

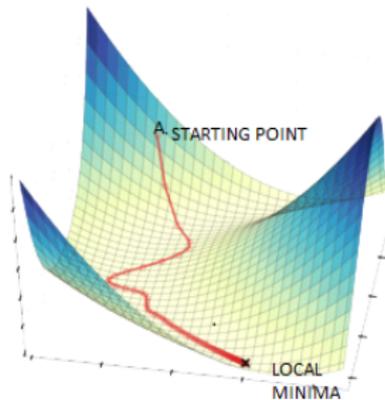
Continuous-Time Perspectives on First-Order Optimization Methods

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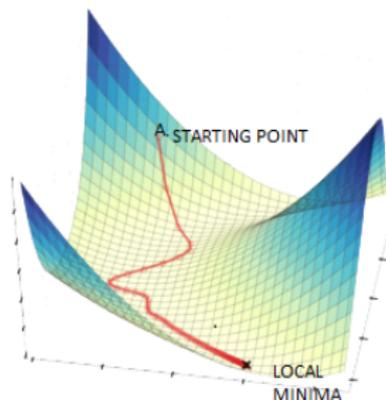
Gradient-based optimization

minimize $f(x)$ using $\nabla f(x)$



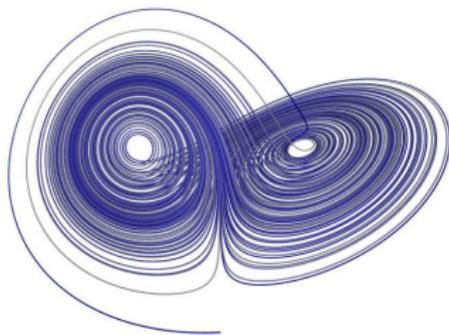
Gradient-based optimization

minimize $f(x)$ using $\nabla f(x)$



- Simplest example: gradient descent
- Almost entirely focused on differentiation
- Toolkit is (relatively) small

Dynamical systems



- Simplest example: ordinary differential equation (ODE)
- Interplay between differentiation and integration
- A much larger toolkit

Connecting dynamical systems with optimization?

Leverage the power of ODEs to analyze optimization methods



Connecting dynamical systems with optimization?

Leverage the power of ODEs to analyze optimization methods



- Long history (see monograph of Helmke and Moore '96)

This talk: connecting ODEs with gradient-based methods

*A framework for modeling, analyzing, interpreting,
and designing accelerated optimization methods*

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A framework for modeling, analyzing, interpreting, and designing accelerated optimization methods

- ▶ Develop ODEs as amenable surrogates for accelerated optimization methods

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- ▶ Provide intuitive and generalizable proofs

This talk: connecting ODEs with gradient-based methods

A framework for modeling, analyzing, interpreting, and designing accelerated optimization methods

- ▶ Develop ODEs as amenable surrogates for accelerated optimization methods
- ▶ Provide intuitive and generalizable proofs
- ▶ Suggest new accelerated methods

Collaborators

- Stephen Boyd (Stanford)
- Emmanuel Candès (Stanford)
- Shuxiao Chen (UPenn)
- Simon Du (CMU)
- Yicong Jiang (Harvard)
- Michael Jordan (Berkeley)
- Bin Shi (Berkeley)
- Da Wu (UPenn)

Gradient descent

f is convex and ∇f is L -Lipschitz: $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$

- $\|b - Ax\|^2$: least squares
- $-b^T(Ax + x_0) + 1^T \log(1 + \exp(Ax + x_0))$: logistic regression
- $\frac{1}{2}\|b - Ax\|^2 + \lambda\|x\|_1$: lasso

Gradient descent for minimizing f

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

Gradient descent

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Gradient descent for minimizing f

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

- Convergence rate

$$f(x_k) - f^* \leq O\left(\frac{1}{k}\right)$$

if $s = 1/L$, where $f^* = \min f(x)$

- $\nabla f(x_k)$ replaced by proximal subgradient if f is composite (lasso)

Accelerating the convergence

Nesterov's accelerated gradient method '83

$$x_k = y_{k-1} - s \nabla f(y_{k-1})$$
$$y_k = x_k + \underbrace{\frac{k-1}{k+2}(x_k - x_{k-1})}_{\text{momentum}}$$

from $x_0 = y_0$

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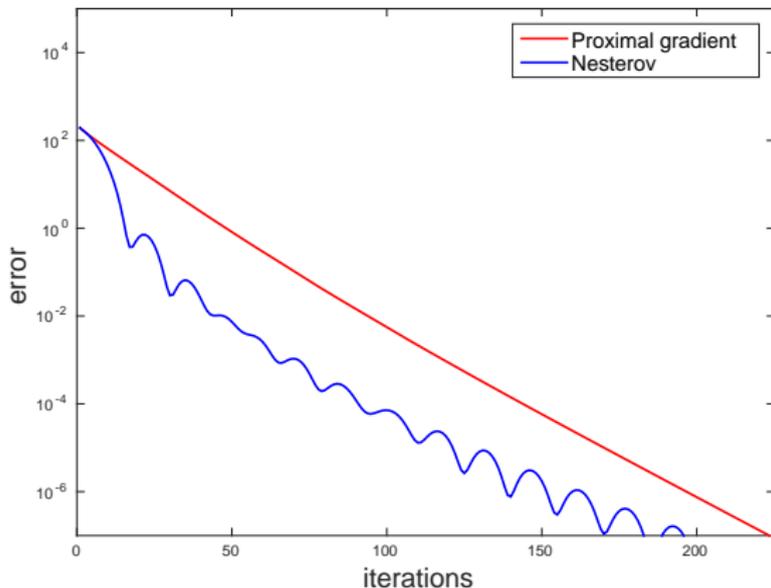
- For L -smooth convex f , Nesterov proved that for $0 < s \leq 1/L$

