TWO TIME DISCRETIZAZIONS FOR GRADIENT FLOWS EXACTLY REPLICATING ENERGY DISSIPATION

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Gradient flows

$$u'(t) + D\phi(u(t)) = 0, \quad \text{for a.e. } t \in (0,T), \quad u(0) = u_0 \tag{1}$$

- $t \mapsto u(t) \in H$: trajectory in a Hilbert space H
- ϕ : given potential
- $D(\phi)$: Fréchet differential (for ϕ smooth)
- u_0 : prescribed initial datum

For all $[s,t] \subset [0,T]$, solutions to (1) fullfill the energy equality

$$\phi(u(t)) + \int_s^t \|u'(r)\|^2 \mathrm{d}r = \phi(u(s)) \tag{2}$$

and this can be rewritten as

$$\phi(u(t)) + \frac{1}{2}\int_s^t \|u'(r)\|^2 \mathrm{d}r + \frac{1}{2}\int_s^t \|D\phi(u(r))\|^2 \mathrm{d}r = \phi(u(s)). \tag{3}$$

Observe: (1) $\Leftrightarrow$ (3) $\rightleftarrows\!\!\!\!\!/\;$ (2)

Discretization of (1)

Let a partition $\{0 = t_0 < t_1 < \cdots < t_N = T\}$ be given and indicate by $\tau_i = t_i - t_{i-1}$ its time steps.

Implicit Euler Scheme

Given u_0, solve

$$\frac{u_i - u_{i-1}}{\tau_i} + D\phi(u_i) = 0 \quad \text{for } i = 1, \ldots, N.$$

which can be equivalenty reformulated in **variational terms** as:

$$u_i \in \arg\min_{u \in H} \left(\phi(u) + \frac{\tau_i}{2}\left\|\frac{u - u_{i-1}}{\tau_i}\right\|^2 \right) \quad \text{for } i = 1, \ldots, N.$$

Scheme A

Given u_0, let $u_i = u_{i-1}$ if $D\phi(u_{i-1}) = 0$ or

$$\frac{u_i - u_{i-1}}{\tau_i} + D\phi(u_i) + (\phi(u_i) - \phi(u_{i-1}) - (D\phi(u_i), u_i - u_{i-1}))\frac{u_i - u_{i-1}}{\|u_i - u_{i-1}\|^2} = 0 \quad \text{if } D\phi(u_{i-1}) \neq 0.$$

for $i = 1, \ldots, N$

which can be equivalenty formulated as:

$$\phi(u_i) + \tau_i \left\|\frac{u_i - u_{i-1}}{\tau_i}\right\|^2 = \phi(u_{i-1}) \text{ and } D\phi(u_i) \text{ is parallel to } u_i - u_{i-1}.$$

Scheme B

Given u_0, solve

$$\phi(u_i) + \frac{\tau_i}{2}\left\|\frac{u_i - u_{i-1}}{\tau_i}\right\|^2 + \frac{\tau_i}{2}\|D\phi(u_i)\|^2 - \phi(u_{i-1}) = 0 \quad \text{for } i = 1, \ldots, N$$

which is a discrete version of (3).

Scheme A

Existence Let $\phi \in C^1(\mathbb{R}^d)$ be bounded from below and let $D\phi(u_{i-1}) \neq 0$. Then there exists $u_i \in \mathbb{R}^d \setminus \{u_{i-1}\}$ solving the scheme A.

Convergence Let $\phi \in C^1(\mathbb{R}^d)$ be bounded from below.

(i) There exists a subsequence which is not relabeled such that $\widehat{u}^n \to u$ weakly in $H^1(0,T;\mathbb{R}^d)$ as $n \to \infty$, where u solves (1).

