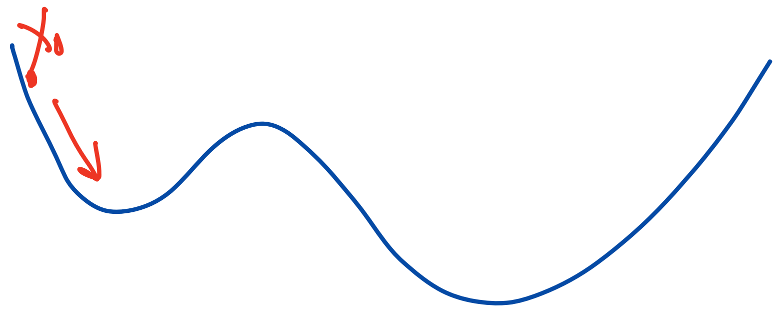
Supplement

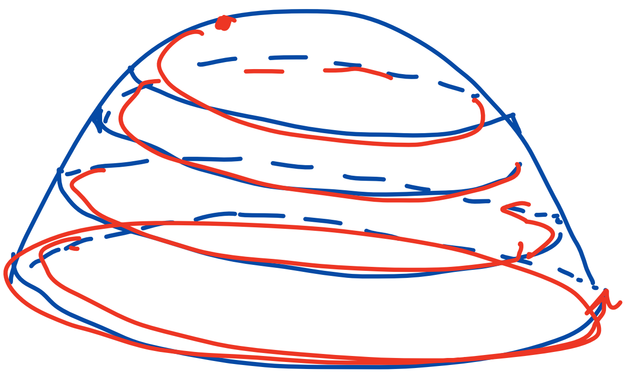
Consider $\min_{x} E(x)$

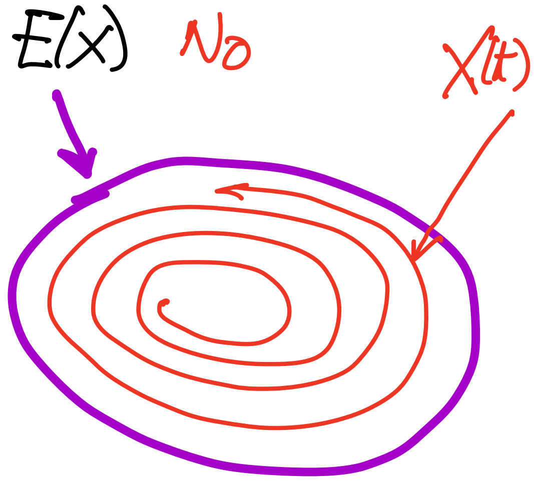
$$\dot{x} = -\nabla E(x)$$

① $E(x(t)) \longrightarrow \min_{x} E(x)$ No (local min)



② $x(t) \longrightarrow x_* \in \arg\min_{x} E(x)$ No





Even if ① and ② are true, how fast is the convergence (according to $\dot{x} = -\nabla E(x)$) ?

Convergence rate?

When E is strongly convex, $D^2E(x) \geq \lambda I$

$\Rightarrow$ exponential convergence with rate λ

eg. $\quad E(x) = \frac{1}{2}\langle Ax, x\rangle \qquad \overset{(\text{sym})}{A} \geq \lambda I$

