MRI pulse design via discrete-valued optimal control

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Motivation: Magnetic resonance imaging

Magnetic resonance imaging (MRI):

- popular for medical imaging (and spectroscopy)
- safe, radiation-free
- versatile
- simple image reconstruction (Fourier transform)
- but: complicated physics
  (compare CT: simple physics, complicated mathematics)

MRI in a nutshell

Basic steps in MR scan:

1. magnetic field is applied, aligns proton spins
2. radio pulse at resonance frequency is absorbed by hydrogen nuclei, re-radiated over time at same frequency
3. decaying time-dependent signal is measured by receiver coil

Fundamental principles of MRI:

- signal amplitude proportional to hydrogen density
- signal frequency proportional to magnetic field strength

Spatial encoding

Problem:

- measured time-dependent signal is composite over whole volume, no spatial information

Solution:

- use spatially dependent magnetic fields to map resonance frequency to spatial location

But: linear superposition of (x, y, z) fields is not unique

$\rightsquigarrow$ sequential application of fields to encode (x, y, z) separately

Spatial encoding

Slice selection (z):

- use z-proportional magnetic field during RF excitation
- $\rightsquigarrow$ only thin slice has resonance at RF pulse frequency, contributes to measured signal

Not considered here:

Frequency encoding (x):

- use x-proportional magnetic field during measurement

Phase encoding (y):

- use y-proportional magnetic field before measurement to change phase offset of signal

$\rightsquigarrow$ FFT of time/phase-dependent data gives image

$\rightsquigarrow$ MRI is controlled imaging $\rightsquigarrow$ optimal control

1 Overview

2 Optimal control of Bloch equation

3 MR pulse design

4 Discrete-valued pulses

5 Conclusion

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Mathematical model

Bloch equation

$$\frac{d}{dt}M(t) = \gamma M(t) \times B(t) + R(M(t)), \qquad M(0) = M_0$$

- $M(t) \in \mathbb{R}^3$ describes temporal evolution of spin ensemble
- $B(t)$ controlled time-dependent magnetic field
- γ gyromagnetic ratio $\rightsquigarrow$ resonance frequency $\omega = \gamma B_0$
- $R(M) = \left(-M_x \frac{1}{T_2}, -M_y \frac{1}{T_2}, (-M_z - M_0)\frac{1}{T_1}\right)^T$ relaxation term (T_1, T_2 tissue parameters)

Mathematical model

Slice selection (in rotating frame):

$$B(t) = \left(u_x(t)B_1, u_y(t)B_1, G_z(t)z\right)^T$$

$G_z(t)$ slice-selective gradient field, B_1 static magnetic field

Bloch equation

$$\begin{cases} \dfrac{d}{dt}M(t;z) = A(u(t);z)M(t;z) + b(z), & t > 0, \\ M(0;z) = M^0(z), \end{cases}$$

$$A(u;z) = \begin{pmatrix} -\frac{1}{T_2} & \gamma G_z(t)z & \gamma u_y(t)B_1 \\ -\gamma G_z(t)z & -\frac{1}{T_2} & \gamma u_x(t)B_1 \\ -\gamma u_y(t)B_1 & -\gamma u_x(t)B_1 & -\frac{1}{T_1} \end{pmatrix} \qquad b(z) = \begin{pmatrix} 0 \\ 0 \\ \frac{M_0}{T_1} \end{pmatrix}$$

Optimal control problem

Goal:

- compute control $u(t) = (u_x(t), u_y(t))$ such that $M(T) \approx M_d$
- $\rightsquigarrow$ control-to-state mapping $S^{(\omega)} : u \longrightarrow M(T; z)$
- $M_d(z)$ desired magnetization state $\rightsquigarrow$ slice selection
- ($M_d = M_d^{(\omega)}$ selective to resonance frequency $\rightsquigarrow$ spectroscopy)
- in addition: control with minimal specific absorption rate (SAR)

$$\min_{u \in L^2} \frac{1}{2} \sum_{\omega} \int_{-a}^{a} \left| S^{(\omega)}(u) - M_d^{(\omega)} \right|_2^2 dt + \frac{\alpha}{2} \int_0^T |u(t)|_2^2 \, dt$$

