



Gradient Flow. Accelerated gradient flow.

Daniil Merkulov

Optimization methods. MIPT

Gradient Flow

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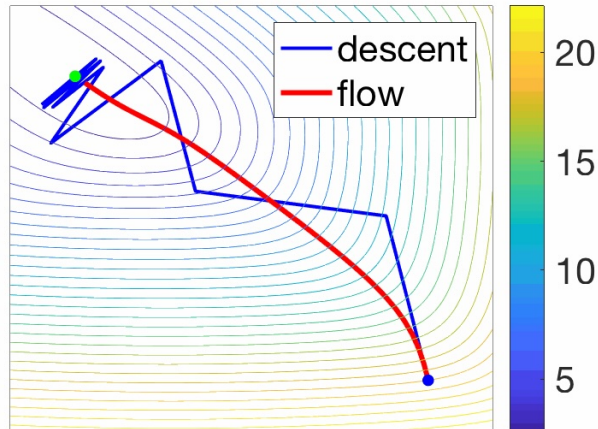
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$k = 100$

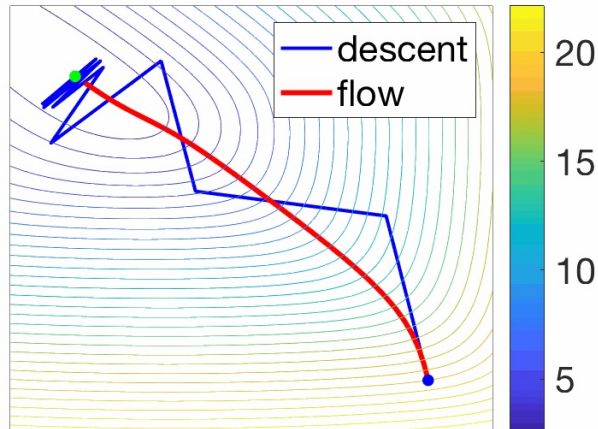


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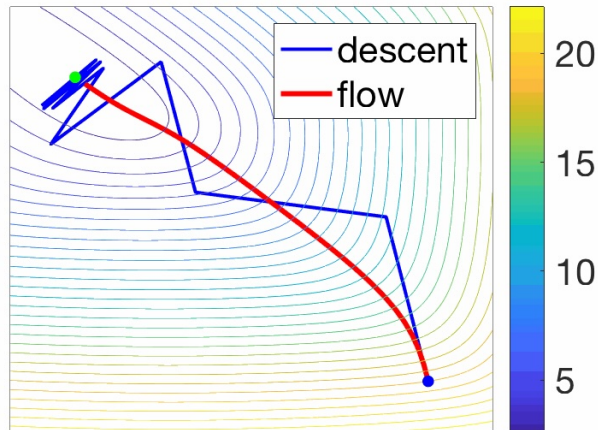


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- **Analytical solution in some cases.** For example, one can consider quadratic problem with linear gradient, which will form a linear ODE with known exact formula.
- **Different discretization leads to different methods.** We will see, that the continuous-time 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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Explicit Euler discretization:

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$$\begin{aligned} \frac{x_{k+1} - x_k}{\alpha} &= -\nabla f(x_{k+1}) \\ \frac{x_{k+1} - x_k}{\alpha} + \nabla f(x_{k+1}) &= 0 \end{aligned}$$

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(PPM)

Convergence analysis. Convex case.

1. Simplest proof of monotonic decrease of GF:

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

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 $\nabla f = 0$ (potentially including minima, maxima and saddle points).

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

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

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3. Finally,

$$f(x(t)) - f^* \leq \exp(-2\mu t)[f(x(0)) - f^*],$$

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Remember one of the forms of Nesterov Accelerated Gradient

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

The corresponding ¹ ODE is:

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

¹A 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*

$$E(t) = t^2(f(X(t)) - f^*) + 2\left\|X(t) - x^* + \frac{t}{2}\dot{X}(t)\right\|^2.$$

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*

$$\boxed{f(X(t)) - f^* \leq \frac{2\|x_0 - x^*\|^2}{t^2}}. \quad (\text{AGF-rate})$$

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

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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:

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

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 $x(t)$

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! Fokker-Planck equation

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

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- NAG-GS: Semi-Implicit, Accelerated and Robust Stochastic Optimizer
- Introduction to Gradient Flows in the 2-Wasserstein Space
- Stochastic Modified Equations and Dynamics of Stochastic Gradient Algorithms I: Mathematical Foundations
- Understanding Optimization in Deep Learning with Central Flows