$$f(x_k) - f^* \leq O\left(\frac{1}{k^2}\right)$$

- Optimal rate with access to first-order information
- Generalized to composite minimization (Beck and Teboulle '09)

Solving SLOPE using Nesterov's method

$$\min_x f(x) \triangleq \underbrace{\frac{1}{2} \|b - Ax\|^2}_{\text{smooth}} + \underbrace{\sum_{i=1}^n \lambda_i |x|_{(i)}}_{\text{nonsmooth but convex}}$$



Error denotes $f(x_k) - f^*$; design matrix A is 1000×10000

Mysteries of acceleration

Common wisdom: momentum reduces zig zags and smooths paths

$$x_k = y_{k-1} - s \nabla f(y_{k-1})$$
$$y_k = x_k + \frac{k-1}{k+2} (x_k - x_{k-1})$$

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- What is the underlying mechanism?
- Why $\frac{k-1}{k+2}$?

Mysteries of acceleration

Common wisdom: momentum reduces zig zags and smooths paths

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$$y_k = x_k + \frac{k-1}{k+2} (x_k - x_{k-1})$$

- What is the underlying mechanism?
- Why $\frac{k-1}{k+2}$?
- Existing approaches: generalized estimate sequence (Baes '09), Chebyshev polynomials (Hardt '13), linear coupling (Allen-Zhu and Orecchia '14), optimized first-order method (Drori and Teboulle '14), control theory (Lessard et al '16)

Outline

1. A second-order ODE

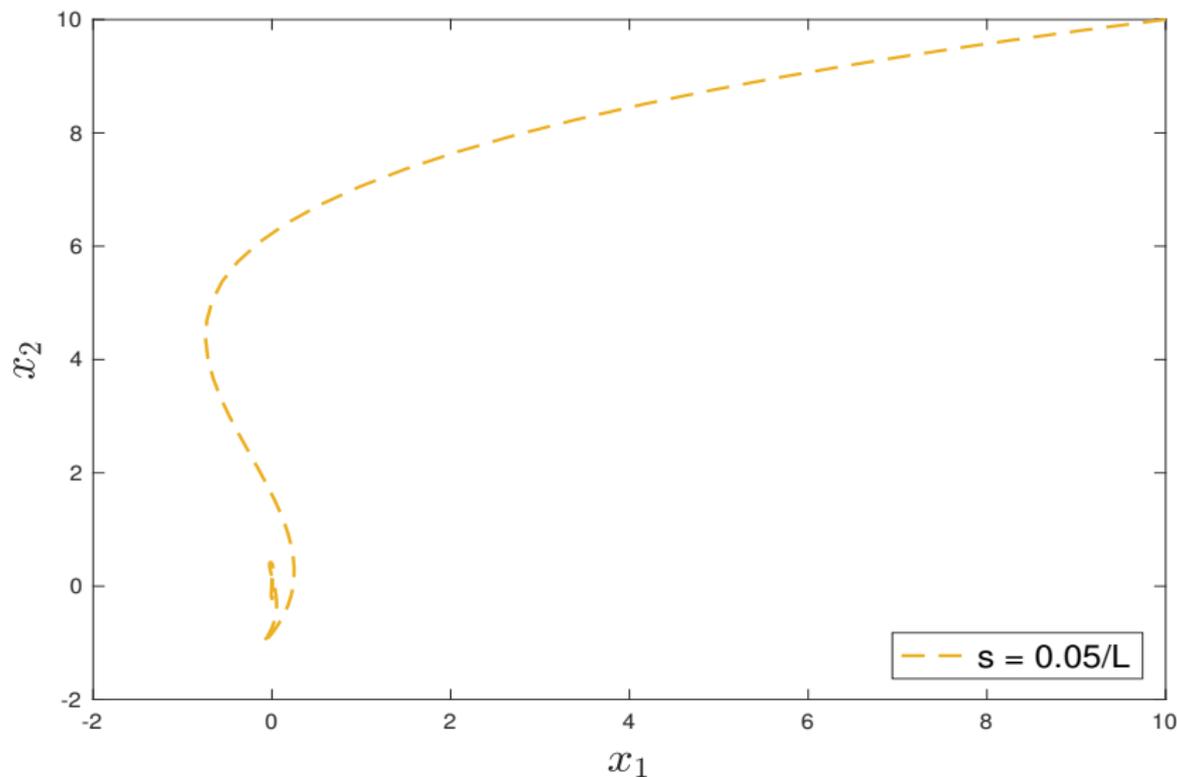
2. High-resolution ODEs

3. Concluding remarks

The beginning of the story...

