Convergence to equilibrium for the θ-scheme applied to gradient systems with analytic nonlinearities

Morgan PIERRE, University of Poitiers, France

Warwick, EFEF 2010, May 20-21, 2010

Consider the gradient flow

$$U'(t) = -\nabla F(U(t)) \quad t \geq 0, \tag{1}$$

where $U = (u_1, \ldots, u_d)^t$, $F \in C^{1,1}_{loc}(\mathbf{R}^d, \mathbf{R})$. For every solution $U(t)$, we have

$$F(U(t)) + \int_0^t \|U'(s)\|^2 ds = F(U(0)), \quad t \geq 0.$$

If U is a solution of (1) which is bounded on $[0, +\infty)$, then

$$\omega(U(0)) := \{U^\star \;:\; \exists t_n \to +\infty,\; U(t_n) \to U^\star\}$$

is a non-empty compact connected subset of

$$\mathcal{S} = \{V \in \mathbf{R}^d \;:\; \nabla F(V) = 0\}.$$

Moreover, $d\big(U(t), \omega(U(0))\big) \to 0$ as $t \to +\infty$.

Does $U(t) \to U^\star$ as $t \to +\infty$?

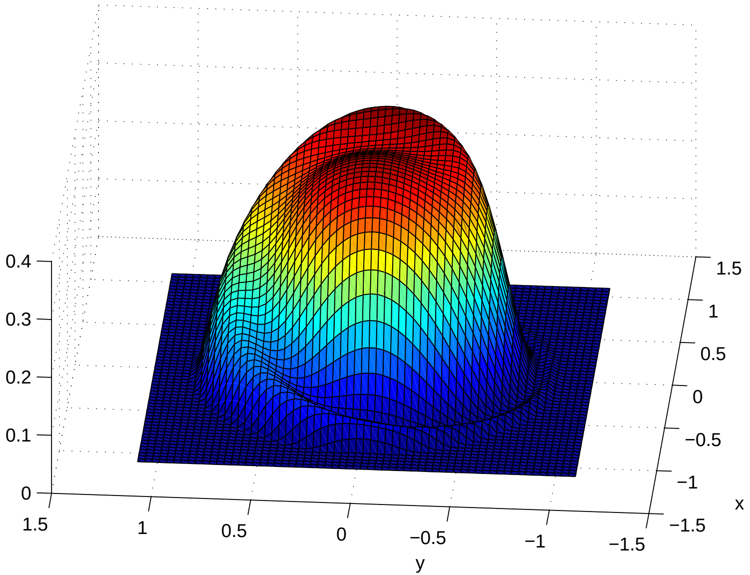
If $d = 1$, it is obvious by monotonicity.
If $d \geq 2$, it is obviously true if $\mathcal{S}$ is discrete, but it is no longer true in general: counterexamples in Curry'44, Palis and De Melo'82, Zoutendijk'88, Bertsekas '95. The following counter-example ("Mexican hat") is given in Absil, Mahony and Andrews'05 :

$$f(r,\theta) = e^{-1/(1-r^2)} \left[1 - \frac{4r^4}{4r^4 + (1-r^2)^4} \sin(\theta - \frac{1}{1-r^2}) \right],$$

if $r < 1$ and $f(r,\theta) = 0$ otherwise. We have $f \in C^\infty$, $f(r,\theta) > 0$ for $r < 1$ so $r = 1$ is a global minimizer. We can check that the curve defined by

$$\theta = 1/(1-r^2)$$

is a trajectory.



“Mexican hat” function

Theorem (Lojasiewicz'65)

If $F : \mathbf{R}^d \to \mathbf{R}$ is real analytic in a neighbourhood of $U^\star \in \mathbf{R}^d$, there exist $\nu \in (0, 1/2]$, $\sigma > 0$ and $\gamma > 0$ s.t. for all $V \in \mathbf{R}^d$,

$$\|V - U^\star\| < \sigma \Rightarrow |F(V) - F(U^\star)|^{1-\nu} \leq \gamma \|\nabla F(V)\|. \qquad (2)$$

NB: see the preprint of Michel Coste on his web page.
Example: for $d = 1$ and $p \geq 2$, $x \mapsto x^p$ satisfies (2) at $x^\star = 0$ with $\nu = 1/p$. For $d \geq 1$, in the "generic case"' where $\nabla^2 F(U^\star)$ inversible, $\nu = 1/2$.

