On the Links Between Integration Methods and Optimization Algorithms

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Outline

A The gradient flow

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- ▲ The gradient flow
- B Optimization algorithms and ODE: a small review
 - 1 Gradient method
 - 2 Nesterov's method and Accelerated mirror descent

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- B Optimization algorithms and ODE: a small review
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- **C** Linear multi-step methods
 - 1 Generalization
 - 2 How to model Nesterov as a linear multi-step method?

The Gradient Flow

Let $\dot{x} = \frac{dx}{dt}$. The gradient flow is described by the ODE

$$\dot{x} = -\nabla f(x)$$
 ; $x(0) = x_0$

We can prove, if f is strongly convex, that

$$||x(t) - x^*||^2 \le e^{-\mu t} ||x_0 - x^*||^2$$

If the step size is $h = \frac{1}{L}$, then for t = kh we have

$$||x(kh) - x^*||^2 \le e^{-k\frac{\mu}{L}} ||x_0 - x^*||^2$$

We recover the rate of gradient method.

Gradient method

• ODE Proposed:

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

Discretization on the interval $[t_k, t_{k+1}]$: Forward Euler.

$$\dot{x}(t) \approx \frac{x(t_k + h) - x(t_k)}{h} \qquad \nabla f(x(t)) \approx \nabla f(x(t_k))$$

Writing $x_k = x(t_k)$, and assuming $t_k = kh$, we have

$$x_{k+1} = x_k - h\nabla f(x_k)$$

Proximal Gradient method

ODE Proposed:

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

Discretization on the interval $[t_k, t_{k+1}]$: **Backward Euler**.

$$\dot{x}(t) \approx \frac{x(t_k + h) - x(t_k)}{h} \qquad \nabla f(x(t)) \approx \nabla f(x(t_{k+1}))$$

Writing $x_k = x(t_k)$, and assuming $t_k = kh$, we have

$$x_{k+1} = x_k - h\nabla f(x_{k+1}) = \operatorname{prox}_{hf}(x_k)$$

Nesterov's method

Algorithm for convex functions (where $\beta_k = \frac{k-2}{k+1}$):

$$\begin{aligned} x_{k+1} &= y_k - \frac{1}{L} f(y_k) \\ y_{k+1} &= -\beta_k x_k + (1+\beta_k) x_{k+1} \end{aligned}$$

For strongly convex functions, $\beta = \frac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}$ where $\kappa = \frac{\mu}{L}$ is the condition number.

Two different models:

- (A) Su, Boyd, Candes
- **(B)** Wibisono, Wilson, Jordan ; Wilson, Recht, Jordan.

Model (A) (Su, Boyd, Candes)

The authors starts from the algorithm, then takes the limits when the step size $\frac{1}{L}$ goes to zero. The model becomes

$$\ddot{x} + \frac{r}{t}\dot{x} = -\nabla f(x),$$

where r = 3 is called the «magic constant».

They recover the initial algorithm using non-trivial Forward Euler approximation.

They proved that the ODE converge at the accelerated rate, but nothing about the convergence of the discretization.

Model (B) (simplified) (Wibisono, Wilson, Recht, Jordan)

The authors introduce the following ODE,

$$\frac{d}{dt}(x+e^{-\alpha_t}\dot{x}) = -e^{\alpha_t+\beta_t}\nabla f(x),$$

where α_t , β_t should follow the *ideal scaling condition*

$$\dot{\beta}_t \le e^{\alpha_t}.$$

The authors show that

- A (non-trivial) discretization of this ODE models Nesterov's gradient (forward Euler) and accelerated mirror descent (backward Euler).
- The ODE converges at the accelerated rate.
- There exists a "general" discrete Lyapunov function which proves the fast convergence of the discrete scheme (but without any links with the ODE).

For now, each discretization uses **forward** or **backward** Euler method (in a complicated way) on a <u>non-trivial</u> ODE.

Question: What happen if we use a more sophisticated method on a simpler ODE?

Linear multi-step methods Euler method (Forward - explicit):

$$x_{k+1} - x_k = -h\nabla f(x_k)$$

Euler method (backward - implicit):

$$x_{k+1} - x_k = -h\nabla f(x_{k+1})$$

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Generalization:

$$\sum_{i=0}^{s} \rho_i x_{k+i} = -h \sum_{i=0}^{s} \sigma_i \nabla f(x_{k+i})$$

Linear multi-step methods Euler method (Forward - explicit):

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Generalization:

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Introducing the shift operator $E: Ex_k \to x_{k+1}$; $E\nabla f(x_k) \to \nabla f(x_{k+1})$,

$$\left(\sum_{i=0}^{s} \rho_i E^i\right) x_k = -h\left(\sum_{i=0}^{s} \sigma_i E^i\right) \nabla f(x_k)$$

Let ρ and σ be two polynomials of degree s, with $\rho_s = 1$ (by convention). Then

$$\rho(E)x_k = -h\sigma(E)\nabla f(x_k)$$

A linear multi-step methods is uniquely defined by the pair (ρ, σ) .

Linear multi-step methods

Many important characteristics:

- Consistency
- (Order of convergence)
- (Zero-stability)
- (A-stability)
- (G-stability)

...

