0^\pi u^{\star 3}\sin(\phi)d\phi - \frac{4\pi r_1^3}{3} = 0$$

- To minimize the energy $J_\mathrm{i} + J_\mathrm{e}$ under the constraint $J_\mathrm{c} = 0$, we seek a stationary point of the Lagrange functional:

$$L(u) = \frac{1}{2\pi}[J_\mathrm{i}(u) + J_\mathrm{e}(u) - \lambda J_\mathrm{c}(u)]$$

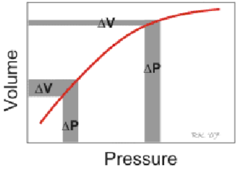
where λ is a Lagrange multiplier.

Modeling the Rubber Band Force

- If a rubber band with cross sectional area A is pulled from a resting state with length $\hat{L}$ to a state with length $\hat{L} + \Delta L$, the countering force F from the rubber band can be modeled with Hook's Law,
$$F = AE\Delta L/\hat{L}$$
where E is Young's modulus.
- Let the cross sectional area be given by $A = \omega \cdot \delta$, where $\omega = z_2 - z_1$ is the width and δ is the thickness.
- If the band is circular, the transverse tension is given by
$$T = F/\omega = E\delta(R - \hat{R})/\hat{R}$$
where $\hat{L} = 2\pi\hat{R}$ and $\hat{L} + \Delta L = 2\pi R$.
- With Laplace's Law for a cylinder
$$\Delta p = T(\kappa_1 + \kappa_2) \quad \Rightarrow \quad R\Delta p = T$$
the radial inwardly directed (i.e., direction $-\hat{\boldsymbol{e}}_R$) force per unit area of the rubber band is given by T/R, i.e.,
$$f(R, z) = E \cdot \delta \cdot (1/R - 1/\hat{R}), \quad z_1 \le z \le z_2$$
where $\hat{R}$ is the resting radius of the band.

Modeling the Membrane Tension

- For the tension it is assumed that $T(u)$ is a constant, which depends upon the function u.
- If the eyeball is spherical with radius r_1, Laplace's Law gives,
$$\Delta p = T(\kappa_1 + \kappa_2) \quad \Rightarrow \quad 2T_1 = p_1 r_1$$
where $p_1 = \Delta p = p_\mathrm{i} - p_\mathrm{a} > 0$ is the pressure difference between outside and inside.
- The relation between pressure and radius (or volume) of a compliant tissue is typically logarithmic,
$$\ln\left(\frac{p_0}{p_1}\right) = \sigma(V_0 - V_1) = \frac{4\pi\sigma}{3}(r_0^3 - r_1^3)$$
where (p_0, r_0) is a departure from the state (p_1, r_1) of the eyeball. This is the *Friedenwald Law* and σ is the *ocular rigidity*.



Compliance curve for a biological tissue such as an artery. At low pressures and volumes, compliance ΔV/ΔP is much greater than at high pressures and volumes.

- The tension which fits to the departure (p_0, r_0) is
$$T_0 = \frac{1}{2} r_0 p_0 = \frac{1}{2} r_0 p_1 \exp\left[\frac{4\pi\sigma}{3}(r_0^3 - r_1^3)\right]$$

Modeling the Membrane Tension

- For a departure from spherical form the tension is modeled with a Hookian supplement to the Laplace Law:

$$T(u) = T_0(u) + E_{\mathrm{m}} \cdot \delta_{\mathrm{m}} \cdot [S(u) - S_0(u)]/S_0(u)$$

where

$V(u)$ = volume of the eyeball with geometry u, i.e., $V(u) = \frac{2\pi}{3} \int_0^\pi u^3 \sin(\phi) d\phi$

$S(u)$ = area of the eyeball with geometry u, i.e., $S(u) = 2\pi \int_0^\pi u(u^2 + u_\phi^2)^{\frac{1}{2}} \sin(\phi) d\phi$

$r_0(u)$ = radius of the spherical eyeball with volume $V(u)$

$p_0(u)$ = pressure of the spherical eyeball with volume $V(u)$, i.e., $p_0(u) = p_1 \exp[\frac{4\pi\sigma}{3}(r_0(u)^3 - r_1^3)]$

$T_0(u)$ = tension of the spherical eyeball with volume $V(u)$, i.e., $T_0(u) = \frac{1}{2} r_0(u) p_0(u)$

$S_0(u)$ = area of the spherical eyeball with radius $r_0(u)$

E_{m} = Young's modulus of the membrane

δ_{m} = thickness of the sclera+choroid

Stationarity of the Lagrangian

- The stationarity conditions for the Lagrangian $L(u,\lambda) = \frac{1}{2\pi}[J_{\mathrm{i}}(u) + J_{\mathrm{e}}(u) - \lambda J_{\mathrm{c}}(u)]$ are:

$$-\left\{ T(u)\frac{uu_\phi}{\sqrt{u^2+u_\phi^2}}\sin\phi \right\}_\phi + T(u)\frac{2u^2+u_\phi^2}{\sqrt{u^2+u_\phi^2}}\sin\phi$$

$$= \left\{ f(u\sin\phi, u\cos\phi)\frac{(u\cos\phi)_\phi}{\sqrt{u^2+u_\phi^2}} + (p_1+\lambda) \right\} u^2\sin\phi, \quad 0<\phi<\pi,$$

$$u_\phi = 0, \quad \phi = 0,\pi, \qquad \int_0^\pi u^3\sin\phi d\phi = 2r_1^3$$

- With the pre-operative state (r_1, p_1) (according to Friedenwald) and the above solution (u,λ) set $p = p_1 + \lambda$.
- Let the *Cerclage Operator* for the intra-operative state be:

$$\mathcal{C}(r_1) = (u,p) \quad \text{with} \quad \mathcal{C}(r_1)[u] = u, \quad \mathcal{C}(r_1)[p] = p$$

Solution Approach

- The intra-operative problem:
  Given the pre-operative state (r_1, p_1) (according to Friedenwald), compute $\mathcal{C}(r_1) = (u, p)$ where
  - $u =$ intra-operative geometry
  - $p =$ intra-operative pressure
- The post-operative problem:
  Given a target pressure $p_t \approx p_1$,
  - find (r_0, p_0) (according to Friedenwald)
  - for a band-free spherical eyeball
  - with reduced volume $V_0 = 4\pi r_0^3/3$

  where $\mathcal{C}(r_0) = (u, p_t)$ holds.
- Solution approach for the post-operative problem is a bisection method, where the following is used iteratively.
- Solution approach for the intra-operative problem: An approximate Newton iteration is applied

$$\begin{bmatrix} A(u) & K(u) \\ K^*(u) & 0 \end{bmatrix} \begin{bmatrix} v \\ \lambda \end{bmatrix} = \begin{bmatrix} F(u,p) \\ G(u) \end{bmatrix} \qquad \begin{matrix} u = u + \alpha v \\ p = p + \alpha\lambda \end{matrix}$$

  where

Solution Procedure

$$A(u)v = -\left\{ \frac{T(u)u\sin\phi}{\sqrt{u^2+u_\phi^2}} v_\phi \right\}_\phi + \frac{T(u)u\sin\phi}{\sqrt{u^2+u_\phi^2}} v \quad \approx -\frac{\delta F}{\delta u}(u;v)$$

$$K(u)\lambda = -\lambda u^2 \sin\phi \quad \approx -\frac{\delta F}{\delta p}(p;\lambda), \quad K^*(u)v = -\int_0^\pi v u^2 \sin\phi d\phi \quad \approx -\frac{\delta G}{\delta u}(u;v)$$

$$F(u,p) = -A(u)u - T(u)\sin\phi\sqrt{u^2+u_\phi^2} + \left[f(u\sin\phi, u\cos\phi)\frac{(u\cos\phi)_\phi}{\sqrt{u^2+u_\phi^2}} + p \right] u^2 \sin\phi$$

$$G(u) = \int_0^\pi u^3 \sin\phi d\phi - 2r_1^3$$

Theorem: $\exists!$ solution (v,λ), when v has a certain smoothness.

- Solution method: cell centered finite differences:

$$\begin{bmatrix} A_h(\boldsymbol{u}) & K_h(\boldsymbol{u}) \\ K_h^{\mathrm{T}}(\boldsymbol{u}) & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v} \\ \lambda \end{bmatrix} = \begin{bmatrix} F_h(\boldsymbol{u},p) \\ G_h(\boldsymbol{u}) \end{bmatrix} \qquad \begin{array}{l} \boldsymbol{u} = \boldsymbol{u} + \alpha\boldsymbol{v} \\ p = p + \alpha\lambda \end{array}$$

Algorithm

For the calculation of the post-operative state:

- Given are the band radius $\hat{R}$ in resting state and the target pressure $p_\mathrm{t} \approx p_1$, where p_1 is the pre-operative pressure.
- Set $r_\mathrm{a} = \hat{R}$ and compute p_a according to Friedenwald. No band force $\Rightarrow \mathcal{C}(r_\mathrm{a}) = (u = r_\mathrm{a}, p = p_\mathrm{a})$.
- Set $p_\mathrm{b} = p_\mathrm{t}$ and compute r_b according to Friedenwald. Then start with $(u = r_\mathrm{b}, p = p_\mathrm{b})$ and iterate to compute $\mathcal{C}(r_\mathrm{b})$.
- Since $\mathcal{C}(r_\mathrm{a})[p] < p_\mathrm{t} < \mathcal{C}(r_\mathrm{b})[p]$ holds, start the bisection method with the interval $[r_\mathrm{a}, r_\mathrm{b}]$ to solve $\mathcal{C}(r_0)[p] = p_\mathrm{t}$.
- The desired post-operative geometry u is given by $\mathcal{C}(r_0)[u]$.

Material Properties

- From the Fürstenfeld lab report:

Measured Cerclage Parameters	
Young's Modulus E_b	24453 mmHg
Thickness δ_b	0.75 mm
Width ω_b	2 mm
Resting Radius $\hat{R}$	10.35 mm

- The cerclage was marked, relaxed and measured directly to determine $\hat{R}$.
- For the following sclera and choroid properties from the literature were summed:

Measured Eyeball Parameters	
Young's Modulus E_m	21753 mmHg
Thickness δ_m	1 mm
Ocular Rigidity σ	1/80

- The (p, V)-curve was generated through direct injection of water.

Experimental Procedures

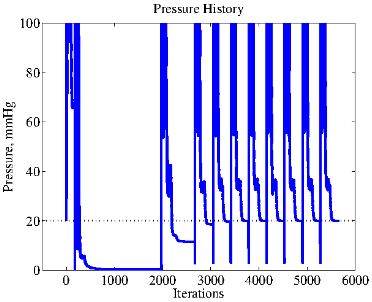
- Eyeball and cerclage states were measured directly.
- Inelastic threads were used to measure the radii.
- The band was wrapped around the eyeball at the equator, pulled, tied and marked.

		measured	computed
pre-operative:	p_1, mmHg	23.00	
	r_1, mm	12.25	
intra-operative:	$\mathcal{C}(r_1)[p]$, mmHg	76.00	67.88
	$\min \mathcal{C}(r_1)[u]$, mm	11.94	10.94
post-operative:	$\mathcal{C}(r_0)[p]$, mmHg	20.00	20.00
	$\min \mathcal{C}(r_0)[u]$, mm	11.22	10.43

- Pressures were measured directly.
- Fluid was extracted to reduce the pressure: $p_t = 20 \neq 23 = p_1$.

Simulation Results

- Post-operative target pressure is $p_{\mathrm{t}} = 20$.
- There holds $p_{\mathrm{a}} \approx 0$ for $r_{\mathrm{a}} = \hat{R}$.
- Start with the pre-operative pressure $p_{\mathrm{b}} = p_1 = 20$ and corresponding radius r_{b}.



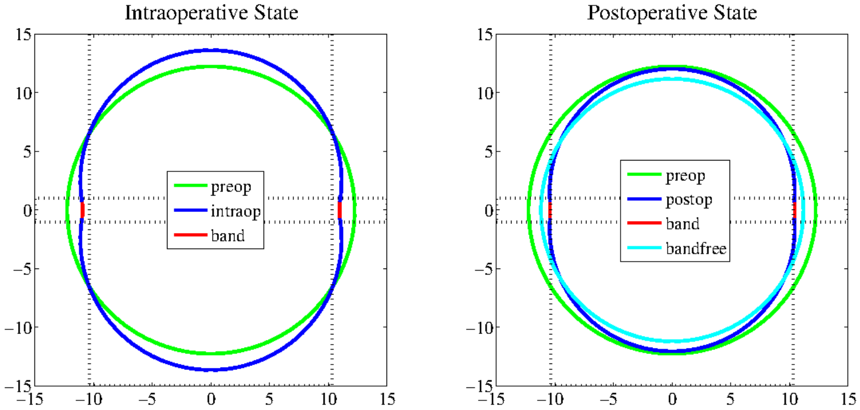
- Continue the bisection method to find $r_0 \in [r_{\mathrm{a}}, r_{\mathrm{b}}]$, so that $\mathcal{C}(r_0)[p] = p_{\mathrm{t}} \in [p_{\mathrm{a}}, p_{\mathrm{b}}]$ holds.

Simulation Results

Input Parameters:

r_1	12.25 mm	E_b	24453 mmHg	E_m	21753 mmHg	σ	1/80
p_1	23 mmHg	δ_b	0.75 mm	δ_m	1 mm	α	0.5
p_t	20 mmHg	$-z_1, z_2$	1 mm	$\hat{R}$	10.35 mm	N	101

Graphical representation:



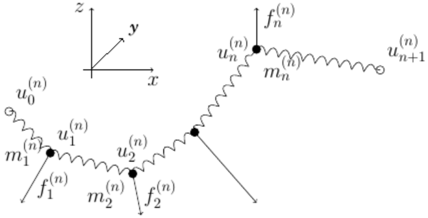
Simulation Results

pre-operativ		intra-operativ	
p_1	23.00 mmHg	$\mathcal{C}(r_1)[p]$	67.88 mmHg
r_1	12.25 mm	$\min \mathcal{C}(r_1)[u]$	10.94 mm
		$\max \mathcal{C}(r_1)[u]$	13.64 mm
T_1	141.0 mm·mmHg	$T(u)$	377.8 mm·mmHg
post-operativ, band-free		**post-operativ**	
p_0	3e-09 mmHg	$\mathcal{C}(r_0)[p]$	20.00 mmHg
r_0	11.20 mm	$\min \mathcal{C}(r_0)[u]$	10.43 mm
		$\max \mathcal{C}(r_0)[u]$	12.05 mm
T_0	2e-08 mm·mmHg	$T(u)$	104.6 mm·mmHg

- Results are rather satisfying for clinicians.
- The model has enriched the understanding of the eyeball-band-system.
- A wider and rectangular cerclage is preferred over a narrow circular one. The narrow one relaxes while the wide one remains stiff.