Corollary

If $F : \mathbf{R}^d \to \mathbf{R}$ is real analytic, then for any bounded semi-orbit of $U'(t) = -\nabla F(U(t))$, there exists $U^\star \in \mathcal{S}$ s.t. $U(t) \to U^\star$ as $t \to +\infty$.

A proof

$F(U(t))$ is non increasing and so has a limit $F^\star(= 0)$. Let $t_n \to +\infty$ s.t. $U(t_n) \to U^\star$. We have $F(U^\star) = F^\star$ and $U^\star \in \mathcal{S}$. Choose n large enough so that $\|U(t_n) - U^\star\| < \sigma/2$ and $\gamma F(U(t_n))^\nu < \sigma/2$, and define

$$t^+ = \sup\{t \geq t_n \mid \|U(s) - U^\star\| < \sigma \quad \forall s \in [t_n, t)\}.$$

For $t \in [t_n, t^+)$, we have

$$\begin{aligned} -[F(U(t))^\nu]' &= -U'(t) \cdot \nabla F(U(t)) F(U(t))^{\nu-1} \\ &= \|U'(t)\| \|\nabla F(U(t))\| F(U(t))^{\nu-1} \\ &\geq \gamma^{-1} \|U'(t)\|, \end{aligned}$$

so

$$F(U(t_n))^\nu - F(U(t))^\nu \geq \gamma^{-1} \int_{t_n}^{t} \|U'(s)\| ds.$$

Thus $\|U(t) - U(t_n)\| < \sigma/2$, $\forall t \in [t_n, t^+)$ and so $t^+ = +\infty$. QED.

This proof extends to many situations:

- For any other scalar product on $\mathbf{R}^d$:

$$AU'(t) = -\nabla F(U(t)),$$

  where A is positive definite (symmetric or not).
- Generalizations in infinite dimension (Simon, Jendoubi, Haraux, Chill,. . .)
  - Semilinear heat equation:

$$u_t = \Delta u - f(u), \quad t \geq 0, \ x \in \Omega.$$

  - Cahn-Hilliard equation: forth order in space (Hoffman, Rybka, Chill, Jendoubi)
  - Cahn-Hilliard equation with dynamic boundary conditions (Wu, Zheng, Chill, Fasangova, Pruss)
  - Cahn-Hilliard-Gurtin equations (Miranville and Rougirel): gradient-like flow

NB: 160 citations for the paper of Simon (most cited paper)
50 citations for the paper of Jendoubi'98 (most cited paper)

- Generalization to second-order gradient-like flows:

$$\epsilon U''(t) + U'(t) = -\nabla F(U(t)), \quad t \geq 0,$$

  where $\epsilon > 0$: Haraux and Jendoubi'98
- Damped wave equation

$$\epsilon u_{tt} + u_t = \Delta u - f(u), \quad t \geq 0, \; x \in \Omega.$$

  Haraux, Jendoubi, Chill,...
- Cahn-Hilliard equation with inertial term (Grasselli, Schimperna, Zelig, Miranville, Bonfoh)
- (optimal) convergence rates for 1st and 2nd order

Questions:

- If we consider some **time discretizations** of the equations above, can we obtain similar results of convergence to equilibrium ?
- In particular, what happens for the **backward Euler scheme** ?
- What **restriction on the time step** do we have ?

The **backward Euler scheme** reads: let $U^0 \in \mathbf{R}^d$, and for $n \geq 0$, let U^{n+1} solve

$$\frac{U^{n+1} - U^n}{\Delta t} = -\nabla F(U^{n+1}), \tag{3}$$

where $\Delta t > 0$ is fixed and $F \in C^1(\mathbf{R}^d, \mathbf{R})$. Since existence is not obvious, we rewrite (3) in the form:

$$U^{n+1} \in \operatorname{argmin} \left\{ \frac{\|V - U^n\|^2}{2\Delta t} + F(V) \ : \ V \in \mathbf{R}^d \right\}. \tag{4}$$

In optimization, (4) is known as the **proximal algorithm**.
In particular, U^{n+1} satisfies

$$F(U^{n+1}) + \frac{1}{2\Delta t}\|U^{n+1} - U^n\|^2 \leq F(U^n).$$

By induction, any sequence defined by (4) satisfies

$$F(U^n) + \frac{1}{2\Delta t} \sum_{k=0}^{n-1} \|U^{k+1} - U^k\|^2 \leq F(U^0), \quad \forall n \geq 0 \qquad (5)$$

This is a **Liapounov stability** result.
By (5), it is easy to prove that if $(U^n)_{n \in \mathbf{N}}$ is a bounded sequence defined by the proximal algorithm (4), then

$$\omega(U^0) := \left\{ U^\star \in \mathbf{R}^d \ : \ \exists n_k \to +\infty, \ U^{n_k} \to U^\star \right\}$$

is a non-empty compact connected subset of $\mathcal{S}$. Moreover, $d(U^n, \omega(U^0)) \to 0$ as $n \to +\infty$.