$$\dot{x} = -\nabla E(x) = -Ax$$

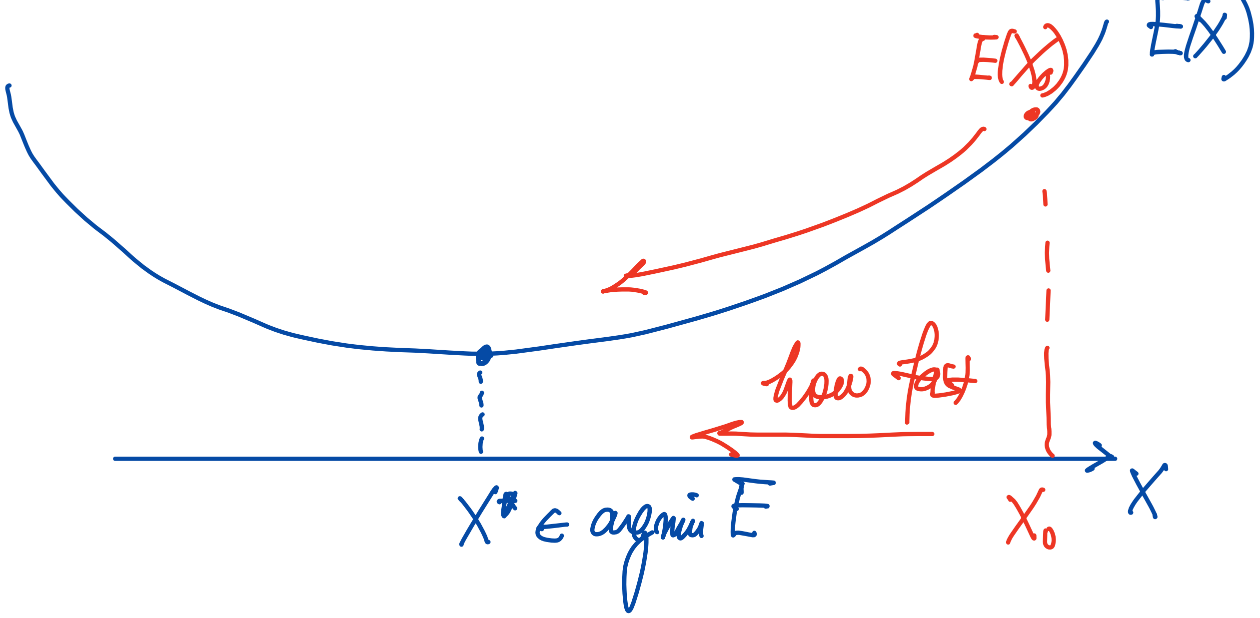
$$\frac{d}{dt}\left(\frac{1}{2}\|x(t)\|^2\right) = \langle x, \dot{x}\rangle = -\langle x, Ax\rangle \leq -\lambda\|x\|^2$$

$$\frac{d}{dt}\|x(t)\|^2 \leq -2\lambda\|x(t)\|^2$$

$$\Longrightarrow \quad \|x(t)\|^2 \leq \|x(0)\|^2 e^{-2\lambda t}$$

$$\Longrightarrow \quad \|x(t)\| \leq \|x(0)\| e^{-\lambda t}$$

What if E is just convex?



$$\boxed{E(X(t)) - \min E \leq \frac{\|X_0 - X_*\|^2}{2t} \sim O\left(\frac{1}{t}\right)}$$

dim independent

<u>Proof</u> Introduce a "new functional"