Large Deformations in a Bungee Cord

- A large deformation model for a bungee cord will be developed from a force balance, starting with a discrete approximation and moving to a continuum formulation.
- Consider a discrete mass-spring system with point masses $\{m_i\}_{i=1}^{n}$ located at positions $\{u_i\}_{i=1}^{n} \in \mathbb{R}^3$ with u_0 and u_{n+1} determined by boundary conditions. Define the displacement state $\vec{u} = \{u_i\}_{i=0}^{n+1}$.
- To each mass m_i there is an externally applied force f_i.
- The masses are connected by springs extending from position u_i to u_{i+1} for $i = 0, \ldots, n$.



Large Deformations in a Bungee Cord

- The magnitude of the force exerted by a single spring which has changed from an unloaded state at length l_0 to a loaded state at length l is modeled by *Hooke's Law*,

$$F(l) = \kappa(l - l_0)$$

  where κ is the spring constant (Nm^{-1}).
- The work done when changing the length from l_0 to l is

$$W_{\mathrm{s}}(l) = \int_{l_0}^{l} F(s)ds = \frac{\kappa}{2}(l - l_0)^2$$

  which increases the elastic energy stored in the spring.
- The total elastic energy in all springs at the state $\vec{u}$ is

$$J_{\mathrm{s}}(\vec{u}) = \frac{1}{2}\sum_{i=0}^{n} \kappa_i(\|u_{i+1} - u_i\| - l_i)^2$$

  where κ_i and l_i are the individual spring parameters.
- The work done to bring a mass m from a reference position 0 to position $||u||\tau$, $\tau = u/\|u\|$, against the external force f is

Large Deformations in a Bungee Cord

$$W_{\mathrm{m}}(u) = -\int_0^{\|u\|} f \cdot \tau ds = -f \cdot \tau \|u\| = -f \cdot u.$$

where, e.g., with gravity $f = (0, 0, -mg)^\top$ and $u \cdot f < 0$, the potential energy increases.

- The total potential energy of the masses is

$$J_{\mathrm{m}}(\vec{u}) = -\sum_{i=1}^{n} f_i \cdot u_i$$

- The total energy of the system at the state $\vec{u}$ is

$$J(\vec{u}) = J_{\mathrm{s}}(\vec{u}) + J_{\mathrm{m}}(\vec{u}) = \frac{1}{2}\sum_{i=0}^{n} \kappa_i(\|u_{i+1} - u_i\| - l_i)^2 - \sum_{i=1}^{n} f_i \cdot u_i$$

- To transform this to a continuum formulation, let the cord have a total length L and define the parameterization,

$$s_i = \frac{i}{n+1}L, \quad l_i = \frac{L}{n+1}$$

and set

$$\kappa_i = \tilde{\kappa}(s_{i+\frac{1}{2}}), \quad f_i = \int_{s_{i-\frac{1}{2}}}^{s_{i+\frac{1}{2}}} f(s) ds$$

Large Deformations in a Bungee Cord

where $\tilde{\kappa}$ is a continuous function describing elastic properties of the string (Nm^{-1}), and f is an integrable function giving the load density (Nm^{-1}).

- The *spring constant* κ_i is transformed to a material property κ (N) independent of length according to

$$\tilde{\kappa}(s_{i+\frac{1}{2}}) = \kappa_i = \frac{A_i E_i}{l_i} = \frac{\kappa(s_{i+\frac{1}{2}})}{L/(n+1)}$$

where A_i is cross-sectional area and E_i is the modulus of elasticity.

- The total energy can be written as

$$J(\vec{u}) = \frac{1}{2}\sum_{i=0}^{n} \kappa_i(\|u(s_{i+1}) - u(s_i)\| - l_i)^2 - \sum_{i=1}^{n} f_i \cdot u(s_i)$$
$$= \frac{1}{2}\sum_{i=0}^{n} \kappa_i \left(\frac{\|u(s_{i+1}) - u(s_i)\|}{s_{i+1} - s_i}\frac{L}{n+1} - \frac{L}{n+1}\right)^2 - \sum_{i=1}^{n}\int_{s_{i-\frac{1}{2}}}^{s_{i+\frac{1}{2}}} f(s)\cdot u(s_i)ds$$

Large Deformations in a Bungee Cord

$$= \sum_{i=0}^{n} \frac{\kappa_i}{2} \frac{L^2}{(n+1)^2} \left(\left\| \frac{u(s_{i+1}) - u(s_i)}{s_{i+1} - s_i} \right\| - 1 \right)^2 - \sum_{i=1}^{n} \int_{s_{i-\frac{1}{2}}}^{s_{i+\frac{1}{2}}} f(s) \cdot u(s_i) ds$$

or with $\kappa_i L^2/(n+1)^2 = \kappa(s_{i+\frac{1}{2}})(s_{i+1} - s_i)$,

$$J(\vec{u}) = \sum_{i=0}^{n} \frac{\kappa(s_{i+\frac{1}{2}})}{2} \left(\left\| \frac{u(s_{i+1}) - u(s_i)}{s_{i+1} - s_i} \right\| - 1 \right)^2 (s_{i+1} - s_i) - \sum_{i=1}^{n} \int_{s_{i-\frac{1}{2}}}^{s_{i+\frac{1}{2}}} f(s) \cdot u(s_i) ds$$

which gives the following as $n \to \infty$,

$$J(u) = \frac{1}{2} \int_0^L \kappa(s)(\|u_s(s)\| - 1)^2 ds - \int_0^L f(s) \cdot u(s) ds$$

- Minimizing $J(u)$ with respect to the displacement u gives the static equilibrium state of the cord.
- Now consider modeling the dynamic state.

Non-Linear Hyperbolic IBVP for a Cord

- Let the rest length of a bungee cord be parameterized by $s \in \Omega = (0, 1)$ so the total length L of the cord is 1.
- Let $u(s, t) = (x(s, t), y(s, t), z(s, t)) \in \mathbb{R}^3$ represent the cord at position s and at time t.
- Let the cord be fastened at one end, $u(0, t) = 0$, with known initial position and velocity, $u(s, 0) = u_0(s)$, $u_t(s, 0) = u_1(s)$.
- The cord is loaded externally by $f(s, t) \in \mathbb{R}^3$ (force per unit length) and internally through tension related to the elastic modulus $\kappa(s)$ (force units).
- The density of the cord is $\rho(s)$ (mass per unit length).
- The *Principle of Least Action* used to model the dynamic shape of the cord over the time interval $t \in [0, T]$ is to find a stationary state for the Lagrangian functional (s.t. ICs & BCs)

$$L(u) = \int_0^T \int_0^1 \left[\frac{1}{2}\rho\|u_t\|^2 - \frac{1}{2}\kappa(\|u_s\| - 1)^2 + f \cdot u \right] dsdt$$

  to transform kinetic or potential energy most efficiently to the other type of energy. (cf. Newton's Law!)

Stationary Lagrangian for Non-Linear Mechanics

- Let $Q = \Omega \times (0, T)$ and suppose a test function v is sufficiently smooth with $v = 0$ at $s = 0$, $t = 0, T$. Then,

$$\frac{\delta L}{\delta u}(u; v) = \int_Q \left[\rho u_t \cdot v_t - \kappa(\|u_s\| - 1)\frac{u_s \cdot v_s}{\|u_s\|} + f \cdot v\right]$$

$$= \int_Q v \cdot \left[-\rho u_{tt} + \left(\kappa \frac{\|u_s\| - 1}{\|u_s\|} u_s\right)_s + f\right]$$

$$+ \int_\Omega \rho u_t \cdot v \Big|_{t=0}^{t=T} - \int_0^T \kappa \frac{\|u_s\| - 1}{\|u_s\|} u_s \cdot v \Big|_{s=0}^{s=1}$$

- The necessary optimality condition for a stationary u is

$$\begin{cases} \rho u_{tt} = \left(\kappa \frac{\|u_s\| - 1}{\|u_s\|} u_s\right)_s + f, & \text{for } (s, t) \in Q \\ u(0, t) = 0, \quad (1 - 1/\|u_s\|) u_s(1, t) = 0, & \text{for } t \in [0, T] \\ u(s, 0) = u_0(s), \quad u_t(s, 0) = u_1(s), & \text{for } s \in \Omega \end{cases}$$

where $u_t(s, 0) = u_1(s)$ is imposed initially instead of a final time condition $u(s, T) = u_T(s)$ corresponding to $v(s, T) = 0$.

Conservation Property for the Nonlinear IBVP

- If the cord is very *taut* and $\|u_s\| \gg 1$, the non-linear IBVP reduces to a linear IBVP for the wave equation with $f = 0$,

$$\rho u_{tt} = (\kappa u_s)_s$$

- Note the conservation property,

$$\begin{aligned}\tfrac{1}{2} D_t \int_\Omega \left[\rho \|u_t\|^2 + \kappa \|u_s\|^2\right] &= \int_\Omega [\rho u_t \cdot u_{tt} + \kappa u_s \cdot u_{st}] \\ &= \int_\Omega u_t \cdot [\rho u_{tt} - (\kappa u_s)_s] + \kappa u_s \cdot u_t \Big|_{s=0}^{s=1} = 0\end{aligned}$$

- Thus, the first-order form is often used

$$\begin{pmatrix} \rho^{\frac{1}{2}} u_t \\ \kappa^{\frac{1}{2}} u_s \end{pmatrix}_t = \left(\frac{\kappa}{\rho}\right)^{\frac{1}{2}} \begin{pmatrix} 0 & \partial_s \\ \partial_s & 0 \end{pmatrix} \begin{pmatrix} \rho^{\frac{1}{2}} u_t \\ \kappa^{\frac{1}{2}} u_s \end{pmatrix}$$

since the energy-norm of the state is preserved,

$$\left\| \begin{pmatrix} \rho^{\frac{1}{2}} u_t \\ \kappa^{\frac{1}{2}} u_s \end{pmatrix} (t) \right\|^2 = \int_\Omega \left[\rho \|u_t\|^2 + \kappa \|u_s\|^2\right] = \left\| \begin{pmatrix} \rho^{\frac{1}{2}} u_t \\ \kappa^{\frac{1}{2}} u_s \end{pmatrix} (0) \right\|^2$$

Nonlinear Wave Equation in First Order Form

- Similarly it holds without the taut assumption

$$\frac{1}{2}D_t\int_\Omega\left[\rho\|u_t\|^2+\kappa(\|u_s\|-1)^2-f\cdot u\right]$$
$$=\int_\Omega\left[\rho u_t\cdot u_{tt}+\kappa(\|u_s\|-1)\frac{u_s\cdot u_{st}}{\|u_s\|}-f\cdot u_t\right]$$
$$=\int_\Omega u_t\cdot\left[\rho\cdot u_{tt}-\left(\kappa\frac{\|u_s\|-1}{\|u_s\|}u_s\right)_s-f\right]+\kappa(\|u_s\|-1)\frac{u_s\cdot u_t}{\|u_s\|}\bigg|_{s=0}^{s=1}=0$$

- Since the state $(\rho^{\frac{1}{2}}u_t,\kappa^{\frac{1}{2}}(\|u_s\|-1))$ is problematic, the state $\vec{u}=(u;u_t)$ is used here, with damping $c>0$:

$$\begin{cases}\begin{pmatrix}u\\u_t\end{pmatrix}_t=\begin{pmatrix}0 & 1\\ \omega^2\partial_s(1-1/\|u_s\|)\partial_s & -c\end{pmatrix}\begin{pmatrix}u\\u_t\end{pmatrix}+\begin{pmatrix}0\\g\end{pmatrix} & \text{in } Q\\ \begin{pmatrix}u\\u_t\end{pmatrix}_{t=0}=\begin{pmatrix}u_0\\u_1\end{pmatrix},\quad \begin{pmatrix}u\\u_t\end{pmatrix}_{s=0}=0,\quad (1-1/\|u_s\|)\partial_s\begin{pmatrix}u\\u_t\end{pmatrix}_{s=1}=0\end{cases}$$

- For simplicity assume that $\omega^2=\kappa/\rho$ is a constant and that $g=f/\rho$ is a constant vector (e.g., gravitational force).

Non-Linear Hyperbolic IBVP for a Membrane

Exercise:

- Let the rest area of a membrane be parameterized by $(\xi, \eta) \in \Omega = (0,1)^2$ so the total area A of the membrane is 1.
- Let $u(\xi, \eta, t) = (x(\xi, \eta, t), y(\xi, \eta, t), z(\xi, \eta, t)) \in \mathbb{R}^3$ represent the membrane at position (ξ, η) and at time t.
- Let the membrane be fastened at one end, $u(\xi, 0, t) = (\xi, 0, 0)$, with known initial position and velocity, $u(\xi, \eta, 0) = (\xi, \eta, 0)$, $u_t(\xi, \eta, 0) = (0, 0, 0)$.
- The membrane is loaded externally by $f(\xi, \eta, t) \in \mathbb{R}^3$ (force per unit area) and internally through tension $T(\xi, \eta)$ (force per unit length).
- The membrane density is $\rho(\xi, \eta)$ (mass per unit area).
- For the Lagrangian functional (constrained by ICs & BCs)

$$L(u) = \int_0^T \int_0^1 \int_0^1 \left[\tfrac{1}{2}\rho \|u_t\|^2 - \tfrac{1}{2} T (\|u_\xi \times u_\eta\| - 1)^2 + f \cdot u \right] d\xi d\eta dt$$

show that the necessary optimality condition for a

Non-Linear Hyperbolic IBVP for a Membrane

stationary u in $Q = \Omega \times (0, T)$ (with damping $c > 0$) is

$$\begin{cases} u_{tt} + cu_t = (A(u)u_\xi)_\xi + (B(u)u_\eta)_\eta + g, & \text{for } (\xi, \eta, t) \in Q \\ u(\xi, 0, t) = (\xi, 0, 0), \quad B(u)u_\eta(\xi, 1, t) = 0, & \text{for } \xi \in [0, 1], t \in [0, T] \\ A(u)[u_\xi(\xi, \eta, t) - (1, 0, 0)] = 0, \quad \xi = 0, 1, & \text{for } \eta \in [0, 1], t \in [0, T] \\ u(\xi, \eta, 0) = (\xi, \eta, 0), \quad u_t(\xi, \eta, 0) = 0, & \text{for } (\xi, \eta) \in \Omega \end{cases}$$

where $u_t(\xi, \eta, 0) = u_1(\xi, \eta)$ is imposed initially instead of a final time condition $u(\xi, \eta, T) = u_T(\xi, \eta)$, and

$$[\![a]\!] = \begin{bmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{bmatrix} \quad \text{for} \quad a = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \quad \text{so} \quad \begin{aligned} u \times v &= [\![u]\!] v \\ &= -[\![u]\!]^\top v \end{aligned}$$

and
$$\begin{aligned} A(u) &= \delta(u)[\![u_\eta]\!]^2 \\ B(u) &= \delta(u)[\![u_\xi]\!]^2 \end{aligned} \qquad \delta(u) = \frac{T}{\rho} \frac{1 - \|u_\xi \times u_\eta\|}{\|u_\xi \times u_\eta\|}, \qquad g = \frac{f}{\rho}.$$

- Rewrite this problem in first order form and implement a fully discrete approximation with Matlab. Does a solution exist for all parameters?