Numerical solution: gradient method

Gradient method

$$u^{k+1} = u^k - s^k g(u^k)$$

- gradient

$$g(u^k)(t) = \alpha u(t) + \gamma B_1 \begin{pmatrix} \int_{-a}^{a} M_z(t;z)P_y(t;z) - M_y(t;z)P_z(t;z)\,dz \\ \int_{-a}^{a} M_z(t;z)P_x(t;z) - M_x(t;z)P_z(t;z)\,dz \end{pmatrix}$$

- adjoint state solving (backward in time)

$$\begin{cases} -\dfrac{d}{dt}P(t;z) = A(u(t);z)^T P(t;z), & 0 \leq t < T, \\ P(T;z) = M(T;z) - M_d(z), & \end{cases}$$

- step length s^k (Armijo, backtracking)

Numerical solution: Newton method

Newton method

$$H(u^k)\delta u = -g(u^k), \qquad u^{k+1} = u^k + \delta u$$

- Hessian

$$[H(u^k)h](t) = \alpha h(t) + \begin{pmatrix} \int_{-a}^{a} \delta M(t;z) A_1 P(t;z) + M(t;z) A_1 \delta P(t;z)\, dz \\ \int_{-a}^{a} \delta M(t;z) A_2 P(t;z) + M(t;z) A_2 \delta P(t;z)\, dz \end{pmatrix}$$

$$MA_1P = \gamma B_1 (M_z P_y - M_y P_z) \qquad MA_2P = \gamma B_1 (M_z P_x - M_y P_y)$$

- linearized state

$$\begin{cases} \frac{d}{dt}\delta M(t;z) = A(u^k;z)\delta M(t;z) + A'(h)M, & 0 < t \leq T, \\ \delta M(0;z) = (0,0,0)^T, \end{cases}$$

Numerical solution: Newton method

Newton method

$$H(u^k)\delta u = -g(u^k), \qquad u^{k+1} = u^k + \delta u$$

- Hessian

$$[H(u^k)h](t) = \alpha h(t) + \begin{pmatrix} \int_{-a}^{a} \delta M(t;z) A_1 P(t;z) + M(t;z) A_1 \delta P(t;z)\, dz \\ \int_{-a}^{a} \delta M(t;z) A_2 P(t;z) + M(t;z) A_2 \delta P(t;z)\, dz \end{pmatrix}$$

$$MA_1P = \gamma B_1 (M_z P_y - M_y P_z) \qquad MA_2P = \gamma B_1 (M_z P_x - M_y P_y)$$

- linearized adjoint

$$\begin{cases} -\dfrac{d}{dt}\delta P(t;z) = A(u^k;z)^T \delta P(t;z) + A'(h)^T P, & 0 \le t < T, \\ \qquad \delta P(T;z) = \delta M(T;z). \end{cases}$$

Numerical solution: Newton method

Bilinear control problem: non-convex

- solution of Newton step via CG method
- globalization by trust-region method (truncated CG [Steihaug])

Discretization:

- collocation points z_i (independent, parallel)
- Crank–Nicolson (state piecewise linear, controls piecewise constant)
- adjoint-consistent: adjoint state piecewise constant
- same for linearized state, adjoint
- CG method in weighted inner product (time steps)

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MR pulse design

Goal: multi-slice excitation

- initial magnetization $M_0 = (0, 0, 1)^T$
- gradient G_z from standard Cartesian sequence (2.56 ms)
- window $a = 0.5$ m, $\Delta z = 0.2$ mm (5001 points)
- desired magnetization (slice width 5 mm)

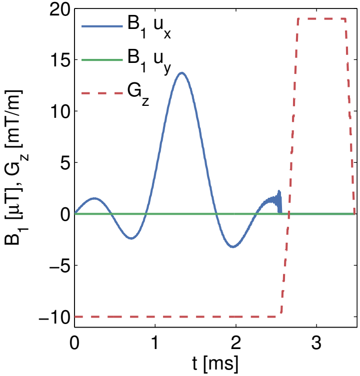
$$M_d(z) = \begin{cases} (\sin(90^\circ), \cos(90^\circ), 0)^T & \text{in slice} \\ (0, 0, 1)^T & \text{out of slice} \end{cases}$$