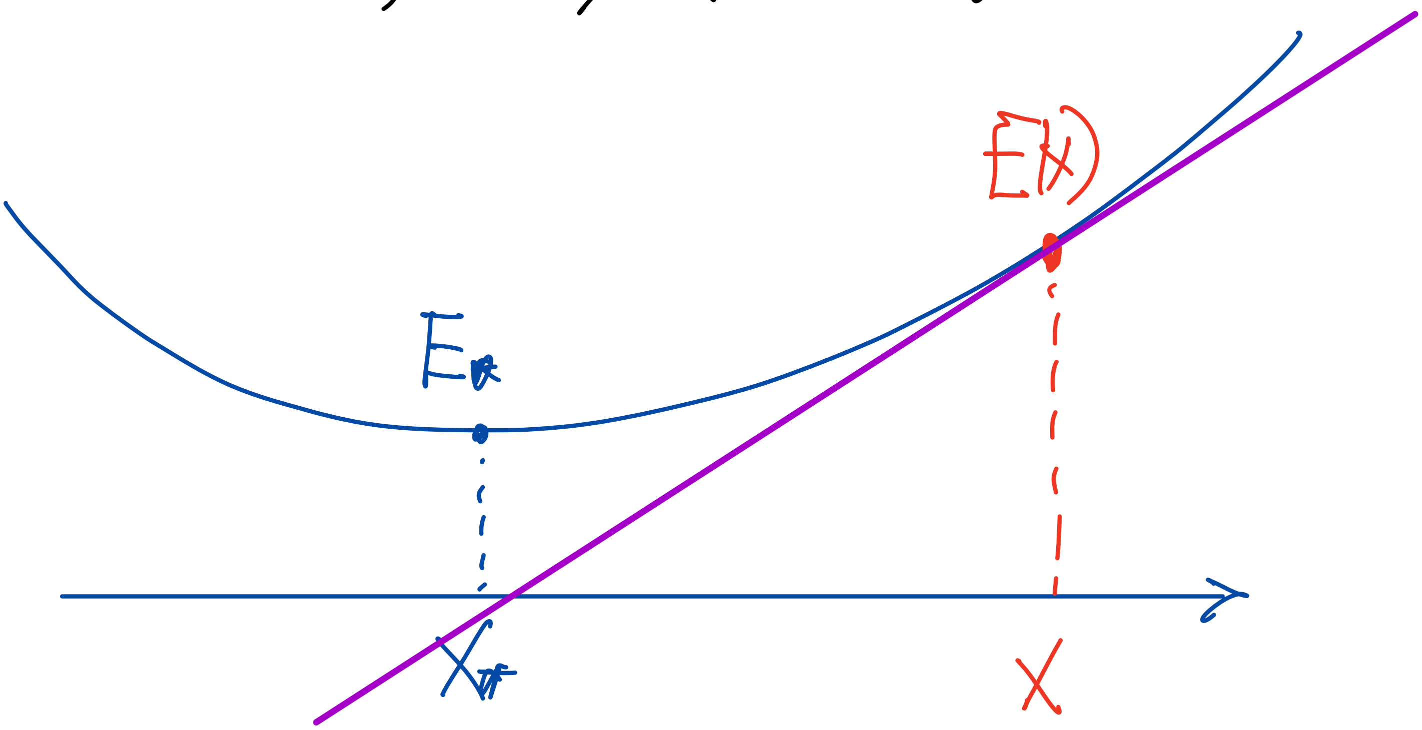
min E

$$F(X(t)) = \frac{\|X(t) - X_*\|^2}{2} + t\left(E(X(t)) - E_*\right)$$

$$\frac{d}{dt} F(X(t))$$

$$= \langle X(t) - X_*, \dot{X} \rangle + \left(E(X(t)) - E_*\right) + t \langle \nabla E(X(t)), \dot{X} \rangle$$

$$= -\langle X(t) - X_*, \nabla E(X) \rangle + \left(E(X) - E_*\right) - t \|\nabla E(X)\|^2$$



$$E_* \geq E(X) + \langle \nabla E(X), X_* - X \rangle$$

$$\frac{d}{dt}\mathcal{F}(X(t))$$

$$= \langle X(t) - X_*, \dot{X} \rangle + (E(X(t)) - E_*) + t\langle \nabla E(X(t)), \dot{X} \rangle$$

$$= -\langle X(t) - X_*, \nabla E(X) \rangle + (E(X) - E_*) - t\|\nabla E(X)\|^2$$

$$\leq 0 \; !$$

$$\Rightarrow \quad \mathcal{F}(X(t)) \leq \mathcal{F}(X(0))$$

$$\frac{\|X(t) - X_*\|^2}{2} + t(E(X(t)) - E_*) \leq \frac{\|X(0) - X_*\|^2}{2}$$

$$\|X(t) - X_*\|^2 \leq \|X(0) - X_*\|^2$$

$$\boxed{E(X(t)) - E_* \leq \frac{\|X(t) - X_*\|^2}{2t}}$$

Nesterov Accelerated Gradient Descent

$$\underbrace{\ddot{X}}_{\text{acc}} = -\underbrace{\frac{3}{t}\dot{X}}_{\text{friction}} - \underbrace{\nabla E(X)}_{\text{force}}$$

$$\boxed{E(X(t)) - E_* \le \frac{2\|X(0) - X_*\|^2}{t^2} \sim O\left(\frac{1}{t^2}\right)}$$

Introduce a "new functional"

$$F(X) = t^2\left(E(X) - E_*\right) + 2\left\|X - X_* + \frac{t\dot{X}}{2}\right\|^2$$

$$\frac{d}{dt}F(X(t))$$

$$= 2t\left(E(X) - E_*\right) + t^2\langle \nabla E(X), \dot{X}\rangle$$

$$+ 4\left\langle X - X_* + \frac{t\dot{X}}{2},\ \underbrace{\dot{X} + \frac{\dot{X}}{2} + \frac{t\ddot{X}}{2}}_{\frac{t\ddot{X}}{2} + \frac{3\dot{X}}{2} = -\frac{t\nabla E(X)}{2}}\right\rangle$$

$$= 2t\left(E(x) - E_*\right) + \underbrace{t^2\langle \nabla E(x), \dot{x}\rangle}$$

