

Gradient Flow. Accelerated gradient flow.

Daniil Merkulov

Optimization methods. MIPT

Gradient Flow intuition

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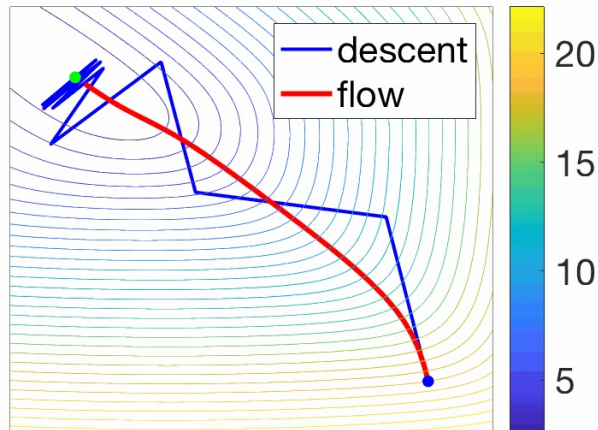
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$k = 100$

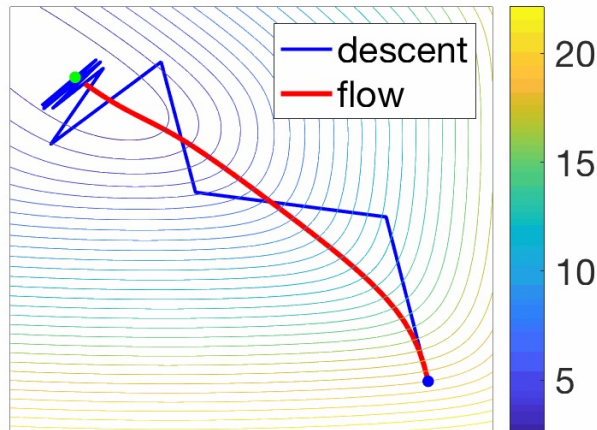


- **Simplified analyses.** The gradient flow has no step-size, so all the traditional annoying issues regarding the choice of step-size, with line-search, constant, decreasing or with a weird schedule are unnecessary.

Figure 1:  Source

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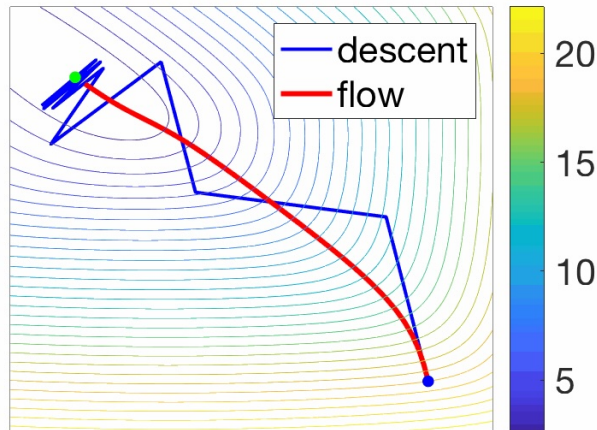


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- **Analytical solution in some cases.** For example, one can consider quadratic problem with linear gradient, which will form a linear ODE with known exact formula.
- **Different discretization leads to different methods.** We will see, that the continuous-time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

Consider Gradient Flow ODE:

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

Explicit Euler discretization:

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! Proximal operator

$$\text{prox}_{\alpha f}(x_k) = \arg \min_{x \in \mathbb{R}^n} \left[\alpha f(x) + \frac{1}{2} \|x - x_k\|_2^2 \right]$$

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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$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) \quad \Rightarrow \quad \nabla f(y)^\top (x - y) \leq f(x) - f(y)$$

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

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

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

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

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3. Finally,

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

Accelerated Gradient Flow

Remember one of the forms of Nesterov Accelerated Gradient

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

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

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:

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

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

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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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