- $u_0 \equiv (0, 0)^T$, $\alpha = 10^{-4}$

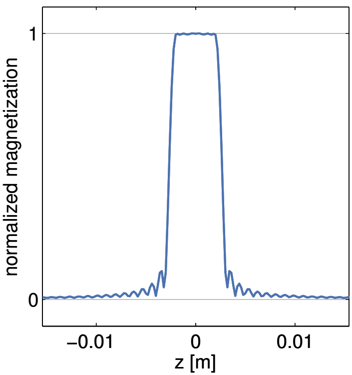
Validation:

- implemented on 3T Siemens MR scanner
- phantom (slice profile homogeneity)
- healthy volunteer (image reconstruction)

Results: slice profile

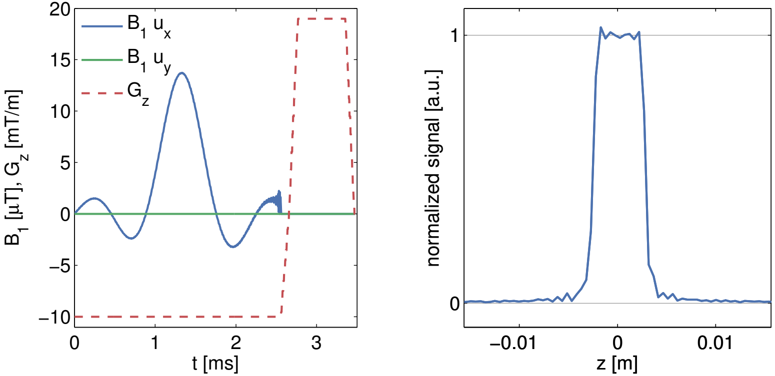


(a) optimized pulse



(b) optimized magnetization $|(M_x, M_y)|_2$

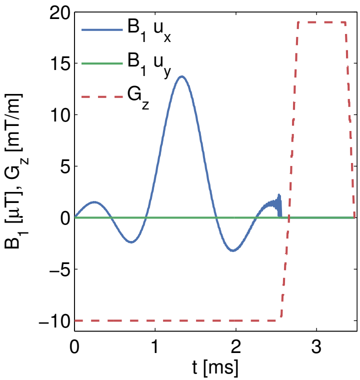
Results: slice profile



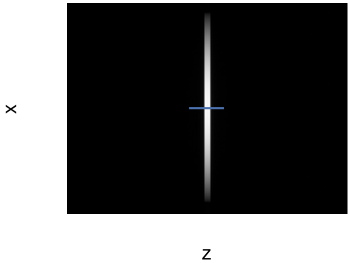
(a) optimized pulse

(b) measured magnetization $|(M_x, M_y)|_2$

Results: slice profile

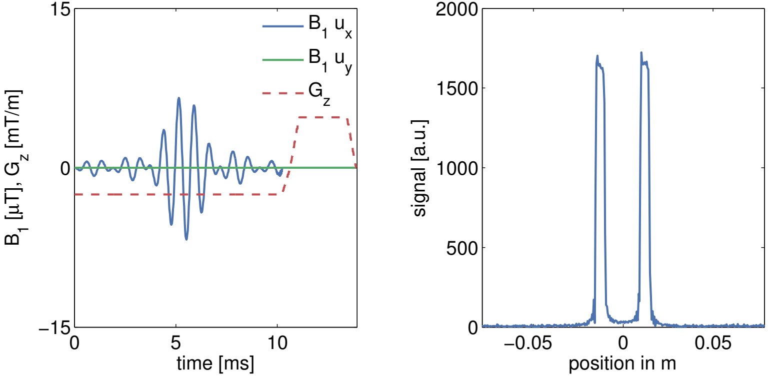


(a) optimized pulse



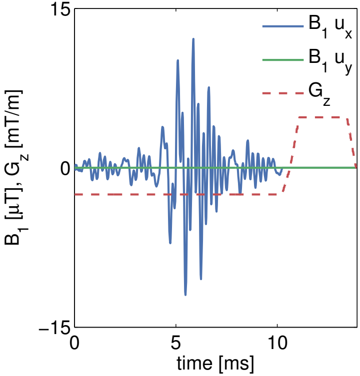
(b) reconstruction

Results: multi-slice excitation

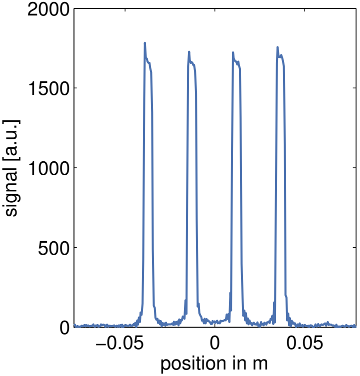


(a) optimized pulse (b) measured magnetization

Results: multi-slice excitation

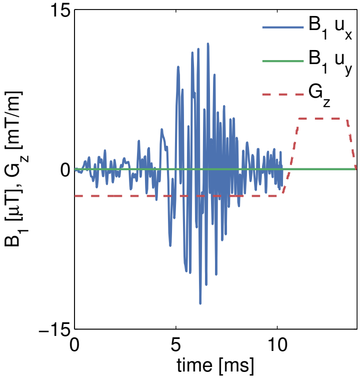


(a) optimized pulse

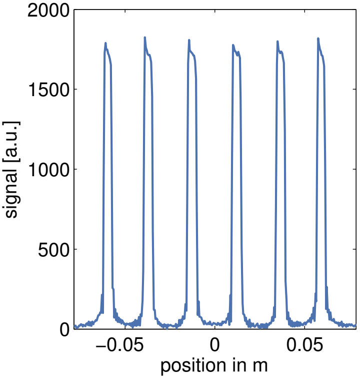


(b) measured magnetization

Results: multi-slice excitation

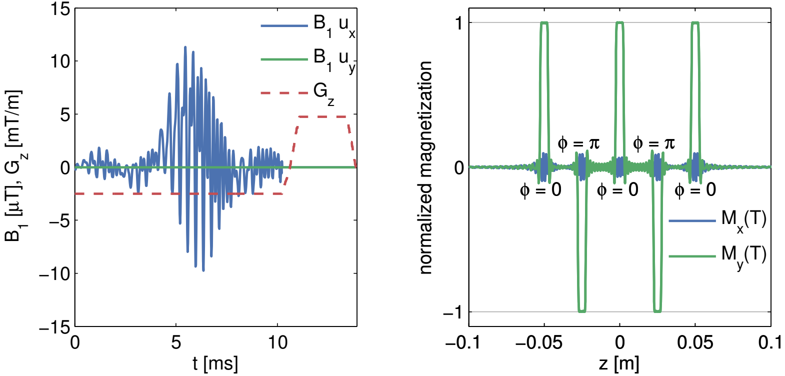


(a) optimized pulse



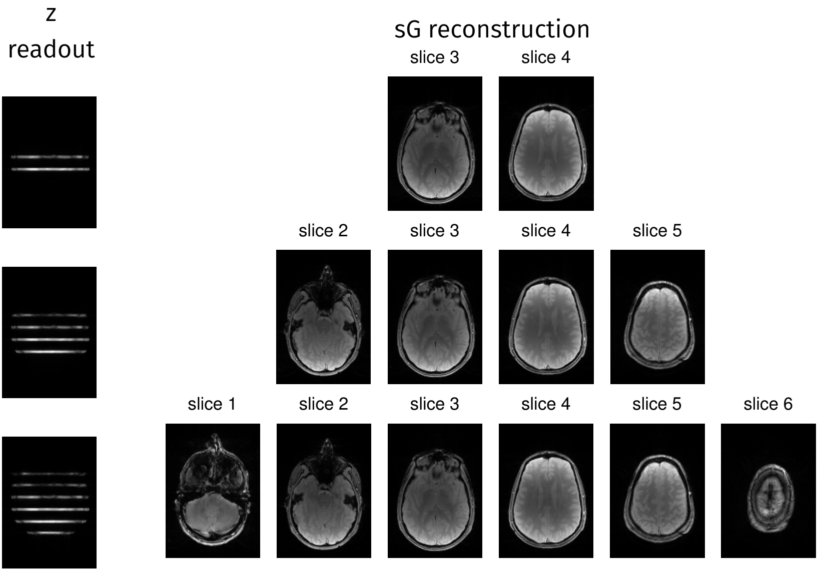
(b) measured magnetization

Results: multi-slice reconstruction



(a) optimized pulse (b) optimized magnetization

Results: multi-slice reconstruction



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Discrete control