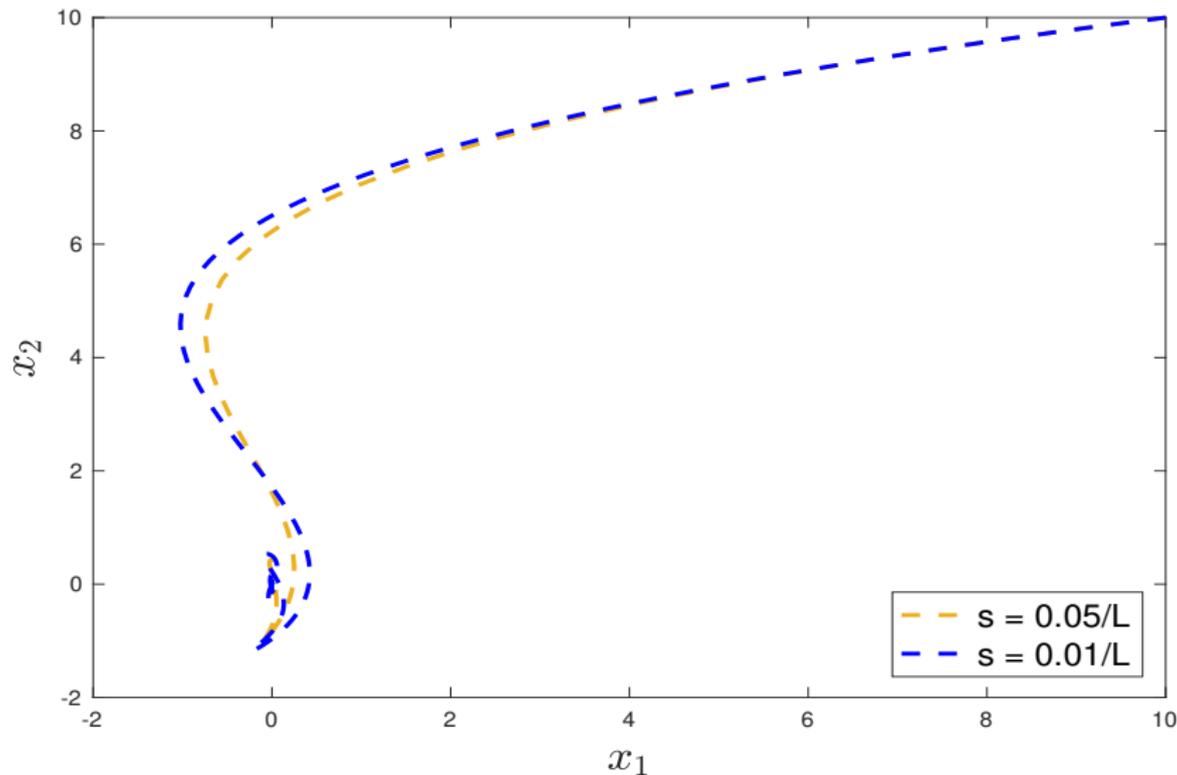
Trajectories of Nesterov's method

Iterates from minimizing $f(x) = \frac{5}{2}x_1^2 + \frac{1}{2}x_2^2$



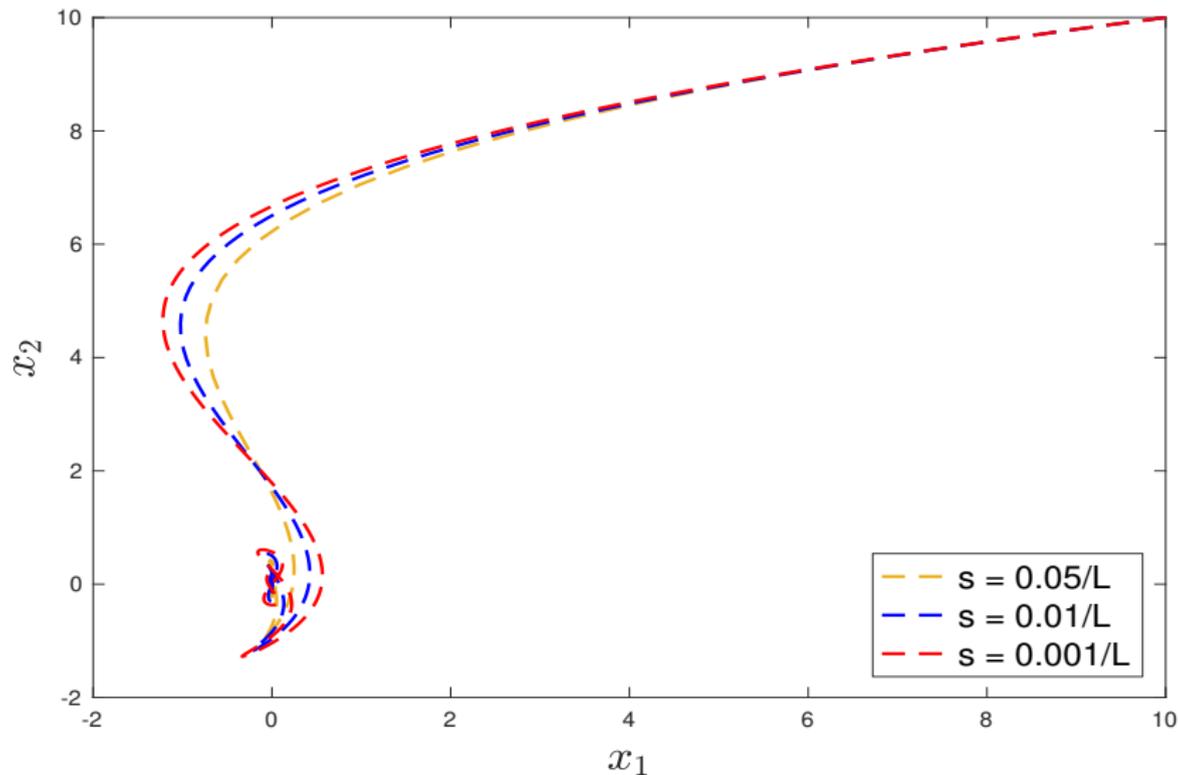
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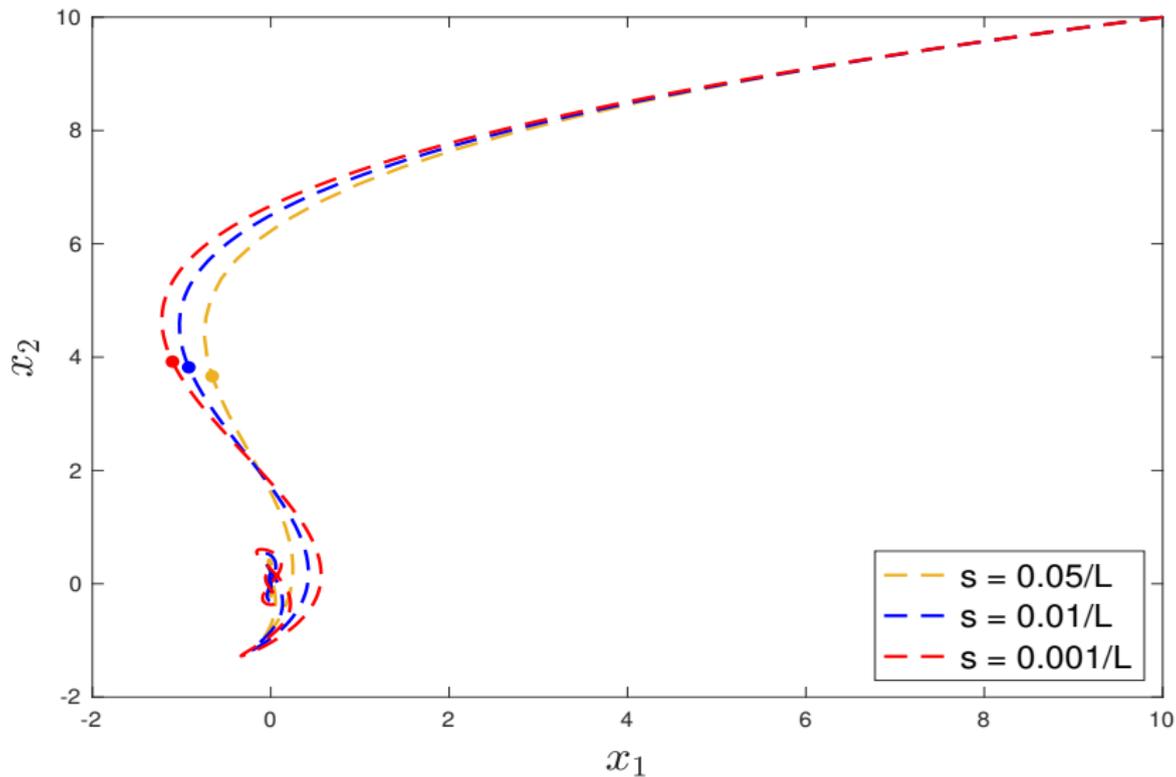
Trajectories of Nesterov's method

Iterates from minimizing $f(x) = \frac{5}{2}x_1^2 + \frac{1}{2}x_2^2$



Time scaling

Iterates at $k = 2.5/\sqrt{\text{step size}}$



The limit of Nesterov's method

Nesterov's method

$$x_k = y_{k-1} - s \nabla f(y_{k-1})$$

$$y_k = x_k + \frac{k-1}{k+2} (x_k - x_{k-1})$$

Theorem

Taking $s \rightarrow 0$, Nesterov's method converges to the ODE

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

with $X(0) = x_0, \dot{X}(0) = 0$ in the sense $\lim_{s \rightarrow 0} \max_{k \leq \frac{T}{\sqrt{s}}} \|x_k - X(k\sqrt{s})\| = 0$

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- Solution exists and unique
- A second-order ODE
- Time parameter $t \approx k\sqrt{\text{step size}} \propto \sqrt{\text{step size}}$

Derivation I

Nesterov's method in one-line

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

↓

$$\frac{x_{k+1} - x_k}{\sqrt{s}} = \frac{k-1}{k+2} \frac{x_k - x_{k-1}}{\sqrt{s}} - \sqrt{s}\nabla f(y_k)$$