Conservation Laws

- For simplicity only conservation laws in 2D space-time are formulated, i.e., $(x,t) \in (-\infty,\infty) \times [0,\infty)$, e.g.,
  - a gas in a pipe,
  - traffic along a street.
- Let $\rho(x,t)$ be the mass density, so
$$\text{mass in } [x_1,x_2] \text{ at time } t \text{ is } \int_{x_1}^{x_2} \rho(x,t)dx$$
- Let $v(x,t)$ be the velocity, so
$$\text{mass flux in } (x,t) = \rho(x,t)v(x,t)$$
- The most fundamental formulation of mass conservation is,
$$\int_{x_1}^{x_2} \rho(x,t_2)dx - \int_{x_1}^{x_2} \rho(x,t_1)dx =$$
$$\int_{t_1}^{t_2} \rho(x_1,t)v(x_1,t)dt - \int_{t_1}^{t_2} \rho(x_2,t)v(x_2,t)dt$$
$$\forall x_1,x_2 \in (-\infty,\infty), \forall t_1,t_2 \in [0,\infty)$$
- This and the following are equivalent *weak* formulations,
$$\int_{-\infty}^{+\infty} \phi(x,0)\rho(x,0)dx + \int_0^{+\infty}\int_{-\infty}^{+\infty} [\phi_t(x,t) + \phi_x(x,t)v(x,t)]\rho(x,t)dxdt = 0$$
$$\forall \phi \in C_0^\infty(\mathbb{R}^2)$$
- If ρ and v are sufficiently smooth, the differences above can be represented in terms of corresponding partial derivatives:

Euler Equations

- With $$\rho(x,t_2) - \rho(x,t_1) = \int_{t_1}^{t_2} \rho_t dt$$
  and $$\rho(x_2,t)v(x_2,t) - \rho(x_1,t)v(x_1,t) = \int_{x_1}^{x_2} (\rho v)_x dx$$
  follows
  $$\int_{t_1}^{t_2} \int_{x_1}^{x_2} [\rho_t + (\rho v)_x] dxdt = 0$$
  As x_1, x_2 and t_1, t_2 are arbitrary, the differential form of the conservation law is obtained,
  mass conservation: $$\rho_t + (\rho v)_x = 0$$
- Other additional conservation laws are similarly derived,
  momentum conservation: $$(\rho v)_t + (\rho v^2 + p)_x = 0$$
  energy conservation: $$E_t + (v(E+p))_x = 0$$
  for the three Euler Equations of gas dynamics, where the pressure is determined by the equation of state
  $p = (\gamma - 1)(E - \frac{1}{2}\rho v^2)$ with $\gamma = c_p/c_v = 1.4$.
- For simplicity only mass conservation will be investigated.
- If v is given *a priori* in terms of ρ through $\rho v = f(\rho)$, the scalar conservation law is obtained,
  $$\rho_t + f(\rho)_x = 0$$

Scalar Conservation Laws

- If v is a constant a, there results the linear convection equation,
$$\rho_t + a\rho_x = 0$$
- If sufficiently smooth initial conditions are given through $\rho(x,0) = \rho_0(x)$, the solution is
$$\rho(x,t) = \rho_0(x - at)$$
i.e., $\rho_t(x,t) + a\rho_x(x,t) = \rho_0'(x - at)(-a) + a\rho_0'(x - at) = 0.$
- Since this solution always satisfies the weak formulation of mass conservation, it is also a *weak* solution, even if ρ_0 is not smooth.
- With this solution, the profile ρ_0 is shifted unchanged downstream in the course of time.
- The equation $\rho_t + a\rho_x = d\rho_{xx}$ with diffusion $d\rho_{xx}$ is more realistic. If diffusion is very small, the inviscid limit is just an idealization.
- Since a solution of a nonlinear scalar conservation law is typically not unique, the most realistic solution is determined from ρ^0 as the limit of ρ^ϵ as $\epsilon \to 0$ in:
$$\rho_t^\epsilon + f(\rho^\epsilon)_x = \epsilon\rho_{xx}^\epsilon$$

Characteristics

- The solution $u(x,t) = u_0(x - at)$ to the linear convection equation,
$$u_t + au_x = 0, \quad u(x,0) = u_0(x)$$
remains constant along the line
$$x - at = x_0$$
These are *characteristics* of the PDE.
- If the velocity $a(x)$ depends upon the spatial variable x, the PDE $u_t + (au)_x = 0$ can be re-written as
$$(\partial_t + a(x)\partial_x)u(x,t) = -a'(x)u(x,t)$$
Along the *characteristic curve* $x(t)$, given by
$$x'(t) = a(x(t)), \quad x(0) = x_0$$
u satisfies an ODE
$$D_t u(x(t),t) = -a'(x(t))u(x(t),t), \quad u(x(0),0) = u_0(x_0)$$
- The solution u is not always a constant on the characteristic curve, but the solution values on two different characteristic curves are determined independently from each other.

Non-Smooth Data

Exercise: Show that the function $u(x,t) = u_0(x - at)$ satisfies the weak formulation of the convection equation

$$u_t + au_x = 0, \quad u(x,0) = u_0(x).$$

- The solution to the heat equation

  $$v_t^\epsilon = \epsilon v_{xx}^\epsilon, \quad v^\epsilon(x,0) = u_0(x)$$

  is given by

  $$v^\epsilon(x,t) = \frac{1}{\sqrt{4\pi\epsilon t}} \int_{-\infty}^{+\infty} e^{-\frac{(x-y)^2}{4\epsilon t}} u_0(y) dy$$

  and is therefore very smooth for $t > 0$.

Exercise: Show that the regularized equation

$$u_t^\epsilon + au_x^\epsilon = \epsilon u_{xx}^\epsilon, \quad u^\epsilon(x,0) = u_0(x)$$

is solved with $u^\epsilon(x,t) = v^\epsilon(x - at, t)$.

Def: The function $\lim_{\epsilon \to 0} u^\epsilon$ is called the *vanishing viscosity solution* to the convection equation.

Exercise: Show that the vanishing viscosity solution agrees here with $u_0(x - at)$. For simplicity, assume that u_0 is continuous with compact support.

Burger's Equation

- For typical examples of scalar conservation laws
$$u_t + f(u)_x = 0$$
the curvature behavior of f is globally consistent, i.e., either $f''(u) > 0$ or $f''(u) < 0$.
- If ρ and p in the conservation of momentum of the Euler equations are constant, the simplification is comparable to the inviscid Burger's Equation,
$$u_t + (u^2/2)_x = u_t + uu_x = 0$$
- The viscous Burger's Equation is
$$u_t + uu_x = \epsilon u_{xx}$$
- The characteristics of the inviscid equation satisfy
$$x'(t) = u(x(t), t), \quad x(0) = x_0$$
and the solution is constant along a characteristic,
$$D_t u(x(t), t) = u_t(x(t), t) + u_x(x(t), t)x'(t) = u_t + uu_x = 0$$
- If the initial values $u(x, 0) = u_0(x)$ are sufficiently smooth, this method can be used to determine u for t small enough. Otherwise, *shocks* develop.

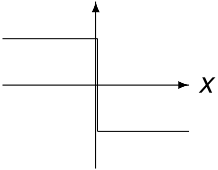
Shocks

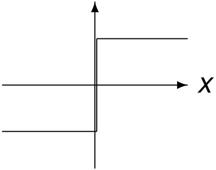
- For the Burger's Equation u is determined initially by:

$$u_t + u(x,0)u_x = 0$$

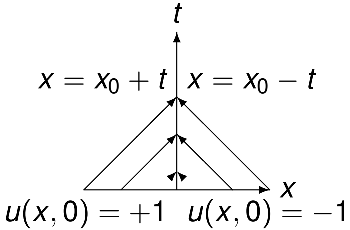
- With, e.g., initial values,

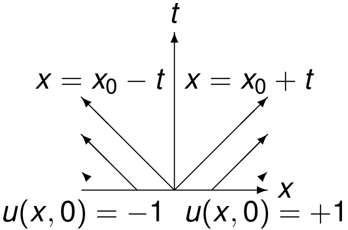
$u(x,0) = -\mathrm{sgn}(x)$ $\quad$ $u(x,0) = \mathrm{sgn}(x)$





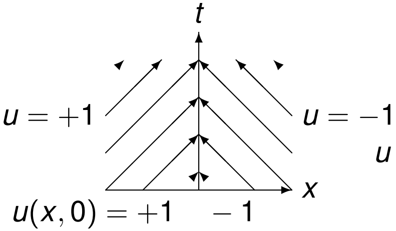
the characteristics are given by:

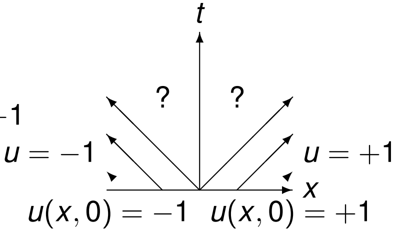




Shocks

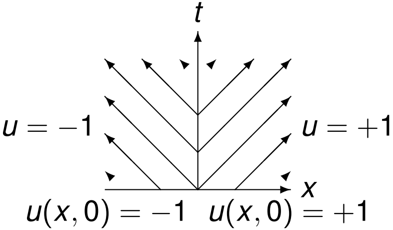
- Since u is piecewise constant in this simple example, the characteristic curves remain lines up to a discontinuity in the solution:





- The vanishing viscosity solution appears to the left.

- In the second case consider a simple solution:
- However, this is not a vanishing viscosity solution.

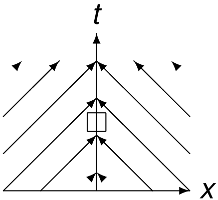


Shocks

- In both cases there is a discontinuity at $x = 0$, $t \geq 0$. To evaluate these solutions, the weak form is investigated:
- For arbitrary x_1, x_2, arbitrary t_1, t_2:

$$\int_{x_1}^{x_2} [u(x,t_2) - u(x,t_1)]dx + \frac{1}{2}\int_{t_1}^{t_2} [u^2(x_2,t) - u^2(x_1,t)]dt = 0$$

- Check for the 1. case with the test cell $[-\varepsilon, +\varepsilon] \times [t_1, t_2]$:



$u(x,t) = +1$ $u(x,t) = -1$

$$\int_{-\varepsilon}^{0} [u(x,t_2)_{=+1} - u(x,t_1)_{=+1}]dx +$$

$$\int_{0}^{+\varepsilon} [u(x,t_2)_{=-1} - u(x,t_1)_{=-1}]dx +$$

$$\frac{1}{2}\int_{t_1}^{t_2} [u^2(+\varepsilon,t)_{=(-1)^2} - u^2(-\varepsilon,t)_{=(+1)^2}]dt = 0$$

- Other test cells are simpler still.

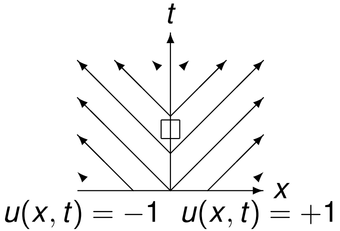
Shocks

- Check for the 2. case with the test cell $[-\varepsilon, +\varepsilon] \times [t_1, t_2]$

$$\int_{-\varepsilon}^{0} [u(x,t_2)_{=-1} - u(x,t_1)_{=-1}]dx +$$

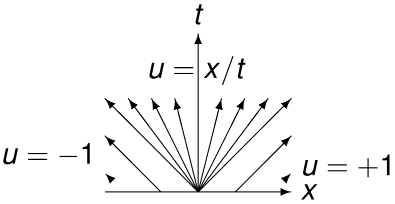
$$\int_{0}^{\varepsilon} [u(x,t_2)_{=+1} - u(x,t_1)_{=+1}]dx +$$

$$\frac{1}{2}\int_{t_1}^{t_2} [u^2(+\varepsilon,t)_{=(+1)^2} - u^2(-\varepsilon,t)_{=(-1)^2}]dt = 0$$



- Other test cells are simpler still.
- The following solution is more natural in the 2. case:

$$u(x,t) = \begin{cases} -1, & x \le -t \\ x/t, & -t \le x \le t \\ +1, & t \le x \end{cases}$$



This is the vanishing viscosity solution.

The Riemann Problem

- The Riemann Problem for a conservation law is an initial value problem, in which the initial values are piecewise constant with a single discontinuity.
- Consider $u_t + uu_x = 0$ with initial values
$$u_0(x) = \begin{cases} u_{\mathrm{l}}, & x < 0 \\ u_{\mathrm{r}}, & x > 0 \end{cases}$$
- For the case $u_{\mathrm{l}} > u_{\mathrm{r}}$ there is a unique weak solution $u(x,t) = u_0(x - st)$, where
$$s = (u_{\mathrm{l}} + u_{\mathrm{r}})/2$$
is the *shock-velocity*.

Exercise: Show that this is a weak solution of Burger's Equation.