Question : does $U^n \to U^\star$ as $n \to +\infty$?

Some answers

- if $d = 1$ or if $\mathcal{S}$ is discrete, yes (use that $\omega(U^0)$ is connected)
- If $d \geq 2$, numerical simulations on the "Mexican hat" function idicate that convergence to equilibrium is not true in general.

Theorem (B.Merlet and M.P.'10)

Assume that $F : \mathbf{R}^d \to \mathbf{R}$ *is real analytic and that*

$$F(V) \to +\infty \text{ as } \|V\| \to +\infty. \tag{6}$$

Let $(U^n)_n$ *be a sequence defined by the proximal algorithm* (4)*.*
There exist $U^\infty \in \mathcal{S}$ *s.t.* $U^n \to U^\infty$ *as* $n \to +\infty$*.*

Remark: A more general version by **Attouch and Bolte'09**:

- variable stepsize $0 < \Delta t_\star \leq \Delta t_n \leq \Delta t^\star < +\infty$
- $F : \mathbf{R}^d \to \mathbf{R}$ real analytic replaced by $F : dom(F) \subset \mathbf{R}^d \to \mathbf{R}$ continuous and satisfies a Lojasiewicz property
- (6) replaced by $\inf F > -\infty$ and $(U^n)_n$ bounded.

A proof

Energy estimate

$$\frac{\|U^{n+1}-U^n\|^2}{2\Delta t}+F(U^{n+1})\le F(U^n),\quad \forall n\ge 0. \tag{7}$$

We can find a subsequence $(U^{n_k})_k$ s.t. $U^{n_k}\to U^\infty\in\mathcal{S}$. Recall the Lojasiewicz inequality (with $F(U^\infty)=0$):

$$\forall V\in\mathbf{R}^d,\quad \|V-U^\infty\|<\sigma\Rightarrow |F(V)|^{1-\nu}\le\gamma\|\nabla F(V)\|. \tag{8}$$

Let n s.t. $\|U^{n+1}-U^\infty\|<\sigma$. We have two cases

- **Case 1:** $F(U^{n+1})>F(U^n)/2$**.** Then,

$$\begin{aligned} F(U^n)^\nu-F(U^{n+1})^\nu &= \int_{F(U^{n+1})}^{F(U^n)}\nu x^{\nu-1}dx \\ &\ge \int_{F(U^{n+1})}^{F(U^n)}\nu\left(F(U^n)\right)^{\nu-1}dx \\ &\ge 2^{\nu-1}\nu\left(F(U^{n+1})\right)^{\nu-1}[F(U^n)-F(U^{n+1})]. \end{aligned}$$

$$[F(U^n)]^\nu - [F(U^{n+1})]^\nu \overset{(7)}{\geq} 2^{\nu-2}\nu \frac{\|U^{n+1}-U^n\|^2}{\Delta t[F(U^{n+1})]^{1-\nu}}$$

$$\overset{(3)}{\geq} 2^{\nu-2}\nu\|U^{n+1}-U^n\| \frac{\|\nabla F(U^{n+1})\|}{[F(U^{n+1})]^{1-\nu}} \overset{(8)}{\geq} \frac{2^{\nu-2}\nu}{\gamma}\|U^{n+1}-U^n\|.$$

- **Case 2:** $F(U^{n+1}) \leq F(U^n)/2$. Then

$$\|U^{n+1}-U^n\| \overset{(7)}{\leq} \sqrt{2\Delta t}[F(U^n)-F(U^{n+1})]^{1/2} \leq \sqrt{2\Delta t}[F(U^n)]^{1/2}$$

$$\overset{\text{cas } 2}{\leq} \left(1-\frac{1}{\sqrt{2}}\right)^{-1} \sqrt{2\Delta t} \left([F(U^n)]^{1/2} - [F(U^{n+1})]^{1/2}\right).$$

In both cases, for all n s.t. $\|U^{n+1}-U^\infty\| < \sigma$, we have

$$\|U^{n+1}-U^n\| \leq \frac{2^{2-\nu}\gamma}{\nu}\left([F(U^n)]^\nu - [F(U^{n+1})]^\nu\right) + 5\sqrt{\Delta t}\left([F(U^n)]^{1/2} - [F(U^{n+1})]^{1/2}\right). \quad (9)$$

From this we deduce that $\sum_{n=0}^{+\infty} \|U^{n+1}-U^n\| < +\infty$.

