Gradient Flow. Accelerated gradient flow.

Daniil Merkulov

Optimization methods. MIPT

Gradient Flow

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- Antigradient $-\nabla f(x)$ indicates the direction of steepest descent at the point x.

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$\alpha_k \to 0$ $\qquad \frac{dx}{dt}$

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$\nabla f(x) = Ax$; $\frac{dx(t)}{dt} = -Ax(t)$; $x(0) = x_0$, $x(t) = ?$; $x(\tau) = ?$; $x(t) = e^{-At} \cdot x(0)$; $\frac{dx}{dt} = e^{-At} \cdot x(0) \cdot (-A)$; $f(x) \to \min_{x \in \mathbb{R}^n}$; $n \times 1$, $n \times 1$; дифф. ур-ие градиентного потока

Gradient Flow

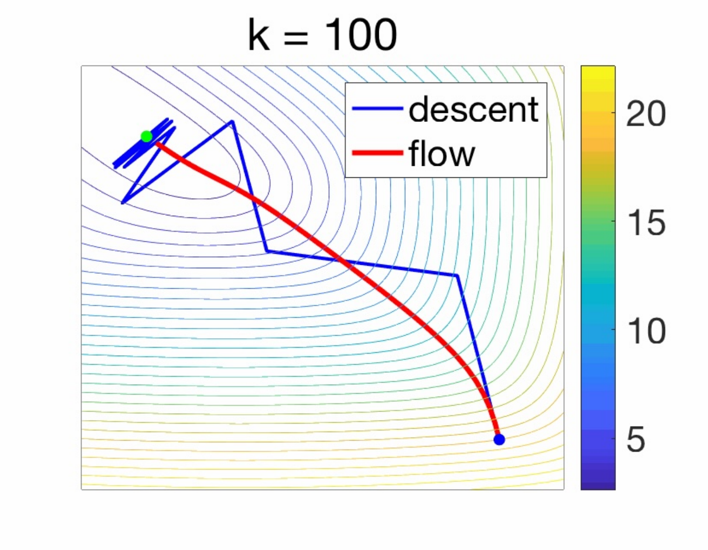

Рис. 1: Source

- **Simplified analyses.** The gradient flow has no step-size, so all the traditional annoying issues regarding the choice of step-size, with line-search, constant, decreasing or with a weird schedule are unnecessary.

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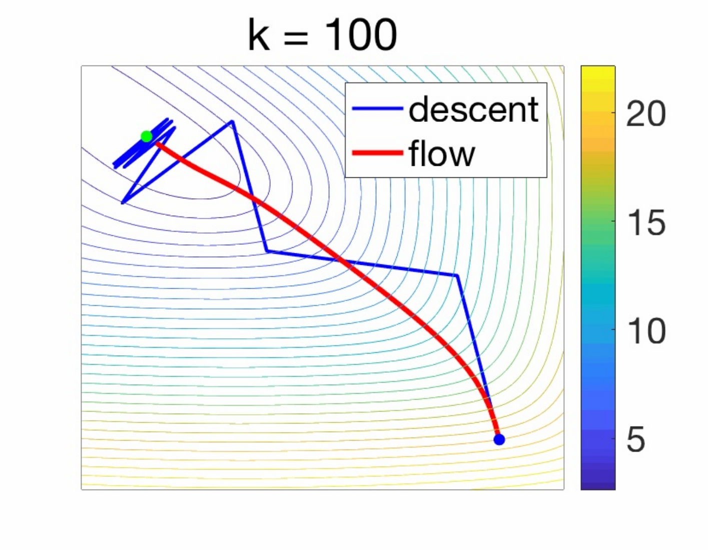

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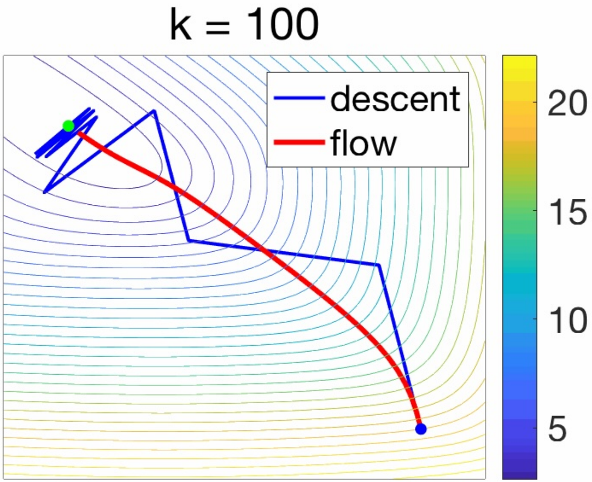

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- **Analytical solution in some cases.** For example, one can consider quadratic problem with linear gradient, which will form a linear ODE with known exact formula.
- **Different discretization leads to different methods.** We will see, that the continuous-time object is pretty rich in terms of the variety of produced algorithms. Therefore, it is interesting to study optimization from this perspective.

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Consider Gradient Flow ODE:

$$\frac{dx}{dt} = -\nabla f(x)$$

Explicit Euler discretization:

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$$\boxed{x_{k+1} = \text{prox}_{\alpha f}(x_k)} \qquad \text{(PPM)}$$

PROXIMAL POINT METHOD

$f(x) + r(x) \to \min_{x \in \mathbb{R}^n}$

PGD $\quad x_{k+1} = \text{PROX}_{\alpha r}(x_k - \alpha \nabla f(x_k))$

Convergence analysis. Convex case.