Exercise: Show that $u_t + uu_x = \epsilon u_{xx}$, $u(x,0) = u_0(x)$, has a solution $u^\epsilon(x,t) = w^\epsilon(x - st)$, where $s = (u_{\mathrm{l}} + u_{\mathrm{r}})/2$ and
$$w^\epsilon(x) = u_{\mathrm{r}} + \frac{1}{2}(u_{\mathrm{l}} - u_{\mathrm{r}})[1 - \tanh((u_{\mathrm{l}} - u_{\mathrm{r}})x/(4\epsilon))] \begin{cases} \to u_{\mathrm{l}}, & x \to -\infty \\ \to u_{\mathrm{r}}, & x \to +\infty \end{cases}$$
Show that $u^\epsilon(x,t) \stackrel{\epsilon \to 0}{\longrightarrow} u_0(x - st)$.

Non-Uniqueness of the Solution

- For the case $u_\mathrm{l} < u_\mathrm{r}$ there are infinitely many weak solutions.

Exercise: Show that all the following are weak solutions:

$$u(x,t) = \begin{cases} u_\mathrm{l}, & x < s_\mathrm{m} t \\ u_\mathrm{m}, & s_\mathrm{m} t \le x \le u_\mathrm{m} t \\ x/t, & u_\mathrm{m} t \le x \le u_\mathrm{r} t \\ u_\mathrm{r}, & x > u_\mathrm{r} t \end{cases} \qquad \begin{array}{c} \forall u_\mathrm{m} : \\ u_\mathrm{l} \le u_\mathrm{m} \le u_\mathrm{r} \\ s_\mathrm{m} = (u_\mathrm{l} + u_\mathrm{m})/2 \end{array}$$

- Another weak solution is again
$$u(x,t) = u_0(x - st).$$
  - The shock velocity is $s = (u_\mathrm{l} + u_\mathrm{r})/2$.
  - Here characteristics emanate from the shock.
  - This is not the vanishing viscosity solution.
- The vanishing viscosity solution is given by the *expansion wave*
$$u(x,t) = \begin{cases} u_\mathrm{l}, & x < u_\mathrm{l} t \\ x/t, & u_\mathrm{l} t \le x \le u_\mathrm{r} t \\ u_\mathrm{r}, & x > u_\mathrm{r} t \end{cases}$$

Rankine-Hugoniot and Entropy Conditions

- The shock solution $u(x,t) = u_0(x - st)$ is a weak solution to the Riemann Problem only if $s = \frac{1}{2}(u_\mathrm{l} + u_\mathrm{r})$.
- The correct velocity s is determined as follows:
  - For a fixed t and unknown s let $M \gg |st|$. Then $u(-M,t) = u_\mathrm{l}$ and $u(+M,t) = u_\mathrm{r}$ for $u(x,t) = u_0(x - st)$.
  - With $t_1 = t$ and $t_2 = t + dt$ in the weak form of Burger's Equation, taking the limit as $dt \to 0$ gives,
    $$\frac{d}{dt}\int_{-M}^{+M} u(x,t)dx = f(u_\mathrm{l}) - f(u_\mathrm{r}) = \tfrac{1}{2}(u_\mathrm{l} + u_\mathrm{r})(u_\mathrm{l} - u_\mathrm{r})$$
  - The solution $u(x,t) = u_0(x - st)$ satisfies

$$\int_{-M}^{+M} u(x,t)dx = \int_{-M}^{st} u(x,t)dx + \int_{st}^{+M} u(x,t)dx = (M + st)u_\mathrm{l} + (M - st)u_\mathrm{r}$$

and therefore

$$\frac{d}{dt}\int_{-M}^{+M} u(x,t)dx = s(u_\mathrm{l} - u_\mathrm{r}) \quad \Rightarrow \quad s = \tfrac{1}{2}(u_\mathrm{l} + u_\mathrm{r})$$

- In general the *Rankine-Hugoniot* jump conditions hold,
  $$f(u_\mathrm{l}) - f(u_\mathrm{r}) = s(u_\mathrm{l} - u_\mathrm{r})$$
- The vanishing viscosity solution is more easily recognized through the *entropy* condition

$$f'(u_\mathrm{l}) > s > f'(u_\mathrm{r}) \quad \text{or} \quad \frac{f(u) - f(u_\mathrm{l})}{u - u_\mathrm{l}} \ge s \ge \frac{f(u) - f(u_\mathrm{r})}{u - u_\mathrm{r}}, \forall u \in [u_\mathrm{r}, u_\mathrm{l}]$$

that characteristics run into and not out of a shock.

Traffic Flux

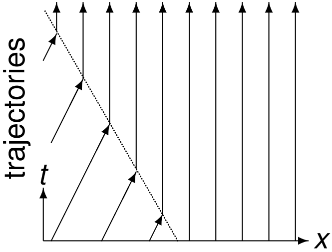
- At the position x along a street and at time t, let $\rho(x,t)$ be the density and $u(x,t)$ the velocity field of vehicles.
- Assume that $0 \leq \rho \leq \rho_{\max}$, where vehicles stand bumper-to-bumber at the $\rho = \rho_{\max}$.
- Conservation of the total number of vehicles gives the conservation law
$$\rho_t + (\rho u)_x = 0$$
or the weak form, depending upon the smoothness of variables.
- It is natural to assume that u depends upon ρ. Here this dependency is modeled as,
$$u(\rho) = u_{\max}(1 - \rho/\rho_{\max})$$
where $u_{\max}$ is the speed limit.
- With this velocity the conservation law becomes
$$\rho_t + f(\rho)_x = 0$$
with the flux
$$f(\rho) = \rho u(\rho) = \rho u_{\max}(1 - \rho/\rho_{\max})$$
which is concave instead of convex,
$$f''(\rho) = -2u_{\max}/\rho_{\max} < 0.$$

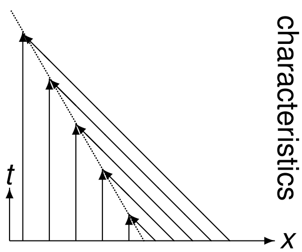
Traffic Flux

- Due to the equation form $\rho_t + f'(\rho)\rho_x = 0$ the characteristics are given by
$$x'(t) = f'(\rho(x(t),t)), \quad f'(\rho) = u_{\max}(1 - 2\rho/\rho_{\max})$$
and trajectories by
$$x'(t) = u(\rho(x(t),t)), \quad u(\rho) = u_{\max}(1 - \rho/\rho_{\max})$$
- For the Riemann Problem
$$\rho_t + f(\rho)_x = 0, \quad \rho(x,0) = \rho_0(x) = \begin{cases} \rho_{\mathrm{l}}, & x < 0 \\ \rho_{\mathrm{r}}, & x > 0 \end{cases}$$
the shock speed is
$$s = \frac{f(\rho_{\mathrm{l}}) - f(\rho_{\mathrm{r}})}{\rho_{\mathrm{l}} - \rho_{\mathrm{r}}} = u_{\max}(1 - (\rho_{\mathrm{l}} + \rho_{\mathrm{r}})/\rho_{\max})$$
with undetermined sign in spite of $u(\rho) > 0$.
- Due to the concave flux it follows from the entropy condition,
$$f'(\rho_{\mathrm{l}}) > s > f'(\rho_{\mathrm{r}}) \quad \Rightarrow \quad \rho_{\mathrm{l}} < \rho_{\mathrm{r}}$$
i.e., otherwise than for Burger's equation with convex flux.
- For $0 \le \rho_{\mathrm{l}} < \rho_{\mathrm{r}} \le \rho_{\max}$ the solution to the Riemann problem is $\rho(x,t) = \rho_0(x - st)$ a traveling shock wave.

A Traffic Jam is Reached

- Example: For the Riemann Problem with $2\rho_l = \rho_r = \rho_{\max}$ one obtains the shock speed
$$s = u_{\max}(1 - (\rho_l + \rho_r)/\rho_{\max}) = -\tfrac{1}{2}u_{\max}$$
the vehicle trajectories $\quad u(\rho) = u_{\max}(1 - \rho/\rho_{\max})$
$$x(t) = x_0 + u(\rho_0(x_0))t = \begin{cases} x_0 + \frac{1}{2}u_{\max}t, & x_0 < 0 \\ x_0, & x_0 > 0 \end{cases} \quad t \text{ small}$$
and the characteristics $\quad f'(\rho) = u_{\max}(1 - 2\rho/\rho_{\max})$
$$x(t) = x_0 + f'(\rho_0(x_0))t = \begin{cases} x_0, & x_0 < 0 \\ x_0 - u_{\max}t, & x_0 > 0 \end{cases} \quad t \text{ small}$$
- A traffic jam is suddenly reached, shown graphically as





Starting from a Traffic Light

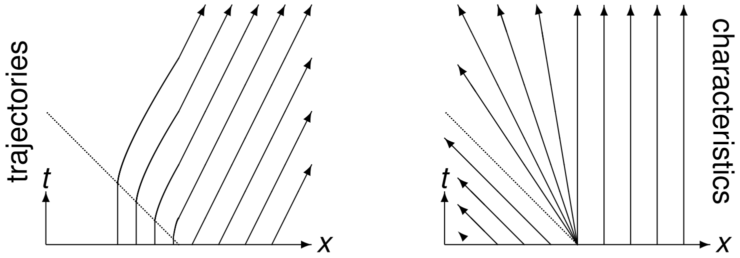
- Example: For the Riemann Problem with $2\rho_{\mathrm{r}} = \rho_{\mathrm{l}} = \rho_{\max}$ the entropy solution has no shock but rather a rarefaction wave with vehicle trajectories $\quad u(\rho) = u_{\max}(1 - \rho/\rho_{\max})$

$$x(t) = x_0 + u(\rho_0(x_0))t = \begin{cases} x_0, & x_0 < 0 \\ x_0 + \frac{1}{2}u_{\max}t, & x_0 > 0 \end{cases} \quad t \text{ small}$$

and the characteristics $\quad f'(\rho) = u_{\max}(1 - 2\rho/\rho_{\max})$

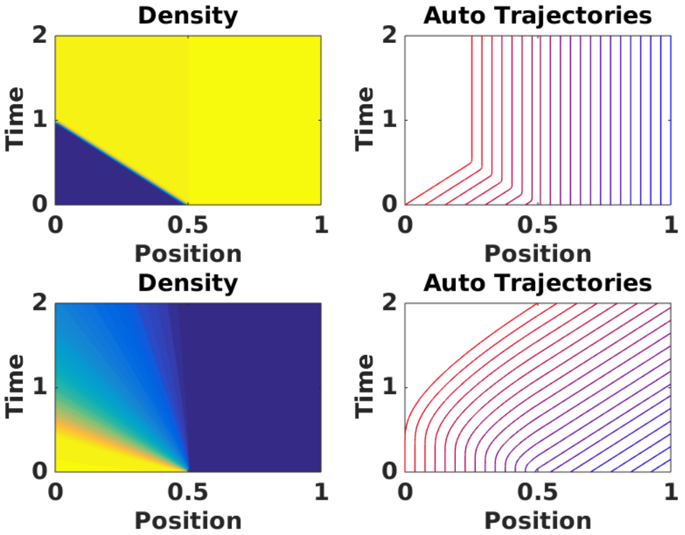
$$x(t) = x_0 + f'(\rho_0(x_0))t = \begin{cases} x_0 - u_{\max}t, & x_0 < 0 \\ x_0, & x_0 > 0 \end{cases}$$

- An acceleration following a rarefaction, seen graphically as



Riemann Problems

- The density together with the trajectories for the last 2 examples:



Sound Speed

Exercise: Traffic starts from a traffic light with an open street in front.

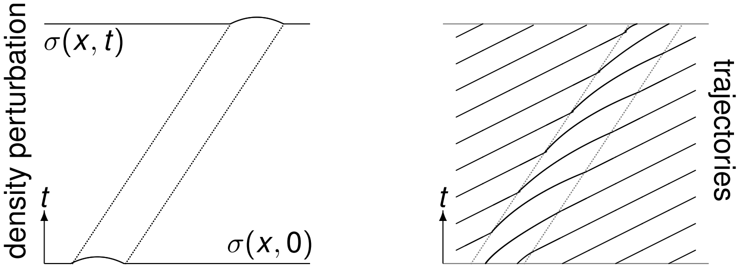
- Solve the Riemann Problem with $\rho_\mathrm{l} = \rho_\mathrm{max}$ and $\rho_\mathrm{r} = 0$.
- Sketch the trajectories and the characteristics.
- Sketch $\rho(x,t)$ and $u(x,t)$ for a fixed time $t > 0$.
- Determine the vehicle velocity $v(t)$ along a trajectory.

Perturbation analysis:

- Let the initial data be nearly constant: $\rho_0(x) = \hat{\rho} + \epsilon\sigma_0(x)$.
- Assume that
$$\rho(x,t) = \hat{\rho} + \epsilon\sigma(x,t), \quad \rho(x,0) = \rho_0(x), \quad \sigma(x,0) = \sigma_0(x)$$
and it follows
$$\rho_t = \epsilon\sigma_t, \quad \rho_x = \epsilon\sigma_x, \quad f'(\rho) = f'(\hat{\rho}) + \epsilon\sigma f''(\hat{\rho}) + \mathcal{O}(\epsilon^2)$$
- With $(\rho_t + f'(\rho)\rho_x)/\epsilon = 0$ it follows
$$\sigma_t + f'(\hat{\rho})\sigma_x = -\epsilon\sigma\sigma_x f''(\hat{\rho}) + \mathcal{O}(\epsilon)$$
- For $0 < \epsilon \ll 1$ the linear PDE holds approximately
$$\sigma_t + f'(\hat{\rho})\sigma_x = 0$$

Sound Speed

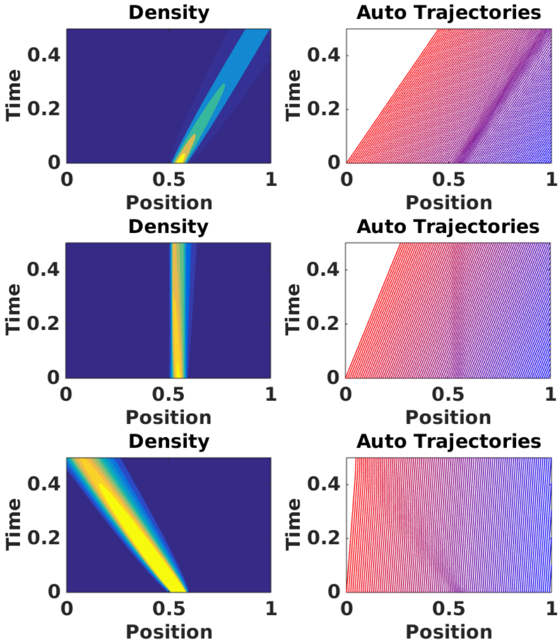
- A density perturbation travels with velocity $f'(\hat{\rho})$, where
$$f'(\hat{\rho}) > 0 \text{ if } \hat{\rho} < \tfrac{1}{2}\rho_{\max}.$$
- The density perturbation travels *backwards* through the auto column.