Derivation II

Let $t_k = k\sqrt{s}$. Assume $x_k = X(t_k)$ for some smooth curve X

$$\frac{x_{k+1} - x_k}{\sqrt{s}} = \dot{X}(t_k) + \frac{1}{2}\ddot{X}(t_k)\sqrt{s} + o(\sqrt{s})$$

$$\frac{x_k - x_{k-1}}{\sqrt{s}} = \dot{X}(t_k) - \frac{1}{2}\ddot{X}(t_k)\sqrt{s} + o(\sqrt{s})$$

$$\sqrt{s}\nabla f(y_k) = \sqrt{s}\nabla f(X(t_k)) + o(\sqrt{s})$$

Comparing coefficients of \sqrt{s} in Nesterov's method gives

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

Ask me anything

The Nesterov ODE

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

A useful surrogate for Nesterov's method?

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Yes

Suggest new accelerated methods?

Yes

Can the ODE do everything for the method?

Ask me anything

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A useful surrogate for Nesterov's method?	I think so
Simplify some proofs for Nesterov's method?	Yes
Suggest new accelerated methods?	Yes
Can the ODE do everything for the method?	Of course not, but we've <i>upgraded</i> the ODE

Ask me anything

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- | | |
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| A useful surrogate for Nesterov's method? | I think so |
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ODE |
| Can the upgraded ODEs do something new? | |

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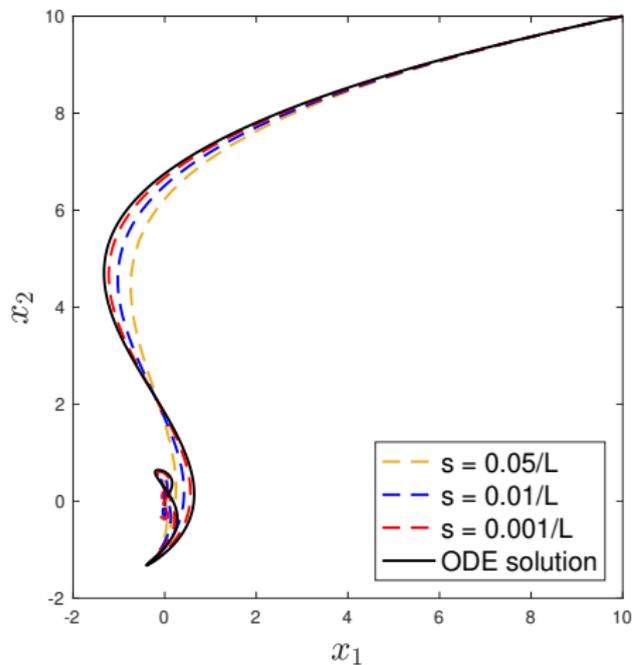
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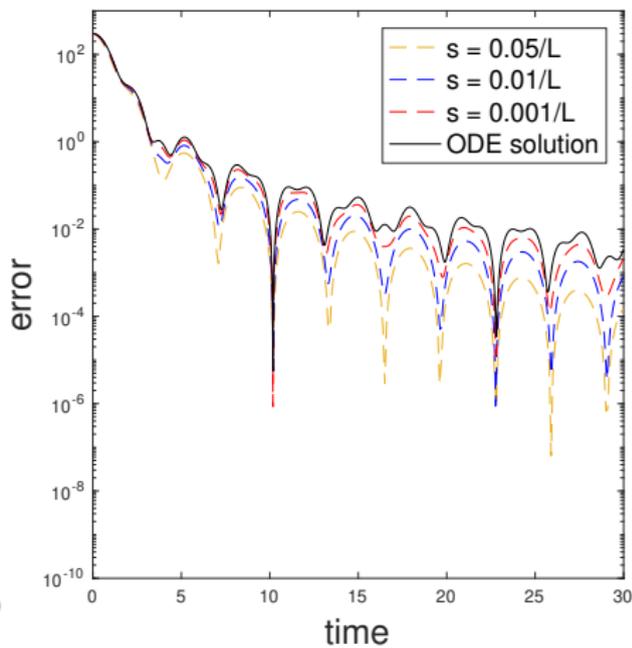
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| Suggest new accelerated methods? | Yes |
| Can the ODE do everything for the method? | Of course not, but we've <i>upgraded</i> the ODE |
| Can the upgraded ODEs do something new? | Yes |

A faithful surrogate

$$f(x) = \frac{5}{2}x_1^2 + \frac{1}{2}x_2^2$$



Trajectories



Convergence

Analogous convergence rate

Theorem (Our)

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

\Downarrow

$$f(X(t)) - f^* \leq \frac{2\|x_0 - x^*\|^2}{t^2}$$

Analogous convergence rate

Theorem (Our)

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

↓

$$f(X(t)) - f^* \leq \frac{2\|x_0 - x^*\|^2}{t^2}$$

Theorem (Nesterov)

$$x_k = y_{k-1} - s\nabla f(y_{k-1})$$

$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$

↓

$$f(x_k) - f^* \leq \frac{2\|x_0 - x^*\|^2}{s(k+1)^2}$$

Analogous convergence rate

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$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$