Consistency

Let (ρ, σ) be a linear multi-step method which generates the sequence x_k on the ODE $\dot{x} = -\nabla f(x)$, using step size h. Assume that the first iterates are exact, i.e.

$$(x_k, x_{k+1}, \dots, x_{k+s-1}) = (x(t_k), x(t_{k+1}), \dots, x(t_{k+s-1})).$$

Then the method is *consistent* if and only if

$$\lim_{h \to 0} \frac{1}{h} \|x_k(h) - x(t_k)\| = 0$$

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Then the method is *consistent* if and only if

$$\lim_{h \to 0} \frac{1}{h} \|x_k(h) - x(t_k)\| = 0$$

This is equivalent to te condition (proof using Taylor expansion)

$$\rho(1) = 0$$
 and $\sigma(1) = \rho'(1)$

Intuition:

- If we start at $x_0 = x^*$, the first condition ensures $x_k = x^*$ for all k.
- If the second condition is not satisfied, then the method presents artificial gain or damping.

(Reminder) Nesterov's method:

$$\begin{aligned} x_{k+1} &= y_k - \frac{1}{L} f(y_k) \\ y_{k+1} &= -\beta_k x_k + (1 + \beta_k) x_{k+1} \end{aligned}$$

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If we expand y_{k+1} ,

$$y_{k+1} = -\beta_k \left(y_{k-1} - \frac{1}{L} \nabla f(y_{k-1}) \right) + (1 + \beta_k) \left(y_k - \frac{1}{L} \nabla f(y_k) \right)$$

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If we separate y_k and $\nabla f(y_k)$,

$$\beta_k y_{k-1} - (1+\beta_k)y_k + y_{k+1} = -\frac{1}{L} \left(-\beta_k \nabla f(y_{k-1}) + (1+\beta_k) \nabla f(y_k)\right)$$

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We will check if the method is consistent (i.e. $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$):

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• First condition: $\rho(1) = 0$

$$\rho(1) = \beta_k - (1 + \beta_k) + 1 = 0$$
 OK

$$\beta_k y_{k-1} - (1+\beta_k) y_k + y_{k+1} = -\frac{1}{L} \left(-\beta_k \nabla f(y_{k-1}) + (1+\beta_k) \nabla f(y_k) \right)$$

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First condition: $\rho(1) = 0$

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 OK

 $\blacksquare \ {\rm Second \ condition:} \ \rho'(1) = \sigma(1) \Leftrightarrow h\rho'(1) = h\sigma(1)$

$$h\rho'(1) = h(-(1+\beta_k)+2) = h(1-\beta_k)$$

$$h\sigma(1) = \frac{1}{L}(-\beta_k+1+\beta_k) = \frac{1}{L}$$

Since we need to have $\rho'(1) = \sigma(1)$, we conclude that $h = \frac{1}{L(1-\beta_k)}$.

The parameters of Nesterov's method are thus (after identification)

•
$$\rho_k = [\beta_k ; -(1 + \beta_k) ; 1]$$

• $\sigma_k = (1 - \beta_k) * [-\beta_k ; 1 + \beta_k ; 0]$
• $h_k = \frac{1}{L(1 - \beta_k)}$

Since $\beta_k \in]0,1[$, the step size is larger.

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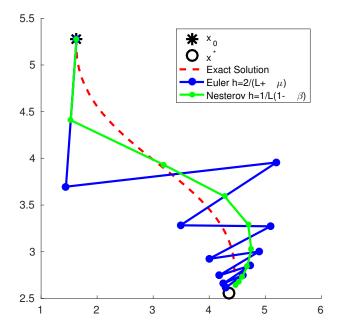
• $\sigma_k = (1-\beta_k) * [-\beta_k; 1+\beta_k; 0]$
• $h_k = \frac{1}{L(1-\beta_k)}$

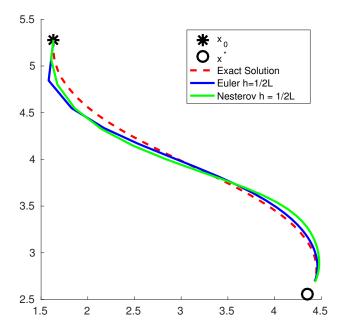
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Intuitive estimation of the rate of convergence:

• (Convex case) If $\beta_k = \frac{k-2}{k+1}$, $h = \frac{1}{L}\frac{k+1}{3}$. It means that we go $\approx k$ times faster than usual gradient method. The rate is $\approx \frac{1}{k^2}$.

• (Strongly convex case) If $\beta_k = \frac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}$, $h = \frac{1}{L}\frac{1+\sqrt{\kappa}}{2}$. We go $\approx \sqrt{\kappa}$ times faster. The rate is $\approx (1-\sqrt{\kappa})^k$





Conclusion

Main contributions:

- Using simple arguments, we have strong links between many algorithms in optimization and integration methods.
- The approach is straightforward, and without any magic tricks we are able to understand why Nesterov's method is faster.
- Using consistency, zero-stability and some optimality argument, we are able to derive a family of two-steps methods (which contains Nesterov's gradient and Polyak's heavy ball).

Future work:

- Proof of convergence.
- The convex case is not so clear: the method change over time.
- Extension to non-Euclidean case?