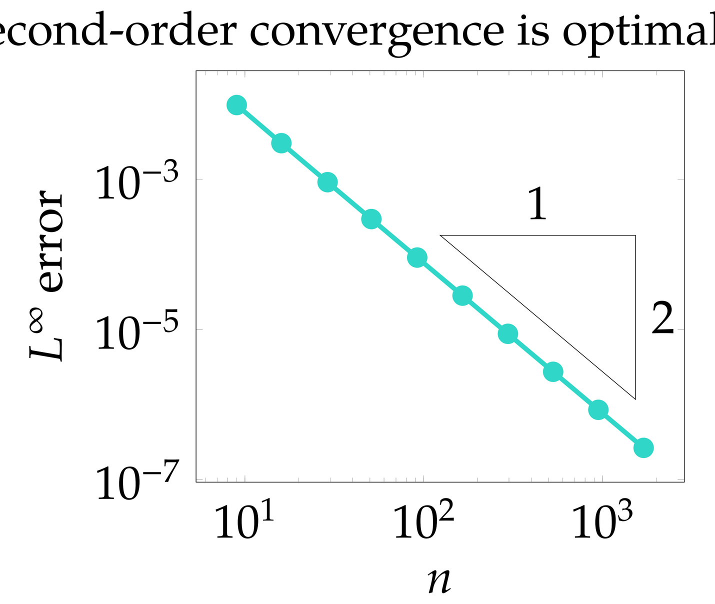
(ii) Let $\phi \in C^{1,1}_{\mathrm{loc}}(\mathbb{R}^d)$. Then the whole sequence $(\widehat{u}^n)$ converges strongly in $W^{1,\infty}(0,T;\mathbb{R}^d)$ and the error bound is $\|u - \widehat{u}^n\|_{W^{1,\infty}(0,T;\mathbb{R}^d)} \leq C\tau^n$.

(iii) Let $\phi \in C^3(\mathbb{R}^d)$ and assume that the condition

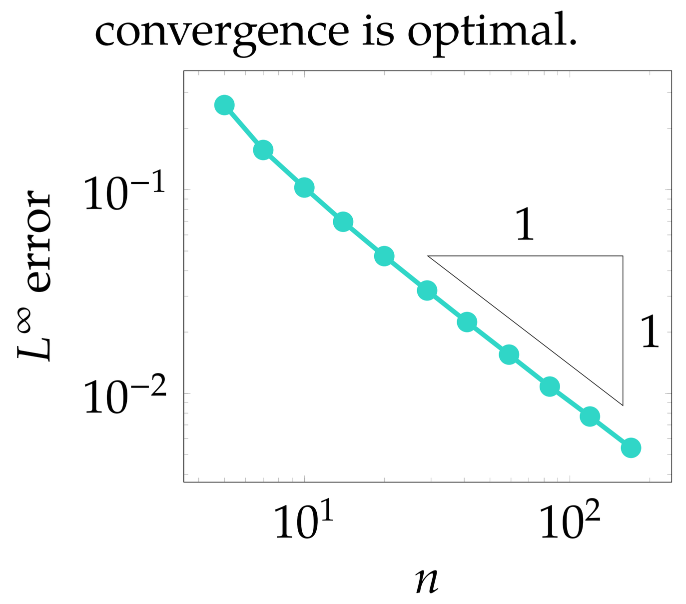
$$D^2\phi(v)w \text{ is parallel to } w \text{ for any } v, w \in \mathbb{R}^d \tag{4}$$

holds. Then $\|u - \widehat{u}^n\|_{W^{1,\infty}(0,T;\mathbb{R}^d)} \leq C(\tau^n)^2$.

If (4) holds, in one dimension, the second-order convergence is optimal.



If (4) does not hold, the first order convergence is optimal.



Scheme B

We look for $u_i \in D(\partial\phi)$ such that

$$\phi(u_i) + \frac{\tau_i}{2}\left\|\frac{u_i - u_{i-1}}{\tau_i}\right\|^2 + \frac{\tau_i}{2}\|\partial\phi(u_i)\|^2 = \phi(u_{i-1}) + \rho_i \tag{5}$$

where ρ_i the residual is nonpositive or small.

Let $\phi = \phi_1 + \phi_2$ have compact sublevels, $\phi_1 : H \to (-\infty, \infty]$ be convex, proper, lower semicontinuous with $\partial\phi_1$ being single-valued, and $\phi_2 \in C^{1,\alpha}_{\mathrm{loc}}(H)$ for $\alpha \in (0,1]$. Furthermore, let $u_{i-1} \in D(\partial\phi)$ be given with $\partial\phi(u_{i-1}) \neq 0$.