↓

$$f(x_k) - f^* \leq \frac{2\|x_0 - x^*\|^2}{s(k+1)^2}$$

- $t^2 \approx s(k+1)^2$

A simple proof

$$\text{Proving } f(X(t)) - f^* \leq \frac{2\|x_0 - x^*\|^2}{t^2}$$

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$$\text{Proving } f(X(t)) - f^* \leq \frac{2\|x_0 - x^*\|^2}{t^2}$$

- Energy functional (Lyapunov)

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

A simple proof

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- Energy functional (Lyapunov)

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

- By convexity of f

$$\begin{aligned}\frac{d\mathcal{E}}{dt} &= 2t(f(X) - f^*) + 4\langle X - x^*, -\frac{t}{2}\nabla f(X)\rangle \\ &= 2t(f(X) - f^*) - 2t\langle X - x^*, \nabla f(X)\rangle \leq 0\end{aligned}$$

A simple proof

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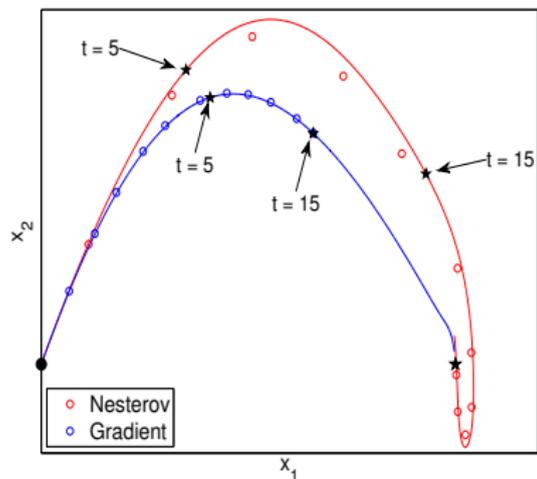
$$\begin{aligned} \frac{d\mathcal{E}}{dt} &= 2t(f(X) - f^*) + 4\langle X - x^*, -\frac{t}{2}\nabla f(X) \rangle \\ &= 2t(f(X) - f^*) - 2t\langle X - x^*, \nabla f(X) \rangle \leq 0 \end{aligned}$$

- $t^2(f(X(t)) - f^*) \leq \mathcal{E}(t) \leq \mathcal{E}(0) = 2\|x_0 - x^*\|^2$

Comparing gradient descent with Nesterov's method

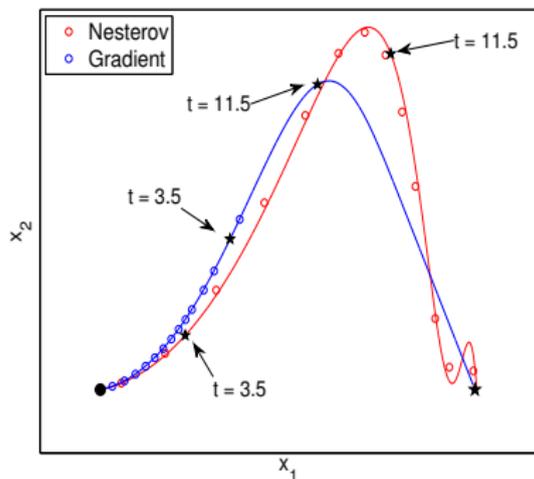
Gradient descent ODE

- $\dot{X} + \nabla f(X) = 0$
- Euler stable step size $O(1/L)$
- Each iteration moves $\propto s$



Nesterov ODE

- $\ddot{X} + \frac{3}{t}\dot{X} + \nabla f(X) = 0$
- Euler stable step size $O(1/\sqrt{L})$
- Each iteration moves $\propto \sqrt{s}$



Suggesting new methods

New ODE

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

Suggesting new methods

New ODE

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

Theorem

Suppose $r > 3$. Then

$$f(X(t)) - f^* \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2t^2}, \quad \int_0^\infty t(f(X(t)) - f^*) dt \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2(r-3)}$$

- Acceleration remains
- If $r < 3$, no acceleration! (see also Attouch et al '17)
- Proof based on $\mathcal{E}(t) = \frac{2t^2}{r-1}(f(X) - f^*) + (r-1)\|X + \frac{t}{r-1}\dot{X} - x^*\|^2$

Generalized Nesterov's methods

Back to the discrete world, from $y_0 = x_0$

$$x_k = y_{k-1} - s \nabla f(y_{k-1})$$

$$y_k = x_k + \frac{k-1}{k+r-1} (x_k - x_{k-1})$$

- r results from $k+r-1 - (k-1)$
- Generalized to composite minimization by replacing $\nabla f(y_{k-1})$ with proximal subgradient

Generalized Nesterov's method

For $r > 3$ and $0 < s \leq 1/L$

$$f(x_k) - f^* \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2s(k+r-2)^2}$$
$$\sum_{k=1}^{\infty} (k+r-1)(f(x_k) - f^*) \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2s(r-3)}$$

