Gradient Flow. Accelerated gradient flow.

Daniil Merkulov

Optimization methods. MIPT

Gradient Flow

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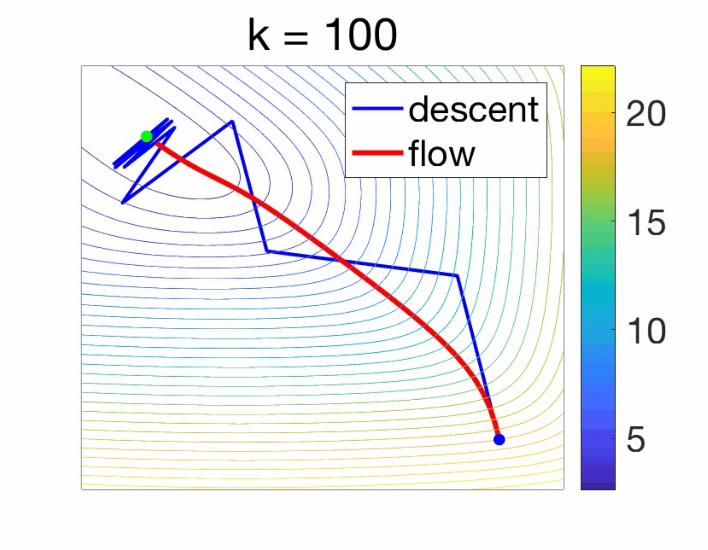

Рис. 1: Source

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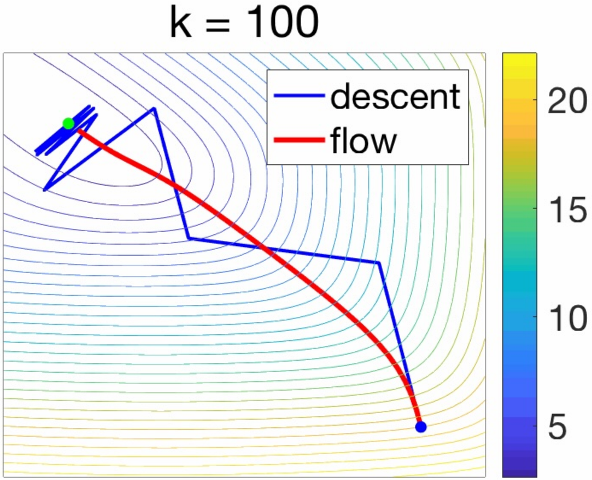

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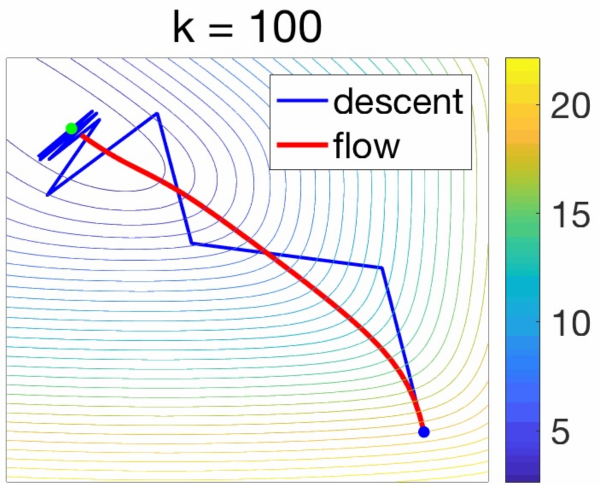

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- **Analytical solution in some cases.** For example, one can consider quadratic problem with linear gradient, which will form a linear ODE with known exact formula.
- **Different discretization leads to different methods.** We will see, that the continuous-time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

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Consider Gradient Flow ODE:

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

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

Convergence analysis. Convex case.

1. Simplest proof of monotonic decrease of GF:

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   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).

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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,

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

Accelerated Gradient Flow

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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:

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

[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 $\dot{E}(t) \le 0$ for all $t > 0$; hence $E(t)$ is non-increasing. Because the second term is non-negative we obtain the *convergence theorem*

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

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

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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:

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

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 $x(t)$

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

! Fokker-Planck equation

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

Sources

- Francis Bach blog

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* Understanding Optimization in Deep Learning with Central Flows