Technical limitation: device can only realize control from discrete set

$$U = \left\{u \in L^2(0,T;\mathbb{R}^2) : u(t) \in \{u_1,\dots,u_d\} \text{ a.e.}\right\}$$

- $u_1,\dots,u_d \in \mathbb{R}^2$ given (fixed amplitude, phases)
- non-convex discrete-valued control problem

$$\min_{u\in U} \frac{1}{2}\sum_{\omega} \|S^{(\omega)}(u) - M_d^{(\omega)}\|_2^2 + \frac{\alpha}{2}\int_0^T |u(t)|_2^2\, dt$$

Multi-bang penalty

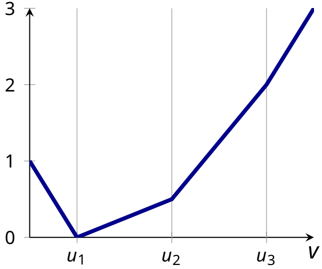
- convex relaxation: replace U by convex hull
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\rightsquigarrow$ promote $u(x) \in \{u_1, \ldots, u_d\}$ by convex pointwise penalty

$$\mathcal{G}(u) = \int_\Omega g(u(x))\,dx$$

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \ldots, u_d$
- not exact relaxation/penalization (in general)!

Multi-bang penalty

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \ldots, u_d$



- motivation: convex envelope of $\frac{1}{2}\|u\|^2 + \delta_U$
- multi-bang (generalized bang-bang) control
- here: vector-valued control

Vector-valued multi-bang: penalty

Here: admissible control set U of d radially distributed states, origin

$$U = \left\{ \binom{0}{0}, \begin{pmatrix} \omega_0 \cos\theta_1 \\ \omega_0 \sin\theta_1 \end{pmatrix}, \dots, \begin{pmatrix} \omega_0 \cos\theta_d \\ \omega_0 \sin\theta_d \end{pmatrix} \right\}$$