Generalized Nesterov's method

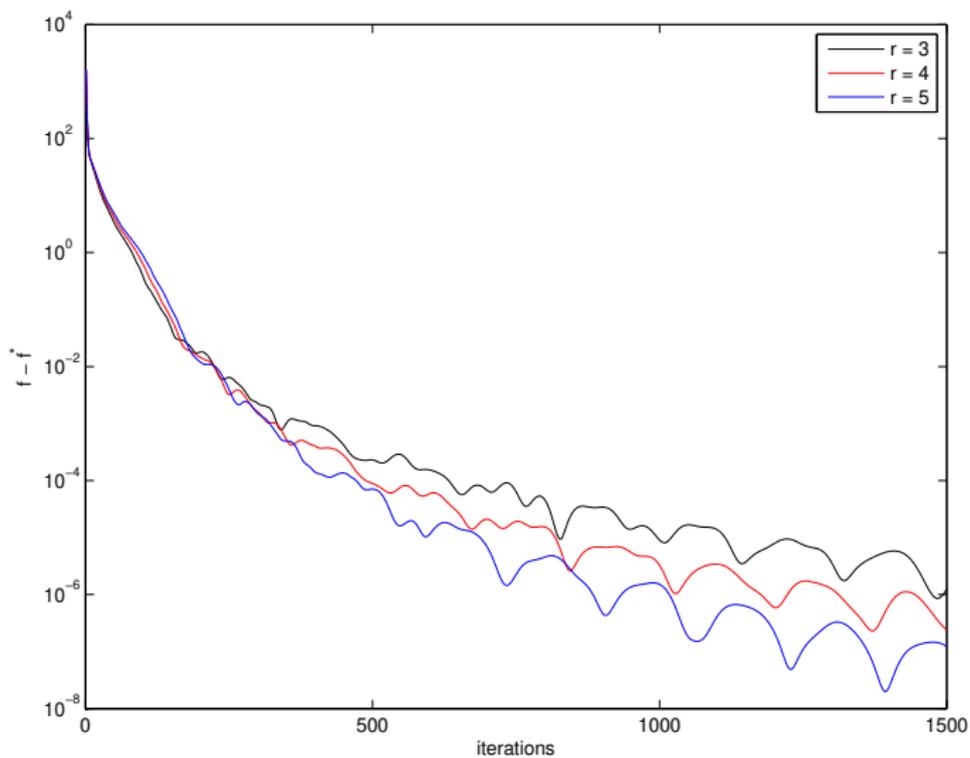
For $r > 3$ and $0 < s \leq 1/L$

$$f(x_k) - f^* \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2s(k+r-2)^2}$$

$$\sum_{k=1}^{\infty} (k+r-1)(f(x_k) - f^*) \leq \frac{(r-1)^2 \|x_0 - x^*\|^2}{2s(r-3)}$$

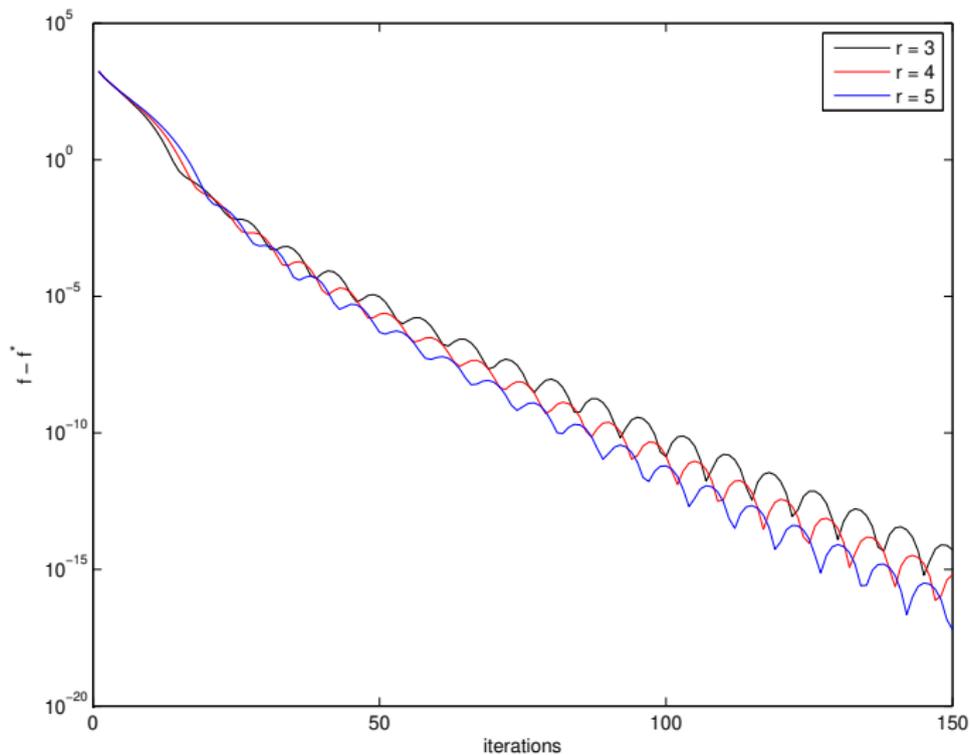
- $O(1/k^2)$ convergence rate remains
- Suggests $f(x_k) - f^* = o(1/k^2)$ asymptotically (Attouch and Peypouquet '16)