- The *sound speed*
$$c = f'(\hat{\rho}) - u(\hat{\rho}) = -u_{\max}\hat{\rho}/\rho_{\max},$$
is the perturbation velocity relative to the auto velocity.
- The density $\hat{\rho} = \frac{1}{2}\rho_{\max}$ is the *sonic point*, at which $c = -u(\hat{\rho})$ holds.

Sound Speed

- supersonic speed $0 > c \approx 0$
- sound speed $c \approx -u_{\max}/2$
- and subsonic speed $c \approx -u_{\max}$

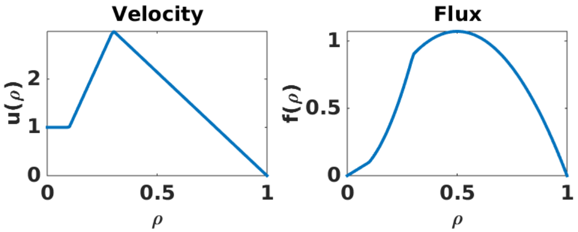


Night-Time Traffic Flow

- For the scalar conservation law $\rho_t + f(\rho)_x = 0$ let

$$u(\rho) = \begin{cases} U_0 & \rho < \rho_\mathrm{a} \\ c\rho & \rho_\mathrm{a} \le \rho \le \rho_\mathrm{b} \\ U_1(\rho_{\max} - \rho) & \rho > \rho_\mathrm{b} \end{cases} \qquad f(\rho) = \rho u(\rho)$$

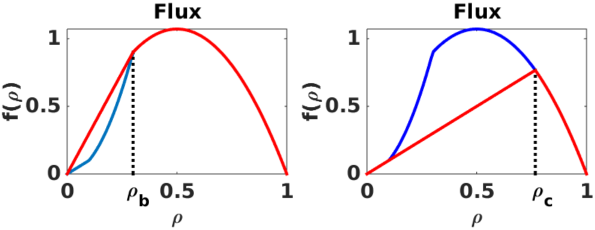
  as graphically represented:



  Here $U_0 = 1$, $\rho_\mathrm{a} = \frac{1}{10}$, $\rho_\mathrm{b} = \frac{3}{10}$, $c = 10$, $U_1 = \frac{30}{7}$, $\rho_{\max} = 1$.
- In the night one drives with velocity
  - U_0 if alone, but faster with
  - $c\rho$, in order to use the illumination ahead, and
  - finally with $U_1(\rho_{\max} - \rho)$ if the density is higher.

Night-Time Traffic Flow

- Solved by an auto following formulation, where $\{x_k(t)\}_{k=1}^N$ represent the positions of the vehicles, and through
  $$x_k' = u(\rho_k(t)), \quad \rho_k(t) = 1/[x_{k+1}(t) - x_k(t)], \quad \rho_N = 0$$
  the kth driver is influenced only by the auto ahead.
  - The solution of the Riemann problem with $\rho_\mathrm{l} = 1$, $\rho_\mathrm{r} = 0$ is graphically represented to the right.



- The alternative formula, $\rho_1 = 1/(x_2 - x_1)$, $\rho_N = 1/(x_N - x_{N-1})$
  $$\rho_k(t) = \tfrac{1}{2}\{1/[x_{k+1}(t) - x_k(t)] + 1/[x_k(t) - x_{k-1}(t)]\}$$
  leads to a non-realistic vanishing viscosity solution.
  - The solution of the Riemann problem with $\rho_\mathrm{l} = 1$, $\rho_\mathrm{r} = 0$ is graphically represented to the left.

Night-Time Traffic Flow

- Entropy solution:

  $\rho(x,0) \in \{\rho_{\mathrm{l}}, \rho_{\mathrm{r}}\}$

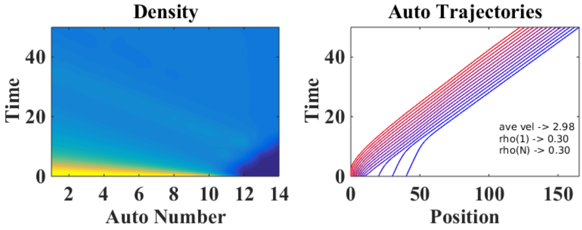
  $\rho_{\mathrm{l}} = 1 > \rho_{\mathrm{r}} \in [0, \rho_a]$

  expansion→shock

  $\rho(x,t) \to \{\rho_{\mathrm{b}}, 0\}$

  $$\frac{f(\rho)-f(\rho_{\mathrm{b}})}{\rho-\rho_{\mathrm{b}}} \geq s(=3) \geq \frac{f(\rho)-f(0)}{\rho-0}$$

  $\forall \rho \in [0, \rho_{\mathrm{b}}]$



- Realistic solution:

  $\rho(x,0) \in \{\rho_{\mathrm{l}}, \rho_{\mathrm{r}}\}$

  $\rho_{\mathrm{l}} = 1 > \rho_{\mathrm{c}} = \frac{23}{30} > \rho_{\mathrm{r}}$

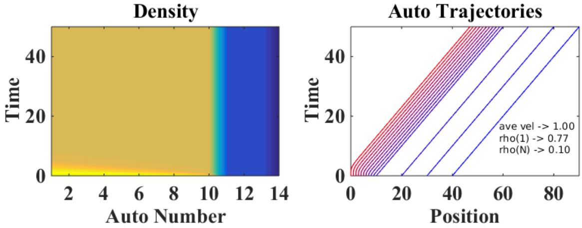
  $\rho_{\mathrm{r}} \in [0, \rho_a]$

  expansion→shock

  $\rho(x,t) \to \{\rho_{\mathrm{c}}, \rho_{\mathrm{r}}\}$

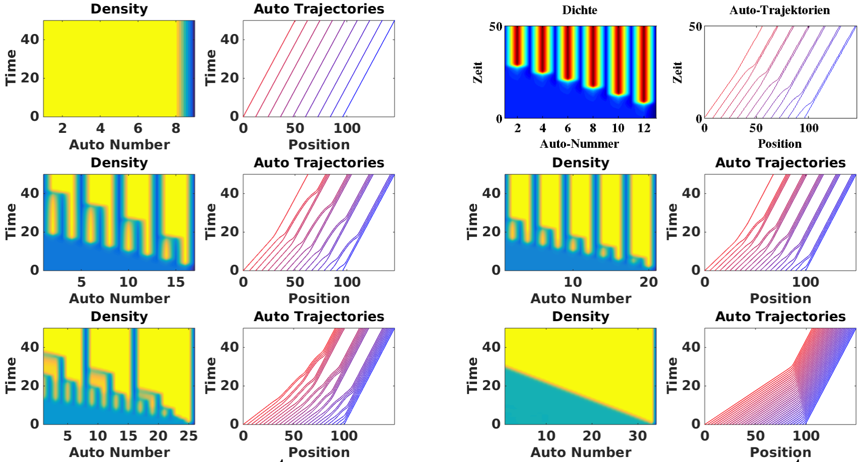
  New condition:

  $(1 =) s \leq f'(\rho_{\mathrm{r}})$



Instability and Clustering

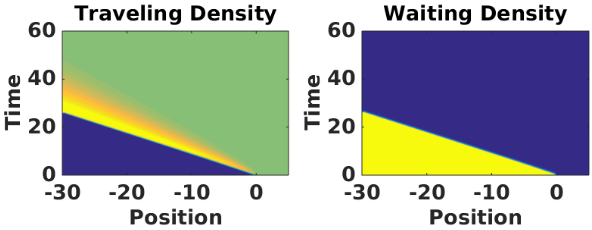
- Results for $\rho_0(x) = \frac{1}{12}, \frac{1}{8}, \frac{1}{6}, \frac{1}{5}, \frac{1}{4}$ and $\frac{1}{3}$.



- For $\rho_0 \leq \rho_a = \frac{1}{10}$ (constant $u = U_0$) or for $\rho_0(x) \geq \rho_b = \frac{1}{3}$ (normal shock) $f(\rho)$ is concave.
- Otherwise clusters arise, since a constant velocity is unstable.

Detonation Waves in Traffic

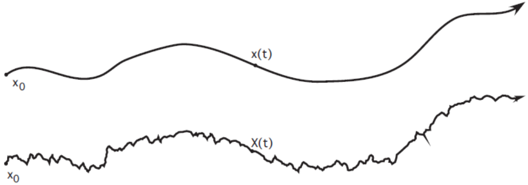
- Let $\rho(x,t)$ be the usual density of the traveling autos.
- Now let $\omega(x,t)$ be the density of standing autos, which are waiting for a spot in the auto column.
- The model of the interaction between these is
$$\omega_t = -\alpha(\rho)\omega, \quad \rho_t + f(\rho)_x = \alpha(\rho)\omega, \quad \alpha(\rho) = \hat{\alpha}(\rho > \rho_\mathrm{i})$$
- An auto enters only when the traveling density reaches the threshold $\rho > \rho_\mathrm{i}$.



- Here $\rho_\mathrm{l} < \rho_\mathrm{i} < \rho_\mathrm{r}$. A traveling traffic jam wave increases over ρ_i. After the shock wave $\rho_\mathrm{peak} > \rho_\mathrm{r}$ holds in a narrow zone.
- Afterward there is a reaction zone with $\rho_\mathrm{peak} > \rho > \rho_\mathrm{r}$, in which all available autos come into the lane.

Differential Stochastic Processes

- For a deterministic model with smooth $\boldsymbol{b} : \mathbb{R}^n \to \mathbb{R}^n$
$$\dot{\boldsymbol{x}}(t) = \boldsymbol{b}(\boldsymbol{x}(t)), \quad t > 0, \qquad \boldsymbol{x}(\boldsymbol{0}) = \boldsymbol{x}_0$$
the solution $\boldsymbol{x} : [0, \infty) \to \mathbb{R}^n$ has a smooth trajectory,



although a non-smooth trajectory might actually be measured.

- Consider a new model with random effects $\boldsymbol{B} : \mathbb{R}^n \to \mathbb{R}^m$,
$$\dot{\boldsymbol{X}}(t) = \boldsymbol{b}(\boldsymbol{X}(t)) + \boldsymbol{B}(\boldsymbol{X}(t))\xi(t), \quad t > 0, \qquad \boldsymbol{X}(0) = \boldsymbol{x}_0$$
where $\boldsymbol{X} : [0, \infty) \to \mathbb{R}^n$ is a stochastic process and
$$\xi : [0, \infty) \to \mathbb{R}^m$$
represents *white noise*.
- How should white noise or even a solution be defined?

Heuristics

- A *Wiener Process* or a *Brownian Motion* $\boldsymbol{W} : [0, \infty) \to \mathbb{R}^m$ will be constructed with the properties:
$$\mathbb{E}[\boldsymbol{W}(t)] = \boldsymbol{0}, \quad \mathbb{E}[\boldsymbol{W}^2(t)] = t, \quad \forall t \geq 0.$$
- White noise $\boldsymbol{\xi} : [0, \infty) \to \mathbb{R}^m$ will be defined,
$$\dot{\boldsymbol{W}}(t) = \boldsymbol{\xi}(t), \quad t \geq 0$$
with expected value
$$\mathbb{E}[\boldsymbol{\xi}(t)] = 0, \quad \forall t \geq 0$$
and autocorrelation function $r_{\boldsymbol{\xi}}(t, s) = \mathbb{E}[\boldsymbol{\xi}(t)^\top \boldsymbol{\xi}(s)]$
$$r_{\boldsymbol{\xi}}(t, s) = c_{\boldsymbol{\xi}}(t - s) = \delta_0(t - s)$$
which has a *flat* spectral density,
$$f(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-\imath \lambda t} c_{\boldsymbol{\xi}}(t) dt = \frac{1}{2\pi}$$
i.e., all frequencies contribute equally.
- The *stochastic differential* equation (SDE)
$$d\boldsymbol{X}(t) = \boldsymbol{b}(\boldsymbol{X}(t))dt + \boldsymbol{B}(\boldsymbol{X}(t))d\boldsymbol{W}(t), \quad \boldsymbol{X}(0) = \boldsymbol{x}_0$$
is said to be satisfied by $\boldsymbol{X} : [0, \infty) \to \mathbb{R}^n$ when
$$\boldsymbol{X}(t) = \boldsymbol{x}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{X}(s))ds + \int_0^t \boldsymbol{B}(\boldsymbol{X}(s))d\boldsymbol{W}(s)$$

(Definition of Integrals?)