Existence Then there exists $u_i \in D(\partial\phi)$ with $u_i \neq u_{i-1}$ and

$$G_i(u_i, u_{i-1}) \leq \frac{L}{1+\alpha}\|u_i - u_{i-1}\|^{1+\alpha},$$

where L is the Hölder constant of $D\phi_2$. In particular, (5) can be solved with $\rho_i \leq L\|u_i - u_{i-1}\|^{1+\alpha}/(1+\alpha)$. In case ϕ is convex, namely $\phi_2 = 0$, and $\|\partial\phi\|$ is strongly continuous along segments in $D(\partial\phi)$, one can find u_i such that $G_i(u_i, u_{i-1}) = 0$.

Convergence Let $u_i^n \in D(\partial\phi)$ be such that $u_0^n = u_0$ and

$$\sum_{i=1}^{N^n} G_i^n(u_i^n, u_{i-1}^n)^+ \to 0 \text{ as } n \to \infty.$$

Then $\widehat{u}^n \to u$ converges strongly in $H^1(0,T;H)$, where u solves the gradient-flow problem (1).

Error control Let $\phi \in C^2(\mathbb{R}^d)$ be bounded from below and u_i, v_i fulfill $u_0 = v_0$, $G_i(u_i, u_{i-1}) = 0$ and $v_i \in \arg\min G_i(\cdot, v_i)$ respectively. Then for all $i = 1, \ldots, N$ we have

$$\|u(t_i) - v_i\| \leq C\tau \quad \text{and} \quad \|u(t_i) - u_i\| \leq C\tau^{1/2}$$

where u is the unique solution of (1).

Extensions of scheme B

For all the following nonlinear evolution equations is it possible to write a scheme B and prove the convergence.

Generalized gradient flows

Let $\psi : H \times H \to [0,\infty)$, such that $\forall u \in H :\ \psi(u,\cdot)$ is convex and lower semicontinuous, the mapping $H \times H \times H \to \mathbb{R}, (u,v,w) \mapsto \psi(u,v) + \psi^*(u,w)$ is weakly lower semicontinuous, $\exists c > 0$, $p > 1$, $\forall u, v, w \in H$: $\psi(u,v) + \psi^*(u,w) \geq c\|v\|^p + c\|w\|^{p'}$:

$$\partial\psi(u,u') + \partial\phi(u) \ni 0 \quad \text{for a.e. } t \in (0,T), \quad u(0) = u_0.$$

The scheme B reads

$$G_i(u,v) := \phi(u) + \tau_i\psi\left(v, \frac{u-v}{\tau_i}\right) + \tau_i\psi^*(v, -\partial\phi(u)) - \phi(v) = 0.$$

GENERIC flows

$$u' = LDE(u) - K\partial\phi(u) \quad \text{for a.e. } t \in (0,T), \quad u(0) = u_0.$$

The equivalent of (3) is

$$\phi(u(t)) + \int_0^t \psi(u' - LDE(u))\mathrm{d}r + \int_0^t \psi^*(-\partial\phi(u))\mathrm{d}r = \phi(u_0)$$

and the scheme B can be extended by considering the functional

$$\overline{G}_i(u,v) := \phi(u) + \tau_i\psi\left(\frac{u-v}{\tau_i} - LDE(u)\right) + \tau_i\psi^*(-\partial\phi(u)) - \phi(v) = 0.$$

Curves of maximal slope

Let (X,d) be a complete metric space and $\phi : X \to [0,\infty]$ be lower semicontinuous. A curve of maximal slope u for the functional ϕ is such that $\phi \circ u$ is nonincreasing, $u(0) = u_0$ and

$$\phi(u(t)) + \frac{1}{2}\int_0^t |u'|^2(s)\mathrm{d}s + \frac{1}{2}\int_0^t |\partial\phi|^2(u(s))\,\mathrm{d}s = \phi(u_0) \text{ for all } t \in [0,T].$$

The scheme B is defined as

$$\widehat{G}_i(u,v) = \phi(u) + \frac{1}{2\tau_i}d^2(u,v) + \frac{\tau_i}{2}|\partial\phi|^2(u) - \phi(v) = 0.$$

Reference

A. Jüngel, U. Stefanelli, L.Trussardi, *Two time discretizations for gradient flows exactly replicating energy dissipation*, submitted (2018)