$$+ 4\left\langle x - x_* + \underbrace{\frac{t\dot{x}}{2}, \; -\frac{t\nabla E(x)}{2}}\right\rangle$$

$$= 2t\left(E(x) - E_*\right) - 2t\langle x - x_*, \nabla E(x)\rangle$$

$$= 2t\left(E(x) - E_* - \langle x - x_*, \nabla E(x)\rangle\right)$$

$$\leq 0$$

$$F(x(t)) \leq F(x(0))$$

$$t^2\left(E(x) - E_*\right) + 2\left\| x - x_* + \frac{t\dot{x}}{2}\right\|^2 \leq 2\|x_0 - x_*\|^2$$

$$\boxed{E(x(t)) - E_* \leq \frac{2\|x_0 - x_*\|^2}{t^2}}$$

How can AI Help Mathematicians?

Amaury Hayat
CERMICS - Ecole des Ponts - Institut Polytechnique de Paris
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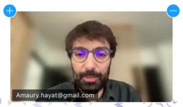
CMAI Colloquium
–
January 22nd 2025



Stability of Dynamical Systems

Today, more than a hundred years later, it is still an open question:

there is still no systematic way to construct a Lyapunov function.

$\rightarrow$ We resort to intuition

Can we train an AI to have better mathematical intuition than us?

$$\dot{x}(t) = \begin{pmatrix} -6x_1^4(t)x_2^5(t) - 3x_1^7(t)x_3^2(t) \\ 3x_1^9(t) - 6x_1^2(t)x_2^5(t)x_3^2(t) \\ -4x_1^2(t)x_3^5(t) \end{pmatrix} \quad \rightarrow \quad \text{Yes, } V(x) = x_1^6 + 2(x_2^6 + x_3^4)$$

Stability of Dynamical Systems

Train an AI to have an intuition of Lyapunov functions

Global Lyapunov functions: a long-standing open problem in mathematics, with symbolic transformers (NeurIPS, Alfarano, Charton, A.H., 2024)

Neural network architecture: Transformer ($\sim$1000 smaller than GPT-3)

Procedure:

1. Generate a set of systems and associated Lyapunov functions.
2. Encode the examples
3. Train the language model (supervised learning)

Heat Equation

$$\frac{\partial u}{\partial t} = \Delta u \quad (= \operatorname{div} \nabla u)$$

$$u(x,0) = u_0(x)$$

$$\frac{d}{dt} \int \frac{1}{2} u^2 \, dx = \int u u_t = \int u \Delta u \, dx$$

$$= - \int |\nabla u|^2 \, dx$$

Suppose $\int u^2 \, dx \leq \frac{1}{\lambda} \int |\nabla u|^2 \, dx$

(Sobolev Type Inequality)

Then $\frac{d}{dt} \int \frac{1}{2} u^2 \, dx \leq -\lambda \int u^2 \, dx$

$$\Rightarrow \int u^2(x,t) \, dx \leq \left(\int u(x,0)^2 \, dx \right) e^{-2\lambda t}$$

i.e. $\|u(\cdot,t)\|_{L^2} \leq \|u(x,0)\| e^{-\lambda t}$

Other versions using heat kernel:

$$u(x,t) = \int u(y,0) \frac{e^{-\frac{|x-y|^2}{2t}}}{t^{n/2}} \, dy$$

1. $$|u(x,t)| \lesssim \|u(\cdot,0)\|_{L^\infty} \int \frac{e^{-\frac{|x-y|^2}{2t}}}{t^{n/2}} \, dy$$

$$= \|u(\cdot,0)\|_\infty$$

$$\|u(\cdot,t)\|_{L^\infty} \leq \|u(\cdot,0)\|_{L^\infty}$$

2. $$|u(x,t)| \lesssim \|u(\cdot,0)\|_{L^1} \left\| \frac{e^{-\frac{|x-y|^2}{2t}}}{t^{n/2}} \right\|_{L^\infty}$$

$$\lesssim \frac{1}{t^{n/2}} \|u(\cdot,0)\|_{L^1} \longrightarrow 0$$

(. . . . . . . many other versions . . . .)