Itô's Formula

- For simplicity suppose $n = 1$ and $X(t)$ solves
$$dX(t) = b(X(t))dt + B(X(t))dW(t)$$
- Which SDE satisfies $Y(t) = u(X(t), t)$, when $u : \mathbb{R}^2 \to \mathbb{R}$ is smooth? A possible first thought is not correct, i.e.,
$$\begin{aligned} dY(t) &\neq u_t(X(t), t)dt + u_x(X(t), t)dX(t) \\ &= (u_t(X(t), t) + b(X(t))dt + u_x(X(t), t)B(X(t))dW(t) \end{aligned}$$
- With the property $\mathbb{E}[W^2(t)] = t$, $\forall t \geq 0$, or $dW(t)^2 = dt$,
$$\begin{aligned} dY(t) &= u_t dt + u_x dX(t) + \tfrac{1}{2} u_{xx} dX^2(t) + \cdots \\ &= u_t dt + u_x(bdt + BdW(t)) \\ &\qquad + \tfrac{1}{2} u_{xx}(bdt + BdW(t))^2 + \cdots \\ &= (u_t + u_x b + \tfrac{1}{2} u_{xx} B^2)dt \\ &\qquad + u_x BdW(t) + \mathcal{O}(dt^{3/2}) \end{aligned}$$

and the system of SDE results

$$\begin{aligned} dX(t) &= b(X(t))dt + B(X(t))dW(t) \\ dY(t) &= [u_t(X(t), t) + u_x(X(t), t)b(X(t)) + \tfrac{1}{2} u_{xx}(X(t), t)B^2(X(t))]dt \\ &\quad + u_x(X(t), t)B(X(t))dW(t) \end{aligned}$$

Itô's Formula

- Example: To solve the SDE,
  $$dY(t) = Y(t)dW(t), \quad Y(0) = 1$$
  one uses the formula,
  $$dY(t) = [u_t + u_x b + \tfrac{1}{2} u_{xx} B^2]dt + u_x B dW(t)$$
  and seeks $u(x, t)$, such that with $(b = 0, B = 1)$
  $$X(t) = W(t), \quad \text{i.e.} \quad dX(t) = dW(t), \quad X(0) = 0$$
  and $y_0 = u(x_0, 0) = u(0, 0) = 1$,
  $$u_x(X, t) = u(X, t) = Y, \quad u_t(X, t) + \tfrac{1}{2} u_{xx}(X, t) = 0.$$
  With $u_{xx} = u_x = u$ follows $u_t = -\frac{1}{2}u$ or $u(X, t) = f(X)e^{-t/2}$ where $f(0) = u(0, 0) = 1$.
  With $f'(X) = u_x e^{t/2} = ue^{t/2} = f(X)$ follows $f(X) = e^X$.
  Solution: $Y(t) = u(X(t), t) = \exp[W(t) - t/2]$
- Example: Let $S(t)$ be the (random) price of a stock at time $t \geq 0$. A model for the price is given by the SDE,
  $$dS(t) = \mu S(t)dt + \sigma S(t)dW(t), \quad S(0) = s_0$$
  where μ is the *drift* and σ ist the *volatility*. Similarly,
  Solution: $S(t) = s_0 \exp[\sigma W(t) + (\mu - \sigma^2/2)t]$

Distribution of a Brownian Motion

- Let the random position of a particle be represented by $X(t)$ with density ρ, $P(X(t) \in [a, b]) = \int_a^b \rho(\xi, t) d\xi$.
- Let the random change of position of the particle in a time interval of length τ be represented by $\delta(\tau)$ with density f, $P(\delta(\tau) \in [a, b]) = \int_a^b f(\xi, \tau) d\xi$.
- Since $P(X(t+\tau) \in [a, b]) = P(X(t) + \delta(\tau) \in [a, b]) = \cdots$ the convolution follows

$$\begin{aligned} \rho(x, t+\tau) &= \int_{-\infty}^{+\infty} \rho(x-y, t) f(y, \tau) dy \\ &= \int_{-\infty}^{+\infty} \left[\rho(x, t) + \rho_x(x, t) y + \tfrac{1}{2} \rho_{xx}(x, t) y^2 + \cdots \right] f(y, \tau) dy \end{aligned}$$

- Since f is a probability density, $\int_{-\infty}^{+\infty} f(y, \tau) dy = 1$.
- With symmetry $f(-y, \tau) = f(y, \tau)$ follows $\int_{-\infty}^{+\infty} y f(y, \tau) dy = 0$.
- Set $D = (1/\tau) \int_{-\infty}^{+\infty} y^2 f(y, \tau) dy > 0$.
- With $\tau \to 0$ follow $\rho_t = \frac{1}{2} D \rho_{xx}$ and the convolution kernel

$$f(x, t) = \exp[-x^2/(2Dt)]/\sqrt{2\pi D t}$$

Distribution of a Brownian Motion

- Let δ be a random variable representing the random walk of a particle stepping spatially left ($\delta = -1$) or right ($\delta = +1$) with
$$P(\delta = -1) = \tfrac{1}{2} = P(\delta = +1), \quad \mathbb{E}(\delta) = 0, \quad \mathbb{V}(\delta) = 1.$$
- Let $\{\delta_k\}_{k=1}^{\infty}$ be independent, all distributed as δ.
- Let $X(t; \Delta t)$ be a random variable representing the position of the particle at time t with temporal steps of Δt with
$$X(t; \Delta t) = \sqrt{D\Delta t}(\delta_1 + \cdots + \delta_{\lfloor t/\Delta t \rfloor}), \quad X(0; \Delta t) = 0$$
so
$$\mathbb{E}[X(t; \Delta t)] = \sqrt{D\Delta t}\lfloor t/\Delta t \rfloor \mathbb{E}(\delta) = 0$$
and
$$\mathbb{V}[X(t; \Delta t)] = D\Delta t \lfloor t/\Delta t \rfloor \mathbb{V}(\delta) = Dt\lfloor t/\Delta t \rfloor/(t/\Delta t).$$
- With the central limit theorem and $Z \sim N(0, 1)$,
$$P(X(t; \Delta t) \in [a, b]) \xrightarrow{\Delta t \to 0} P\left(a \le Z\sqrt{Dt} \le b\right) = \int_{-\infty}^{+\infty} f(x, t)dt$$
with
$$f(x, t) = \exp[-x^2/(2Dt)]/\sqrt{2\pi Dt}.$$

Definition of a Brownian Motion

Def: A 1-*D* stochastic process W is a *Brownian Motion* or a *Wiener Process* if

- $W(0) = 0$ almost surely,
- $W(t) - W(s) \sim N(0, t-s)$, $\forall t \geq s \geq 0$, and
- $\forall$ times $0 < t_1 < \cdots < t_n$ the random variables $W(t_1), W(t_2) - W(t_1), \ldots, W(t_n) - W(t_{n-1})$ are independent.

In particular,

$$W(t) \sim N(0, t), \quad \mathbb{E}[W(t)] = 0, \quad \mathbb{E}[W^2(t)] = t, \quad \forall t \geq 0.$$

Theorem: Let W be a 1D Wiener Process. Let

$$g(x, t|y) = \exp[-(x-y)^2/(2t)]/\sqrt{2\pi t}.$$

Then $\forall n \in \mathbb{N}$, $\forall$ times $0 = t_0 < t_1 < \cdots < t_n$ it holds that

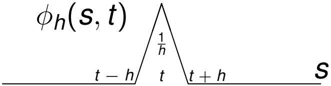
$$P(a_1 \leq W(t_1) \leq b_1, \ldots, a_n \leq W(t_n) \leq b_n) =$$

$$\int_{a_1}^{b_1} \cdots \int_{a_n}^{b_n} g(x_1, t_1|0) g(x_2, t_2 - t_1|x_1) \cdots g(x_n, t_n - t_{n-1}|x_{n-1}) dx_n \cdots dx_1$$

Remark: There are natural counterparts for an *n*-*D* Wiener Process.

Construction of a Brownian Motion

- It holds
  $\mathbb{E}[W(t)W(s)] = \mathbb{E}[(W(s) - W(t) - W(s))W(s)] = \min\{t, s\}$
- It follows
  $$\phi_h(s,t) = \mathbb{E}\left[\frac{W(t+h) - W(t)}{h}\frac{W(s+h) - W(s)}{h}\right] = \frac{1}{h^2}\times$$
  $$\min\{t+h, s+h\} - \min\{t+h, s\} - \min\{t, s+h\} + \min\{t, s\}$$



- With $\phi_h(s,t) \to \delta_0(s-t)$ and formally $\xi(t) = \dot{W}(t)$ the desired formula results heuristically,
  $$\mathbb{E}[\xi(t)] = 0, \quad \mathbb{E}[\xi(t)\xi(s)] = \delta_0(s-t)$$

Def: The *auto correlation function* of a stochastic process X is
$$r_X(t,s) = \mathbb{E}[X(t)X(s)]$$
If $r_X(t,s) = c_X(t-s)$ and $\mathbb{E}[X(t)] = \mathbb{E}[X(s)]$, $\forall t, s \geq 0$, then X is *stationary in the wide sense*.

Construction of a Brownian Motion

Def: For a stochastic process X, which is stationary in the wide sense, i.e., $r_X(t,s) = c_X(t-s)$, the *spectral density* of X is given by

$$f_X(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-\imath\lambda t} c_X(t)dt, \quad \lambda \in \mathbb{R}.$$

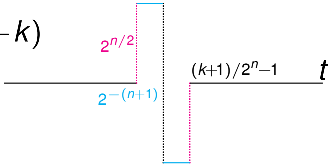
- The desired white noise $\xi(t) = \dot{W}(t)$ should be stationary in the wide sense, i.e., $r_\xi(t,s) = \delta_0(t-s)$, and
$$f_\xi(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-\imath\lambda t}\delta_0(t)dt = \frac{1}{2\pi}, \quad \forall\lambda \in \mathbb{R}$$
i.e., all frequencies contribute equally.
- Construction of the white noise $\xi(t) = \dot{W}(t)$ through random Fourier Series: Let $\{\psi_n\}_{n=0}^\infty$ be a complete orthonormal basis for $L^2(0,1)$. Let $\{A_n\}_{n=0}^\infty$ be independent with $A_n \sim N(0,1)$ given as follows, and with the white noise
$$\xi(t) = \textstyle\sum_{n=0}^\infty A_n\psi_n(t), \quad A_n = \int_0^1 \xi(t)\psi_n(t)dt$$
a Brownian Motion is given by
$$W(t) = \textstyle\int_0^t \xi(s)ds = \sum_{n=0}^\infty A_n \int_0^t \psi_n(s)ds$$

Construction of a Brownian Motion

- An advantageous basis is given by the *Haar functions*:
  $$h_0(t) = 1, \quad h_1(t) = \chi_{[0,1/2]}(t) - \chi_{[1/2,1]}(t)$$
  and

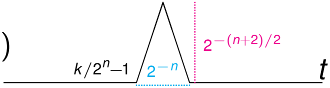
$$h_k(t) = \begin{cases} 2^{n/2}, & (k-2^n) < 2^n t < (k-2^n+1/2) \\ -2^{n/2}, & (k-2^n+1/2) < 2^n t < (k-2^n+1) \\ 0, & \text{otherwise}, \quad \text{where } n = \lfloor \log_2(k) \rfloor. \end{cases}$$

$$h_k(t) = 2^{\frac{\lfloor \log_2(k) \rfloor}{2}} h_1(2^{\lfloor \log_2(k) \rfloor}(t+1)-k)$$



- The *Schauder functions* are given by $\quad s_k(t) = \int_0^t h_k(\tau) d\tau$

$$s_k(t) = 2^{-\frac{\lfloor \log_2(k) \rfloor}{2}} s_1(2^{\lfloor \log_2(k) \rfloor}(t+1)-k)$$



Existence of a Brownian Motion

Theorem: Let $\{A_k\}_{k=0}^{\infty}$ be a sequence of independent random variables on a probability space $(\Omega, \mathcal{U}, P)$ with $A_k \sim N(0,1)$. Then

$$W(t,\omega) = \sum_{k=0}^{\infty} A_k(\omega) s_k(t), \quad t \in [0,1]$$

has the properties:

- The sum converges uniformly for almost every ω.
- W is a Brownian Motion.
- For almost every ω the sample path $t \mapsto W(t,\omega)$ is continuous in t,
- and Hölder continuous with exponent $0 < \gamma < 1/2$.
- For $1/2 < \gamma \leq 1$ and for almost every ω the sample path $t \mapsto W(t,\omega)$ is nowhere Hölder continuous in t with exponent γ,
- and nowhere differentiable in t.

Remark: There are natural counterparts for an n-D Wiener Process.

Itô Integrals

- The solution to the SDE
$$d\boldsymbol{X}(t) = \boldsymbol{b}(\boldsymbol{X}(t), t) + \boldsymbol{B}(\boldsymbol{X}(t), t)d\boldsymbol{W}(t), \quad \boldsymbol{X}(0) = \boldsymbol{X}_0$$
is given by
$$\boldsymbol{X}(t) = \boldsymbol{X}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{X}(s), s)ds + \int_0^t \boldsymbol{B}(\boldsymbol{X}(s), s)d\boldsymbol{W}(s)$$
Since the sample path $t \mapsto W(t, \omega)$ has unbounded variation, the integrals must be defined carefully.
- For $g \in \mathcal{C}^1([0,1])$ with $g(0) = g(1) = 0$ (deterministic) let
$$\int_0^1 g(t)dW(t) = -\int_0^1 g'(t)W(t)dt$$
These random variables have the properties
$$\mathbb{E}[\int_0^1 g(t)dW(t)] = 0, \quad \mathbb{E}[(\int_0^1 g(t)dW(t))^2] = \int_0^1 g^2(t)dt$$
- For $g \in L^2(0,1)$ let $\{g_n\}_{n=0}^{\infty} \subset \mathcal{C}_0^1([0,1])$ be a sequence with $\mathbb{E}[(\int_0^1 g_m(t)dW(t) - \int_0^1 g_n(t)dW(t))^2] = \int_0^1 |g_m(t) - g_n(t)|^2 dt \to 0$ and $\int_0^1 |g(t) - g_n(t)|^2 dt \to 0$ and take
$$\int_0^1 g(t)dW(t) = \lim_{n\to\infty} \int_0^1 g_n(t)dW(t)$$

Itô Integrals

- For stochastic Integrals with random integrands consider defining $\int_0^T W(t)dW(t)$ through Riemann sums.
- For a partition $V_m = \{0 = t_0 < t_1 < \cdots < t_m = T\}$ of $[0, T]$ let $|V_m| = \max_{0 \le k \le m-1} |t_{k+1} - t_k|$. For $\lambda \in [0, 1]$ and $\tau_k(\lambda) = (1 - \lambda)t_k + \lambda t_{k+1}$ let

$$R(V_m, \lambda) = \sum_{k=0}^{m-1} W(\tau_k(\lambda))[W(t_{k+1}) - W(t_k)]$$

Theorem: For $|V_m| \overset{m\to\infty}{\longrightarrow} 0$ and $\lambda \in [0, 1]$ fixed, it holds

$$\mathbb{E}\left[\left(R(V_m, \lambda) - \tfrac{1}{2}W(T)^2 - (\lambda - \tfrac{1}{2})T\right)^2\right] \to 0$$

- i.e., the limit depends upon λ!
- So that the result be *nonanticipating*, $\lambda = 0$ is chosen to obtain the *stochastic Integral of Itô*:

$$\int_0^T W(t)dW(t) = \tfrac{1}{2}W(T)^2 - \tfrac{1}{2}T$$

Itô Integrals

Def: Given a probability space $(\Omega, \mathcal{U}, P)$, a random variable X and the Borel sets $\mathcal{B}$ define the σ-algebra generated by X,

$$\mathcal{U}(X) = \{X^{-1}(B) : B \in \mathcal{B}\}.$$

Def: $\mathcal{W}(t) = \mathcal{U}(W(s) : 0 \leq s \leq t)$ is the *history* of W up to t.