1. Simplest proof of monotonic decrease of GF:

$$\frac{d}{dt}f(x(t)) = \nabla f(x(t))^\top \frac{dx(t)}{dt} = -\|\nabla f(x(t))\|_2^2 \leqslant 0.$$

$\frac{dx(t)}{dt} = -\nabla f(x(t))$

If f is bounded from below, then $f(x(t))$ will always converge as a non-increasing function which is bounded from below. It is straightforward, that GF converges to the stationary point, where $\nabla f = 0$ (potentailly including minima, maxima and saddle points).

Для ур-ия GF $f(x)$ является функцией Ляпунова

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$$f(x) \geqslant f(y) + \nabla f(y)^\top (x - y) \qquad \Rightarrow \qquad \nabla f(y)^\top (x - y) \leqslant f(x) - f(y)$$

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3. Finally, using convexity:

$$\frac{d}{dt}\left[\|x(t) - x^*\|^2\right] = -2(x(t) - x^*)^\top \nabla f(x(t)) \leqslant -2\left[f(x(t)) - f^*\right]$$

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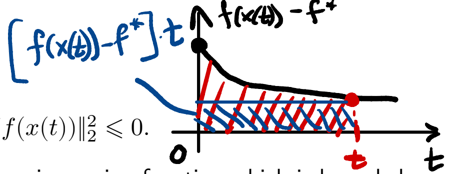

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4. Leading to, by integrating from 0 to t, and using the monotonicity of $f(x(t))$:

$$\boxed{f(x(t)) - f^*} \leqslant \frac{1}{t}\int_0^t [f(x(u)) - f^*]du \leqslant \frac{1}{2t}\|x(0)-x^*\|^2 - \frac{1}{2t}\|x(t)-x^*\|^2 \leqslant \frac{1}{2t}\|x(0)-x^*\|^2. \leq \frac{R^2}{2t}$$

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   We recover the usual rates in $\mathcal{O}\left(\frac{1}{k}\right)$, with $t = \alpha k$.

Convergence analysis. PL case.

1. The analsysis is straightforward. Suppose, the function satisfies PL-condition:

$$\|\nabla f(x)\|^2 \geq 2\mu(f(x) - f^*) \quad \forall x$$

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$$f(x(t)) - f(x^*) = \Psi \qquad \frac{dx}{dt} \leqslant -2\mu x$$

$$\frac{d\Psi}{dt} \leqslant -2\mu\Psi$$

$$\Psi(t) \leqslant \Psi(0) \cdot e^{-2\mu t}$$

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3. Finally,

$$\boxed{f(x(t)) - f^* \leqslant \exp(-2\mu t)[f(x(0)) - f^*],}$$

Accelerated Gradient Flow

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Remember one of the forms of Nesterov Accelerated Gradient

$$
\begin{cases}
x_{k+1} = y_k - \alpha \nabla f(y_k) \\
y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})
\end{cases}
$$

$\sim \frac{1}{k^2}$ $\sqrt{\varkappa} \cdot \log \frac{1}{\varepsilon}$

The corresponding [1] ODE is:

$$
\ddot{X}_t + \frac{3}{t}\dot{X}_t + \nabla f(X_t) = 0
$$

[1] A Differential Equation for Modeling Nesterov's Accelerated Gradient Method: Theory and Insights, Weijie Su, Stephen Boyd, Emmanuel J. Candes

Accelerated Gradient Flow

Define the energy

$$E(t) = t^2\big(f(X(t)) - f^*\big) + 2\Big\|X(t) - x^* + \tfrac{t}{2}\dot{X}(t)\Big\|^2.$$

A direct differentiation using the ODE yields $\dot{E}(t) \leq 0$ for all $t > 0$; hence $E(t)$ is non-increasing. Because the second term is non-negative we obtain the convergence theorem

$$\boxed{f(X(t)) - f^* \;\leq\; \frac{2\left\|x_0 - x^*\right\|^2}{t^2}}. \tag{AGF-rate}$$

Thus AGF enjoys the same $\mathcal{O}(1/t^2)$ rate that discrete NAG achieves in $\mathcal{O}(1/k^2)$ iterations. A similar argument with a restarted ODE gives an exponential rate for μ-strongly convex f.

Stochastic Gradient Flow

Stochastic Gradient Flow

стох градиент

How to model stochasticity in the continuous process? A simple idea would be: $\frac{dx}{dt} = -\nabla f(x) + \xi$ with variety of options for ξ, for example $\xi \sim \mathcal{N}(0, \sigma^2) \sim \sigma^2 \mathcal{N}(0, 1)$.

Therefore, one can write down Stochastic Differential Equation (SDE) for analysis:

стох. диф. ур-ие

$$dx(t) = -\nabla f\left(x(t)\right) dt + \sigma dW(t)$$

Here $W(t)$ is called Wiener process. It is interesting, that one could analyze the convergence of the stochastic process above in two possible ways:

случ. блужд, диффузия, броуновское движ.

- Watching the trajectories of $x(t)$

Эйлер - Маруяма

Stochastic Gradient Flow

How to model stochasticity in the continuous process? A simple idea would be: $\frac{dx}{dt} = -\nabla f(x) + \xi$ with variety of options for ξ, for example $\xi \sim \mathcal{N}(0, \sigma^2) \sim \sigma^2 \mathcal{N}(0, 1)$.

Therefore, one can write down Stochastic Differential Equation (SDE) for analysis:

$$dx(t) = -\nabla f\left(x(t)\right) dt + \sigma dW(t)$$

Here $W(t)$ is called Wiener process. It is interesting, that one could analyze the convergence of the stochastic process above in two possible ways:

- Watching the trajectories of $x(t)$
- Watching the evolution of distribution density function of $\rho(t)$

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! Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \nabla \left(\rho(t) \nabla f\right) + \frac{\sigma^2}{2} \Delta \rho(t)$$

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- Understanding Optimization in Deep Learning with Central Flows