Heat equation as a gradient flow in the space of probability measures:

$$u_t = \Delta u = \operatorname{div} \nabla u = \operatorname{div}\left(u \frac{\nabla u}{u}\right)$$

$$= \operatorname{div}\left(u \nabla \underbrace{\log u}\right) \quad \delta\Big(\underbrace{\int u \log u \, dx}_{\text{Entropy functional}}\Big)$$

$$\operatorname{Ent}(u(\cdot, t)) = \int u \log u \, dx$$

$$\frac{d}{dt} \operatorname{Ent}(u(\cdot, t)) = \int (u_t \log u + u_t) \, dx$$

$$= \int \operatorname{div}(u \nabla \log u) \log u \, dx$$

$$+ \cancel{\int \operatorname{div}(u \nabla \log u) \, dx}$$

$$= - \int u |\nabla \log u|^2 \, dx$$

$$= - \int \frac{|\nabla u|^2}{u} \, dx$$

$$\boxed{\text{"Suppose"} \quad \int u \log u \, dx \leq \frac{1}{\lambda} \int \frac{|\nabla u|^2}{u} dx}$$

Log-Sobolev Inequality

Then $\frac{d}{dt} \operatorname{Ent}(u(\cdot, t)) \leq -\lambda \operatorname{Ent}(u(\cdot, t))$

$$\operatorname{Ent}(u(\cdot, t)) \leq \operatorname{Ent}(u(\cdot, 0)) e^{-\lambda t}$$

Relative Entropy / Kullback-Leibler Divergence

$$\left.\begin{matrix}\operatorname{Ent}(\rho \| \pi), \\ KL(\rho \| \pi)\end{matrix}\right\} = \int \rho \log \frac{\rho}{\pi} \, dx = \begin{cases} \geq 0 \\ = 0 \iff \rho = \pi \end{cases}$$

Suppose $\pi(x) = e^{-U(x)}$, Gibbs measure

Consider $\rho_t = \Delta \rho + \nabla \cdot (\rho \nabla U)$

$$= \nabla \cdot (\nabla \rho + \rho \nabla U)$$

Fokker-Planck Equation

$$= \nabla \cdot \rho \left(\frac{\nabla \rho}{\rho} + \nabla U \right)$$

$$= \nabla \cdot \left[\rho \nabla \big(\underbrace{\log \rho + U}_{\delta \int (\rho \log \rho + \rho U)\, dx} \big) \right]$$

$$= \nabla \cdot \left[\rho \nabla (\log \rho - \log \pi) \right]$$

$$= \nabla \cdot \left[\rho \nabla \log \left(\frac{\rho}{\pi} \right) \right]$$

$$Ent(\rho \| \pi) = \int \rho \log \frac{\rho}{\pi} \, dx$$

$$\frac{d}{dt} Ent(\rho \| \pi)$$

$$\cancel{= \int \nabla \cdot \left[\rho \nabla \log \frac{\rho}{\pi} \right] dx} = 0$$

$$= \int \rho_t \log \frac{\rho}{\pi} \, dx + \int \rho \cancel{\frac{1}{\frac{\rho}{\pi}} \frac{1}{\pi}} \rho_t \, dx$$

$$= \int \nabla \cdot \rho \left[\nabla \log \frac{\rho}{\pi} \right] \log \frac{\rho}{\pi} \, dx$$

$$= - \int \rho \left| \nabla \log \frac{\rho}{\pi} \right|^2 dx$$

$$\boxed{\text{Suppose} \quad \int \rho \log \frac{\rho}{\pi}\, dx \leq \frac{1}{\lambda} \int \rho \left| \nabla \log \frac{\rho}{\pi} \right|^2 dx}$$

$$\Updownarrow \quad f = \frac{\rho}{\pi}$$

$$\int f (\log f) \pi \, dx \leq \frac{1}{\lambda} \int f \left| \nabla \log f \right|^2 \pi \, dx$$

$$= \frac{1}{\lambda} \int \frac{|\nabla f|^2}{f} \pi \, dx$$

$$\boxed{\int f (\log f) \pi \, dx \leq \frac{1}{\lambda} \int \frac{|\nabla f|^2}{f} \pi \, dx}$$

π satisfies Log-Sobolev Ineq.

Then

$$\frac{d}{dt} \mathrm{Ent}(\rho | \pi) \leq -\lambda \, \mathrm{Ent}(\rho | \pi)$$

$$\Rightarrow \quad \boxed{\mathrm{Ent}(\rho(t) | \pi) \leq \mathrm{Ent}(\rho(0) | \pi)\, e^{-\lambda t}}$$