Def: $\mathcal{W}^+(t) = \mathcal{U}(W(s) - W(t) : 0 \leq t \leq s)$ is the *future* of W after t.

Def: $\{\mathcal{F}(t)\}_{t \geq 0} \subseteq \mathcal{U}$ is *nonanticipating* with respect to $\{W(t)\}_{t \geq 0}$ if (a) $\mathcal{F}(s) \subseteq \mathcal{F}(t)$, $\forall t \geq s \geq 0$, (b) $\mathcal{W}(t) \subseteq \mathcal{F}(t)$, $\forall t \geq 0$ und (c) $\mathcal{F}(t)$ is independent of $\mathcal{W}^+(t)$, $\forall t \geq 0$. (called a *filtration*).

Def: A stochastic process $\{G(t)\}_{t \geq 0}$ is *nonanticipating* with respect to $\{\mathcal{F}(t)\}_{t \geq 0}$ when $\mathcal{U}(G(t)) \subseteq \mathcal{F}(t)$, $\forall t \geq 0$.

Def: A stochastic process $\{G(t, \omega) : \omega \in \Omega, t \geq 0\}$ is *progressively measurable* with respect to the filtration $\{\mathcal{F}(t)\}_{t \geq 0}$ if $\{G^{-1}(B, U) : B \in \mathcal{B}([0, \infty)), U \in \mathcal{U}\} \subset \mathcal{B}([0, t]) \otimes \mathcal{F}(t)$, $\forall t \geq 0$.

Itô Integrals

Def: The space $\mathbb{L}^p(0,T)$, $p \geq 1$, consists of real-valued stochastic processes G which are progressively measurable with respect to a given filtration $\{\mathcal{F}(t)\}_{t\geq 0}$ and satisfy

$$\mathbb{E}\left[\int_0^T |G(t)|^p dt\right] < \infty$$

Def: $G \in \mathbb{L}^2(0,T)$ is a step process if $\exists V_m = \{t_0 < t_1 < \cdots < t_m\}$ of $[0,T]$ and $\{G_k\}_{k=0}^m$ with $\mathcal{U}(G_k) \subseteq \mathcal{F}(t_k)$ where

$$G(t) = G_k, \quad t_k \leq t < t_{k+1}, \quad k = 0, \ldots, m-1.$$

Def: For a step process $G \in \mathbb{L}^2(0,T)$

$$\int_0^T G(t)dW(t) = \sum_{k=0}^{m-1} G_k[W(t_{k+1}) - W(t_k)]$$

is the *Itô stochastic integral* of G on $(0,T)$.

Theorem: The integral has the properties

$$\int_0^T (aG + bH)dW = a\int_0^T GdW + b\int_0^T HdW \text{ and}$$

$$\mathbb{E}[\int_0^T GdW] = 0, \quad \mathbb{E}[\int_0^T GdW \int_0^T HdW] = \mathbb{E}[\int_0^T GHdt].$$

Itô's Formula

Theorem: For $G \in \mathbb{L}^2(0,T)$ there exists a bounded step process $\{G^n\}_{n\geq 0} \subset \mathbb{L}^2(0,T)$ where

$$\mathbb{E}\left[\int_0^T |G(t) - G^n(t)|^2 dt\right] \to 0$$

Def: With $G \in \mathbb{L}^2(0,T)$ approximated by a sequence $\{G^n\}_{n\geq 0}$ $\subset \mathbb{L}^2(0,T)$ of bounded step processes as above, i.e.,

$$\mathbb{E}\left[\left(\int_0^T (G^n(t) - G^m(t))dW(t)\right)^2\right] = \mathbb{E}\left[\int_0^T [G^n(t) - G^m(t)]^2 dt\right] \to 0$$

Itô's stochastic integral of G on $(0,T)$ is given by

$$\int_0^T G(t)dW(t) = \lim_{n\to\infty} \int_0^T G^n(t)dW(t)$$

Theorem: Let $\{X(t)\}_{t\geq 0}$ be given with $dX(t) = F(t)dt + G(t)dW(t)$, $F \in \mathbb{L}^1(0,T)$ and $G \in \mathbb{L}^2(0,T)$. Assume $u : \mathbb{R} \times [0,T] \to \mathbb{R}$ is such that u, u_t, u_x, u_{xx} are continuous. Then $Y(t) = u(X(t),t)$ satisfies *Itô's Formula* "u"$= u(X(t),t)$

$$\begin{aligned} dY(t) &= u_t dt + u_x dX(t) + \tfrac{1}{2} u_{xx} G^2(t) dt \\ &= [u_t + u_x F(t) + \tfrac{1}{2} u_{xx} G^2(t)]dt + u_x G(t) dW(t) \end{aligned}$$

Itô's Formula

Theorem: For $F^i \in \mathbb{L}^1(0,T)$ and $G^i \in \mathbb{L}^2(0,T)$ let $\{X^i(t)\}_{t\geq 0}$ be given with $dX^i(t) = F^i(t)dt + G^i(t)dW(t)$, $i = 1, \ldots, n$. Assume $u : \mathbb{R}^n \times [0,T] \to \mathbb{R}$ is such that $u, u_t, u_{x_i}, u_{x_i x_j}$ are continuous, $1 \leq i, j \leq n$. Then $Y(t) = u(X^1(t), \ldots, X^n(t), t)$ satisfies the *generalized Itô formula* "u"$= u(X(t), t)$

$$dY(t) = u_t dt + \sum_{i=1}^{n} u_{x_i} dX^i(t) + \frac{1}{2} \sum_{i,j=1}^{n} u_{x_i x_j} G^i(t) G^j(t) dt$$

- Example, *Itô's product rule*: If $F^i \in \mathbb{L}^1(0,T)$, $G^i \in \mathbb{L}^2(0,T)$ and $dX_i(t) = F_i(t)dt + G_i(t)dW(t)$, $i = 1, 2$, then

$$d(X_1(t)X_2(t)) = X_2(t)dX_1(t) + X_1(t)dX_2(t) + G_1(t)G_2(t)dt$$

- Example, *Itô's integration by parts*:

$$\int_s^r X_2(t)dX_1(t) = X_1(r)X_2(r) - X_1(s)X_2(s) - \int_s^r X_1(t)dX_2(t) - \int_s^r G_1(t)G_2(t)dt$$

Stopping Times

Def: Let a probability space $(\Omega, \mathcal{U}, P)$ and a filtration $\{\mathcal{F}(t)\}_{t\geq 0}$ be given. A random variable $\tau : \Omega \to [0, \infty]$ is called a *stopping time* with respect to the filtration if

$$\{\omega \in \Omega : \tau(\omega) \leq t\} \in \mathcal{F}(t), \quad \forall t \geq 0.$$

Theorem: Let $\boldsymbol{X} : [0, \infty) \to \mathbb{R}^n$ be the solution to the SDE

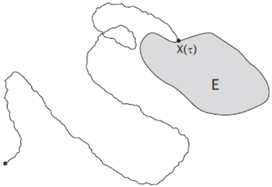
$$d\boldsymbol{X}(t) = \boldsymbol{b}(\boldsymbol{X}(t), t)dt + \boldsymbol{B}(\boldsymbol{X}(t), t)d\boldsymbol{W}(t), \quad \boldsymbol{X}(0) = \boldsymbol{X}_0$$

Let $E \subseteq \mathbb{R}^n$ be given with $E \neq \emptyset$ and E or $\mathbb{R}^n \backslash E$ open. Then

$$\tau = \inf\{t \geq 0 : \boldsymbol{X}(t) \in E\}$$

is a stopping time.

This example motivates the term *stopping time*, although the stochastic process can run further.



Remark: $\sigma = \sup\{t \geq 0 : \boldsymbol{X}(t) \in E\}$ is not a stopping time, since $\{\omega \in \Omega : \sigma(\omega) \leq t\}$ depends upon the future.

Stopping Times

Def: For $G \in \mathbb{L}^2(0,T)$ let τ be a stopping time with $0 \le \tau \le T$. Then

$$\int_0^\tau G(t)dW(t) = \int_0^T \chi_{\{t\le\tau\}}(t)G(t)dW(t)$$

These random variables have the properties

$$\mathbb{E}\left[\int_0^\tau G(t)dW(t)\right] = 0, \quad \mathbb{E}\left[\left(\int_0^\tau G(t)dW(t)\right)^2\right] = \mathbb{E}\left[\int_0^\tau G^2(t)dt\right]$$

- If $\boldsymbol{X} : [0,\infty) \to \mathbb{R}^n$ satisfies

$$d\boldsymbol{X}(t) = \boldsymbol{b}(\boldsymbol{X}(t),t) + \boldsymbol{B}(\boldsymbol{X}(t),t)d\boldsymbol{W}(t), \quad \boldsymbol{X}(0) = \boldsymbol{X}_0$$

where $\boldsymbol{X} = \{X^i\}_{i=1}^n$, $\boldsymbol{b} = \{b^i\}_{i=1}^n$, $\boldsymbol{B} = \{B^{ik}\}_{i,k=1}^{n,m}$

and $u \in \mathcal{C}^2(\mathbb{R}^{n+1},\mathbb{R})$, then "$u$" $= u(X(t),t))$

$$du(\boldsymbol{X}(t),t) = u_t dt + \sum_{i=1}^n u_{x_i} dX^i(t) + \frac{1}{2}\sum_{i,j=1}^n u_{x_i x_j}\sum_{k=1}^m B^{ik}B^{jk}dt$$

or

$$u(\boldsymbol{X}(t),t) - u(\boldsymbol{X}_0,0) = \int_0^t (u_t + Lu)ds + \int_0^t Du\cdot\boldsymbol{B}d\boldsymbol{W}(s)$$

$$Lu = \frac{1}{2}\sum_{i,j=1}^n a^{ij}u_{x_i x_j} + \sum_{i=1}^n b^i u_{x_i}, \quad a^{ij} = \sum_{k=1}^m B^{ik}B^{jk}, \quad Du\cdot\boldsymbol{B}d\boldsymbol{W} = \sum_{i,k=1}^{n,m} u_{x_i}B^{ik}dW^k$$

Stopping Times and PDEs

- This formula holds for $t \in [0, T]$. If τ is a stopping time with $0 \leq \tau \leq T$, then the formula may be evaluated in τ, and there results
$$\mathbb{E}[u(\boldsymbol{X}(\tau), \tau)] = \mathbb{E}[u(\boldsymbol{X}_0, 0)] + \mathbb{E}\left[\int_0^\tau (u_t + Lu) ds\right]$$
L is called a generator. So there is an important connection betweeen SDEs and (deterministic) PDEs.
- For the most important case $\boldsymbol{X} = \boldsymbol{W}$ the generator is
$$Lu = \frac{1}{2}\sum_{i=1}^{n} u_{x_i x_j} = \frac{1}{2}\Delta u$$

Theorem: Let $U \subset \mathbb{R}^n$ be bounded and open with ∂U smooth. Let u be a smooth solution to the PDE,
$$-\frac{1}{2}\Delta u = 1 \text{ in } U, \quad u = 0 \text{ on } \partial U$$
For $x \in U$ let $\boldsymbol{X}(t) = \boldsymbol{W}(t) + x$ and $\tau_x = \inf\{t \geq 0 : \boldsymbol{X}(t) \in \partial U\}$. Then $u(x) = \mathbb{E}[\tau_x]$, $\forall x \in U$.

Follows from $u_t = 0$, $\mathbb{E}[u(\boldsymbol{X}_0)] = u(x)$, $\min\{\tau_x, n\} \xrightarrow{|u|<\infty} \tau_x$

Stopping Times and PDEs

Theorem: Let $U \subset \mathbb{R}^n$ be bounded and open with ∂U smooth. Let $g : \partial U \to \mathbb{R}$ be continuous. Let $u \in \mathcal{C}^2(U) \cap \mathcal{C}(\bar{U})$ be the solution to the PDE,

$$\Delta u = 0 \text{ in } U, \quad u = g \text{ on } \partial U \quad \text{i.e., } u \text{ harmonic}$$

For $x \in U$ set $\boldsymbol{X}(t) = \boldsymbol{W}(t) + x$ and $\tau_x = \inf\{t \geq 0 : \boldsymbol{X}(t) \in \partial U\}$. Then $u(x) = \mathbb{E}[g(\boldsymbol{X}(\tau_x))]$, $\forall x \in U$.

Follows with $u_t = \Delta u = 0$, $\mathbb{E}[u(\boldsymbol{X}_0)] = u(x)$, $u(\boldsymbol{X}(\tau_x)) = g(\boldsymbol{X}(\tau_x))$

- Since Brownian Motion is isotropic, the mean value formula is a result of the last theorem,

$$u(x) = \int_{\Omega \to \partial B(x,r)} g(\underbrace{\boldsymbol{X}(\omega, \tau_x(\omega))}_{y \in \partial B(x,r)}) \underbrace{dP(\omega)}_{dS(y)/|\partial B(x,r)|} = \frac{1}{|\partial B(x,r)|} \int_{\partial B(x,r)} u(y) dS(y)$$

Theorem: Let $U \subset \mathbb{R}^n$ be bounded and open with ∂U smooth. Let $u \in \mathcal{C}^2(U) \cap \mathcal{C}(\bar{U})$ be a solution to the PDE,

$$\Delta u = 0 \text{ in } U, \quad u = 1 \text{ on } \Gamma_1, \quad u = 0 \text{ on } \Gamma_2, \quad \partial U = \Gamma_1 \cup \Gamma_2$$

For $x \in U$, $u(x)$ is the probability that $\boldsymbol{X}(t) = \boldsymbol{W}(t) + x$ meets the boundary at Γ_1 before Γ_2.