- fixed amplitude $\omega_0 > 0$
- phases $0 \leq \theta_1 < \dots < \theta_d < 2\pi$

multi-bang penalty $g = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}$ convex envelope

$$g^*(q) = \left(\left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}\right)^*(q) = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^*(q)$$

$$= \begin{cases} 0 & \langle q, u_i \rangle \leq \frac{1}{2}\omega_0^2 \text{ for all } 1 \leq i \leq d \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & \frac{\theta_{i-1}+\theta_i}{2} \leq \angle q \leq \frac{\theta_i+\theta_{i+1}}{2}, \langle q, u_i \rangle \geq \frac{1}{2}\omega_0^2 \end{cases}$$

Vector-valued multi-bang: subdifferential

Fenchel conjugate

$$g^*(q) = \begin{cases} 0 =: u_0 & q \in \overline{Q}_0 \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & q \in \overline{Q}_i \end{cases}$$

Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i & 0 \leq i \leq d \\ \operatorname{co}\{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} & 0 \leq i_1, \dots, i_k \leq d \end{cases}$$

Vector-valued multi-bang: subdifferential

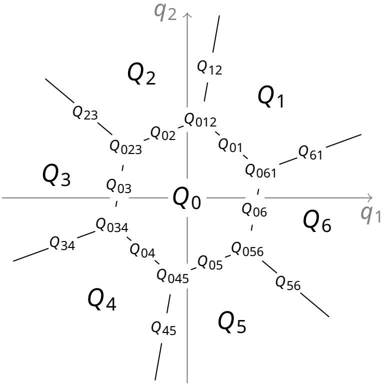
Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i \quad 0 \le i \le d \\ \operatorname{co}\{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} \quad 0 \le i_1, \dots, i_k \le d \end{cases}$$