Corollary (B. Merlet et M.P.)

Let U^∞ s.t. $U(t) \to U^\infty$. Assume that U^∞ is a local minimizer of F, i.e.

$$\exists \rho > 0, \quad \forall V \in \mathbf{R}^N, \ \|V - U^\infty\| < \rho \Rightarrow \quad F(V) \geq F(U^\infty).$$

Let $(U^n_{\Delta t})_n$ be the sequence defined by the backward Euler scheme (which is unique for $\Delta t > 0$ small enough), and let $U^\infty_{\Delta t} := \lim_{n\to+\infty} U^n_{\Delta t}$. Then $U^\infty_{\Delta t} \to U^\infty$, as $\Delta t \to 0$ and $U^0_{\Delta t} \to U_0$.

NB: this is a Liapounov stability result

Applications

- Applies to any other scalar product on $\mathbf{R}^d$:

$$AU'(t) = -\nabla F(U(t)),$$

where A is positive definite (symmetric or not).

  - FD or FE space discrete versions of the Allen-Cahn equation, Cahn-Hilliard equation (Merlet and P.'10), Cahn-Hilliard equation with dynamic boundary conditions (Cherfils, Petcu, P.'10)
  - FE space discrete version of the Cahn-Hilliard-Gurtin equation (Injrou and P.)

- Generalizations in infinite dimension to the semilinear heat equation (Merlet and P.'10)
- Abstract version of the semilinear heat equation in infinite dimension (Attouch, Daniildis, Ley, Mazet'09)

Extension to second-order gradient-like systems case

- Finite dimension : ok
- The damped wave equation as a model problem : ok
- Space discrete version of the Cahn-Hilliard equation with inertial term (ongoin work with M. Grasselli)

$$\epsilon u_{tt} + u_t = -\alpha\Delta^2 u + \Delta f(u).$$

The **mass is no longer preserved**, but it converges exponentially fast to a constant: adapt results of Chill and Jendoubi with vanishing source term.

Perspectives and questions

- Find an abstract version of the damped wave equation ?
- Adapt other results from the continuous case ?
- Find other Liapounov stable schemes ? (implicit schemes, most likely)

An example: the θ-scheme

For $\theta \in [1/2, 1]$, the θ-scheme reads:

$$\frac{U^{n+1} - U^n}{\Delta t} = -\theta \nabla F(U^{n+1}) - (1-\theta)\nabla F(U^n). \qquad (10)$$

Assume that F satisfies

$$(\nabla F(U) - \nabla F(V)\,,\, U - V) \geq -c_F \|U - V\|^2, \qquad \forall U, V \in \mathbf{R}^d, \qquad (11)$$

for some $c_F \geq 0$ (i.e., F is **semiconvex**).

Theorem (Liapounov stability, Stuart and Humphries'94)

If $\theta \in [1/2, 1]$, $\Delta t < 2/c_F$ and $F(V) \to +\infty$ as $\|V\| \to +\infty$, then for all $n \geq 0$,

$$F_{\Delta t}(U^{n+1}) + \left(1 - \frac{c_F \Delta t}{2}\right) \frac{\|U^{n+1} - U^n\|^2}{\Delta t} \leq F_{\Delta t}(U^n),$$

where

$$F_{\Delta t}(V) = F(V) + \frac{(1-\theta)\Delta t}{2} \|\nabla F(V)\|^2.$$

By applying a proof similar to the previous one to the Liapounov function $F_{\Delta t}$, we obtain convergence to equilibrium **if Δt is small enough**. For a discretization of the Allen-Cahn equation, the smallness assumption is

$$\Delta t \leq Ch^2. \tag{12}$$

On the other hand, Liapounov stability holds if $\Delta t < 2/c_F$:
Can (12) be improved ?

Some additional references

- Huang (Sen-Zhong), "Gradient Inequalities", AMS'06
- Attouch, Bolte, Redont, Soubeyran'08: *Alternating minimization...*
- Absil, Mahony and Andrews'05: *Convergence of iterates of descent methods for analytic cost functions*
- Gajewski and Griepentrog'06 : *A descent method for the free energy of multicomponent systems*