Stopping Times and PDEs

Follows with $g = \chi_{\Gamma_1}$ (smoothing, previous theorem) and

$$u(x) = \int_\Omega g(\boldsymbol{X}(\omega, \tau_x(\omega)))dP(\omega) = \int_\Omega \{\omega : X(\omega, \tau_x(\omega)) \in \Gamma_1\} dP(\omega)$$

Theorem: Let $U \subset \mathbb{R}^n$ be bounded and open with ∂U smooth. Let $c, f : U \to \mathbb{R}$ be continuous with $c \geq 0$. Let u be a smooth solution to the PDE,

$$-\frac{1}{2}\Delta u + cu = f \text{ in } U, \quad u = 0 \text{ on } \partial U$$

For $x \in U$ let $\boldsymbol{X}(t) = \boldsymbol{W}(t) + x$ and $\tau_x = \inf\{t \geq 0 : \boldsymbol{X}(t) \in \partial U\}$. Then the *Feynman-Kac formula* holds,

$$u(x) = \mathbb{E}\left[\int_0^{\tau_x} f(\boldsymbol{X}(t)) \exp\left(-\int_0^t c(X(s))ds\right) dt\right]$$

Follows with

$$Z(t) = -\int_0^t c(\boldsymbol{X}(s))ds, \qquad dZ(t) = -c(\boldsymbol{X}(t))dt$$
$$Y(t) = v(Z(t)), v(z) = e^z, \quad dY(t) = v_z dZ = -c(\boldsymbol{X}(t))Y(t)dt$$

$$\begin{aligned} d[u(\boldsymbol{X}(t))Y(t)] &= [\tfrac{1}{2}\Delta u(\boldsymbol{X}(t))dt + Du(\boldsymbol{X}(t)) \cdot d\boldsymbol{W}(t)]Y(t) \\ &+ u(\boldsymbol{X}(t))dY(t) \end{aligned}$$

Stopping Times and PDEs

$$\mathbb{E}[\underbrace{u(\boldsymbol{X}(\tau_x))}_{=0}\,Y(\tau_x)) - \mathbb{E}[\underbrace{u(\boldsymbol{X}(0))]}_{=u(x)} =$$
$$\mathbb{E}[\int_0^{\tau_x} \underbrace{[\tfrac{1}{2}\Delta u(\boldsymbol{X}(t))dt - c(\boldsymbol{X}(t))u(\boldsymbol{X}(t))]}_{=-f(\boldsymbol{X}(t))} \underbrace{Y(t)}_{\exp[-\int_0^t c(\boldsymbol{X}(s))ds]} \; dt]$$

Interpretation: Assume that a Brownian particle can disappear or can be absorbed along the path. Let $c(\boldsymbol{X}(t))h + o(h)$ be the probability that a particle disappears during $[t, t+h]$. For a partition $\{t_k = kh\}_{k=0}^m$ of $[0, t]$ with $h = t/m$ the probability that a particle survives up to time t is approximated by $\prod_{k=1}^m (1 - c(\boldsymbol{X}(t_k))h)$. With $h \to 0$ this converges to $\exp[-\int_0^t c(\boldsymbol{X}(s))ds]$. Therefore,

$u(x) =$ average of $f \circ \boldsymbol{X}$ over sample paths
of particles surviving to hit the boundary ∂U.

Remark: There are natural counterparts of these results for more general generators.

Optimal Stopping Time

- Let $U \subset \mathbb{R}^n$ be bounded and open with ∂U smooth. For $x \in U$ let $\boldsymbol{X} : [0, \infty) \to \mathbb{R}^n$ be a solution to the SDE
$$d\boldsymbol{X}(t) = \boldsymbol{b}(\boldsymbol{X}(t), t) + \boldsymbol{B}(\boldsymbol{X}(t), t)d\boldsymbol{W}(t), \quad \boldsymbol{X}(0) = x$$
with $\tau_x = \inf\{t \geq 0 : \boldsymbol{X}(t) \in \partial U\}$.
- Let θ be a stopping time with respect to the filtration $\{\mathcal{F}(t)\}_{t\geq 0}$. Then
$$J_x(\theta) = \mathbb{E}\left[g(\boldsymbol{X}(\min\{\tau_x, \theta\}) + \int_0^{\min\{\tau_x,\theta\}} f(\boldsymbol{X}(s))ds\right]$$
represents the expected cost of halting at time $\min\{\tau_x, \theta\}$.
- One seeks $\theta_x^* = \operatorname{argmin}_\theta J_x(\theta)$ or $u(x) = \inf_\theta J_x(\theta)$.
- $u(x)$ is the *value function*: the minimal cost when the process starts at x. Given $u(x)$ one can construct θ_x^*.
- For constructing optimality conditions one notes that
$$u(x) \leq J_x(\theta = 0) = g(x), \quad \forall x \in U$$
and
$$u(x) = J_x(\theta \geq \tau_x = 0) = g(x), \quad \forall x \in \partial U$$

Optimal Stopping Time

- Fix $\delta > 0$ small and $x \in U$. If the System is not stopped by time δ, then it moves to $\boldsymbol{X}(\delta)$, and the best which can be achieved to minimize the cost thereafter is $u(\boldsymbol{X}(\delta))$.
- Although $\theta_x^* \in [0, \delta]$, e.g., $u(x) = g(x)$ could still hold, the cost is at least the right side if $\tau_x > \delta$ holds,
$$u(x) \leq \mathbb{E}\left[u(\boldsymbol{X}(\delta)) + \int_0^\delta f(\boldsymbol{X}(s))ds\right]$$
where the inequality follows from the definition of u.
- According to Itô's formula,
$$\mathbb{E}[u(\boldsymbol{X}(\delta))] = u(x) + \mathbb{E}\left[\int_0^\delta Lu(\boldsymbol{X}(s))ds\right]$$
and it follows that
$$0 \leq \mathbb{E}\left[\int_0^\delta f(\boldsymbol{X}(s)) + Lu(\boldsymbol{X}(s))ds\right].$$
With $\delta \to 0$,
$$0 \leq f(x) + Lu(x).$$
- If $u(x) < g(x)$ holds, then $\theta_x^* > \delta$ holds and thus smoothness follows,
$$0 = f(x) + Lu(x).$$
- The optimality conditions are
$$\min\{f + Lu, g - u\} = 0 \text{ in } U, \quad u = g \text{ on } \partial U.$$

Optimal Stopping Time

- Approximation of the solution to the optimality conditions,
$$-Lu^\epsilon + \beta_\epsilon(u^\epsilon - g) = f \text{ in } U, \quad u^\epsilon = g \text{ auf } \partial U$$
where $\beta_\epsilon : \mathbb{R} \to \mathbb{R}$ is a smooth, convex, non-decreasing function with
$$\begin{cases} \beta_\epsilon(s) = 0, & s \leq 0 \\ \lim\limits_{\epsilon\to 0} \beta_\epsilon(s) = \infty, & s > 0 \end{cases}$$
Claim: Under reasonable conditions the convergence is obtained:
$$u^\epsilon \to u, \quad \epsilon \to 0.$$
- The closed set
$$S = \{x \in \bar{U} : u(x) = g(x)\}$$
is the *stopping set*. For $x \in \bar{U}$, $\boldsymbol{X}(0) = x$, define
$$\theta_x^* = \inf\{t \geq 0 : \boldsymbol{X}(t) \in S\}$$
Claim: Under reasonable conditions the relations are satisfied:
$$u(x) = J_x(\theta_x^*) = \inf_\theta J_x(\theta).$$

Options Price Theory

- Let $S(t)$ be the price of a stock at time t, which has initial value s_0 and develops stochastically according to,

$$dS(t) = \mu S(t)dt + \sigma S(t)dW(t), \quad S(0) = s_0.$$

  The *drift* is μ and the *volatility* is σ.
- With a *European Call Option* one has the right to buy a share of a stock at a certain *strike price* p at a certain *strike time* T. Let p and T be fixed for the following.
- A finance firm intends to sell the call option at a price determined by knowing a break-even gain/loss threshold.
- To be determined is a deterministic function $u(s, t)$ representing the anticipated *payoff* for the call option at strike time, given that the stock has value s at time t.
- Then $u(s, t)$ is also the break-even *price* for the call option.
- The stochastic payoff/price for or the value of the call option ist

$$C(t) = u(S(t), t).$$

Options Price Theory

- The firm generates assets to cover this payoff by maintaining a parallel (stochastic) portfolio with value
$$\Pi(t) = \phi(t)S(t) - \psi(t)B(t)$$
by buying (long) holdings ϕ in the stock S itself and by selling (short) ψ shares of a secure bond B, thereby borrowing on those shares with the obligation to buy them.
- For simplicity it is assumed that the interest rate of the secure bond is a constant $r > 0$, i.e., a unit $B(0) = 1$ of presently invested money grows according to $B(t) = e^{rt}$.
- The portfolio Π is constructed to be *self-financing* so that transactions in the time interval $[t, t + dt]$ are performed only with the holding assets given at time t, i.e.,
$$\begin{array}{lcccccc} \Pi(t+dt) & = & \phi(t+dt)S(t+dt) & - & \psi(t+dt)B(t+dt) & = \\ & & \phi(t)S(t+dt) & - & \psi(t)B(t+dt) & \\ \Pi(t) & = & \phi(t)S(t) & - & \psi(t)B(t) & \end{array}$$
or with $dX(t) = X(t+dt) - X(t)$ for each variable X,
$$d\Pi(t) = \phi(t)dS(t) - \psi(t)dB(t).$$

Options Price Theory

- A stochastic process $X(t)$ with $dX(t) = \alpha(t)dt + \beta(t)dW(t)$ is said to be *risk-free* if $\beta(t) = 0$.
- It may seem natural to set the threshold call option price to

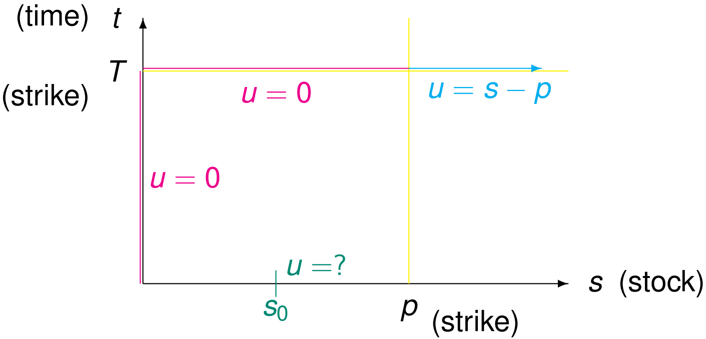
$$e^{-rT}\mathbb{E}[(S(T) - p)^+], \quad x^+ = \max\{x, 0\}$$

  but $X(t) = e^{-rt}(S(t) - p)^+$ is not risk-free, unless $\sigma = 0$.
- A *hedging* strategy is to construct u so that
  ◦ the portfolio Π is *self-financing* and so that
  ◦ the stochastic difference $C(t) - \Pi(t)$ is zero and risk-free.
- If there were otherwise risk, then the firm would be vulnerable to *arbitrage* from others who could siphen off resources such as with the following strategy:
- Start with zero wealth, borrow money by (short) selling a bond, use the borrowed money to buy (long), e.g., a call option, a stock or a portfolio with each, and then use the return on investment to pay the bond debt at a net profit.

Options Price Theory

- Boundary conditions for u are

$$u(s,T) = (s-p)^+, \quad s \geq 0, \quad u(0,t) = 0, \quad 0 \leq t \leq T$$



- With Itô's formula and the SDE for $S(t)$,

"u"$= u(S(t), t)$

$dB(t) = rB(t)dt$

$$\begin{aligned} dC(t) &= u_t dt + u_s dS(t) + \tfrac{1}{2} u_{ss} dS^2(t) \\ &= [u_t + \mu u_s S(t) + \tfrac{1}{2}\sigma^2 u_{ss} S^2(t)]dt + \sigma u_s S(t) dW(t) \\ d\Pi(t) &= \phi(t)dS(t) - \psi(t)dB(t) \\ &= [\mu\phi(t)S(t)dt - r\psi(t)B(t)]dt + \sigma\phi(t)S(t)dW(t) \end{aligned}$$

Options Price Theory

- That $C(t) - \Pi(t)$ be zero and risk-free requires

$$\begin{cases} [u_t + \mu u_s S(t) + \frac{1}{2}\sigma^2 u_{ss} S^2(t)]dt = [\mu\phi(t)S(t) - r\psi(t)B(t)]dt \\ \sigma u_s S(t) dW(t) = \sigma\phi(t)S(t)dW(t) \end{cases}$$

- According to Itô's formula, $\Pi(t)$ satisfies

$$d\Pi(t) = \phi(t)dS(t) - \psi(t)dB(t) + S(t)d\phi(t) - B(t)d\psi(t) + d\phi(t)dS(t)$$

so for $\Pi(t)$ to be self-financing requires

$$S(t)d\phi(t) - B(t)d\psi(t) + d\phi(t)dS(t) = 0.$$

- The system of conditions is solved with the holdings,

$$\phi(t) = u_s(S(t), t), \quad \psi(t) = [u_s(S(t), t)S(t) - u(S(t), t)]e^{-rt}.$$

- Self-financing follows with $u_t + \frac{1}{2}\sigma^2 u_{ss} S^2 = r(u - su_s) = -r\psi B$,

$$\begin{aligned} d\psi &= -re^{-rt}[\phi S - C]dt + e^{-rt}[d(\phi S) - dC] \\ &= -r\psi dt + e^{-rt}[(\phi dS + Sd\phi + d\phi dS) - dC] \Rightarrow \\ Sd\phi + d\phi dS - Bd\psi &= r\psi B dt - \phi dS + dC \\ &= -[u_t + \tfrac{1}{2}\sigma^2 u_{ss} S^2]dt - u_s[\mu S dt + \sigma S dW] \\ &\quad + [u_t + \mu u_s S + \tfrac{1}{2}\sigma^2 u_{ss} S^2]dt + \sigma u_s S dW = 0. \end{aligned}$$

Options Price Theory

- The result is the *Black-Scholes-Merton PDE*:

$$\begin{cases} u_t + rsu_s + \frac{1}{2}\sigma^2 s^2 u_{ss} - ru = 0, & s > 0, \quad 0 \le t \le T \\ u(s,T) = (s-p)^+, & s \ge 0, \quad 0 \le t \le T \\ u(s,t) = 0, & s = 0, \quad 0 \le t \le T \end{cases}$$

- The desired threshold call option price is $u(s_0, 0)$.
- The explicit solution is given by

$$u(s,t)$$

$$= \frac{s}{2}\left[1 + \operatorname{erf}\left(\frac{\ln(s/p) + (r + \sigma^2/2)(T-t)}{\sqrt{2}\sigma\sqrt{T-t}}\right)\right]$$

$$-\frac{p}{2}\left[1 + \operatorname{erf}\left(\frac{\ln(s/p) + (r - \sigma^2/2)(T-t)}{\sqrt{2}\sigma\sqrt{T-t}}\right)\right] e^{-r(T-t)}$$