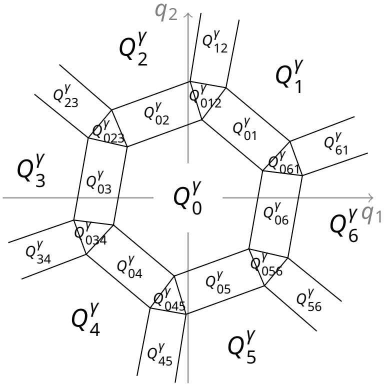
Moreau–Yosida regularization

$$(\partial g^*)_\gamma(q) = \begin{cases} u_i & q \in Q_i^\gamma \\ \left(\frac{\langle q, u_i \rangle}{\gamma \omega_0^2} - \frac{\alpha}{2\gamma}\right) u_i & q \in Q_{0,i}^\gamma \\ \frac{u_i + u_{i+1}}{2} + \frac{\langle q, u_i - u_{i+1} \rangle (u_i - u_{i+1})}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma \\ \frac{q}{\gamma} - \frac{\alpha}{\gamma}\left(\frac{\omega_0}{|u_i + u_{i+1}|_2}\right)^2 (u_i + u_{i+1}) & q \in Q_{0,i,i+1}^\gamma \end{cases}$$

Vector-valued multi-bang: subdifferential



(a) subdomains for ∂g^*



(b) subdomains for $(\partial g^*)_\gamma$

Vector-valued multi-bang: Newton method

Newton derivative

$$D_N(\partial g_\gamma^*)(q) = \begin{cases} 0 & q \in Q_i^\gamma \\ \frac{u_i u_i^T 1}{\gamma \omega_0^2} & q \in Q_{0,i}^\gamma \\ \frac{(u_i - u_{i+1})(u_i - u_{i+1})^T}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma \\ \frac{1}{\gamma}\,\mathrm{Id} & q \in Q_{0,i,i+1}^\gamma \end{cases}$$

Superposition operator:

$$\left[D_N H_\gamma(p)\right](t) := D_N\left(\partial g_\gamma^*\right)(p(t)) \quad \text{a.e.} \quad t \in [0,T]$$

Vector-valued multi-bang: Newton method

Semismooth Newton system

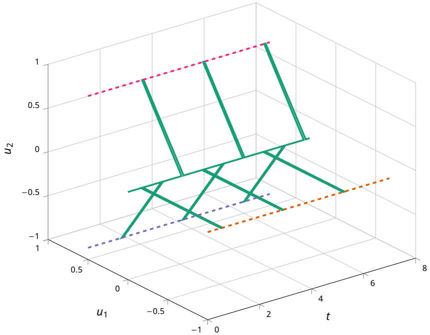
$$\left(\mathrm{Id} - D_N H_\gamma(\mathcal{F}'(u^k))\mathcal{F}''(u^k)\right)\delta u = -u^k + \partial\mathcal{G}_\gamma^*(\mathcal{F}'(u^k))$$

- matrix-free Krylov method for semismooth Newton step
- $\mathcal{F}'$, $\mathcal{F}''$ via linearized, adjoint Bloch equation
- discretization, adjoint as before

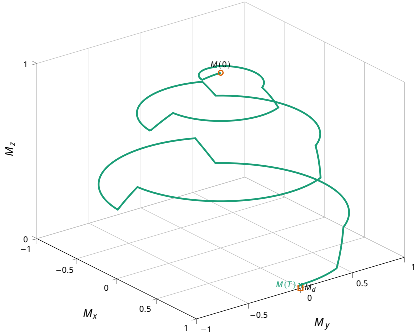
Numerical examples

- goal: shift magnetization from $M_0 = (0,0,1)^T$ at $t = 0$
  to $M_d = (1,0,0)^T$ at $t = T$
- $d = 3, 6$ radially distributed admissible control states
- $n = 1, 4$ isochromats with different resonance frequencies
  1. shift all isochromats
  2. shift only one isochromat
- $\alpha = 10^{-1}$, $\omega_0 = 1$
- example motivated by [Dridi/Lapert/Salomon/Glaser/Sugny ’15]

Numerical examples



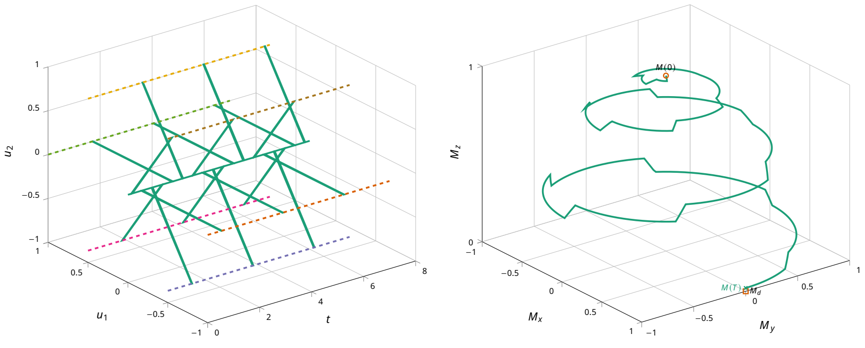
(a) control $u(t)$



(b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 3$ control states

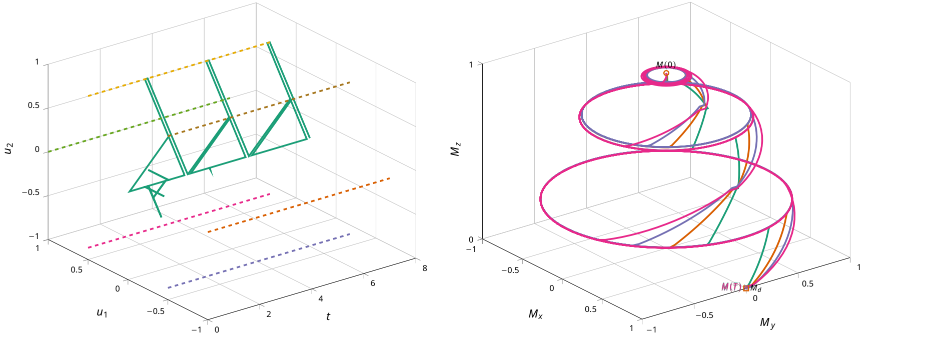
Numerical examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 6$ control states

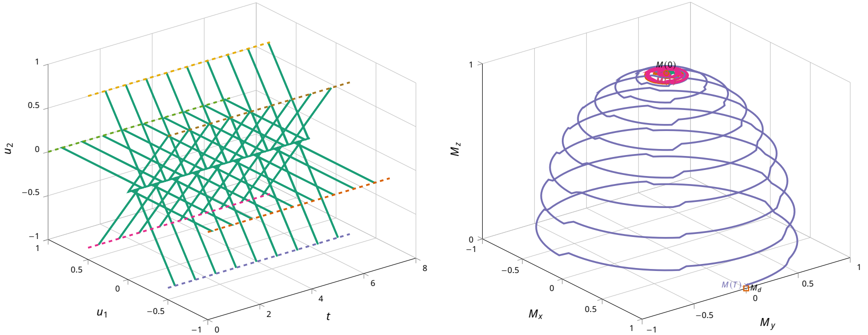
Numerical examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 4$ isochromats, same target

Numerical examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $J = 4$ isochromats, different targets

Conclusion

Optimal control for MR pulse design

- allows designing low energy pulses
- allows incorporating full physical model
- allows accelerated imaging
- allows incorporating structural constraints

Outlook:

- joint optimization of RF pulse and gradient
- (joint) optimization of frequency, phase encoding
- joint optimization and reconstruction

Preprints, codes:

`http://homepage.uni-graz.at/c.clason/publikationen`