Numerical Examples I



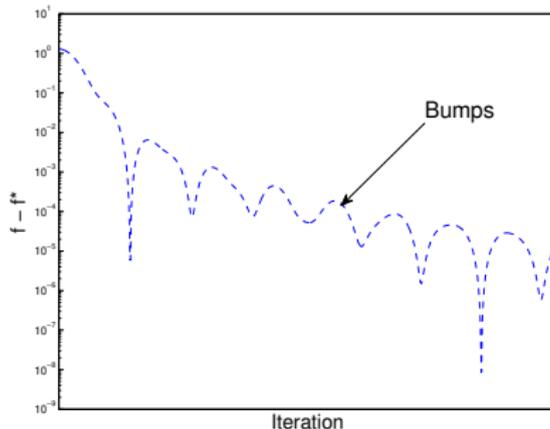
$$\min \frac{1}{2} \|Ax - b\|^2 + \lambda \|x\|_1$$

Numerical Examples II



$$\min \frac{1}{2} \|Ax - b\|^2, \quad \text{s.t. } x \succeq 0$$

Restarting Nesterov's method I



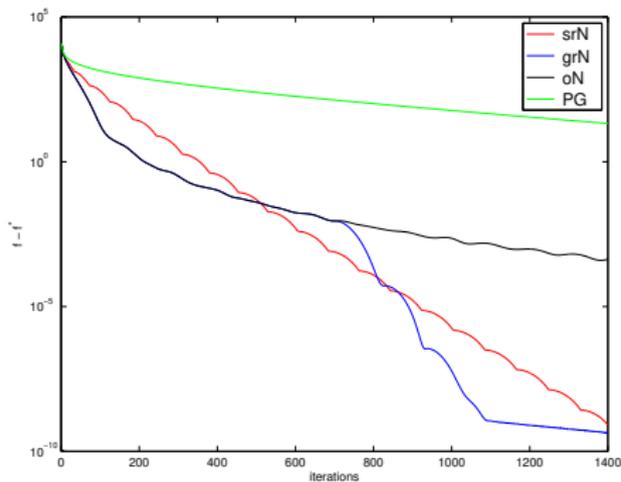
Cause

If $\frac{\beta}{t}$ is small, friction is too low

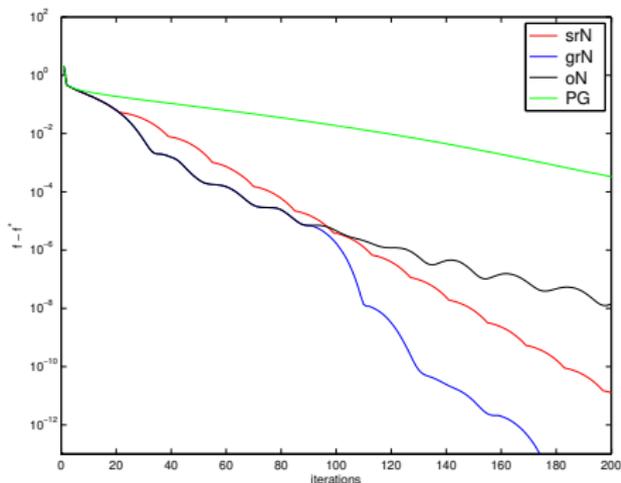
- Time is set to zero whenever velocity starts to decrease
- Early restarting ideas (O'Donoghue and Candès '12)

Restarting Nesterov's method II

Our restarting (srN), gradient restarting (grN) (O'Donoghue and Candès '12), Nesterov's method (oN), and proximal gradient (PG)



$$\min \frac{1}{2} \|Ax - b\|^2 \quad \text{s.t. } \|x\|_1 \leq C$$



$$\min \frac{1}{2} \|X_{\text{obs}} - M_{\text{obs}}\|_F^2 + \lambda \|X\|_*$$

Acceleration and monotonicity simultaneously?

- Nesterov's method achieves acceleration, but is not monotone
- Gradient descent is monotone, but not accelerated

Acceleration and monotonicity simultaneously?

- Nesterov's method achieves acceleration, but is not monotone
- Gradient descent is monotone, but not accelerated

Theorem

*If a first-order method can be represented as a linear combination of several iterates and the gradient, then it **cannot** be both accelerated and monotone*

Outline

1. A second-order ODE

2. High-resolution ODEs

3. Concluding remarks

Methods for strongly convex functions

Let f be μ -strongly convex and L -smooth

Polyak's heavy-ball method

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

Nesterov's method

$$y_{k+1} = x_k - s \nabla f(x_k)$$

$$x_{k+1} = y_{k+1} + \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}} (y_{k+1} - y_k)$$

- Polyak suggests $\alpha = (1 - \sqrt{\mu/L})^2$

They look similar

Let f be μ -strongly convex and L -smooth

Nesterov's method

$$\begin{aligned}y_{k+1} &= x_k - s\nabla f(x_k) \\x_{k+1} &= y_{k+1} + \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}} (y_{k+1} - y_k)\end{aligned}$$

Equivalent to

$$x_{k+1} = x_k + \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}} (x_k - x_{k-1}) - \underbrace{s\nabla f(x_k) - \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}} s (\nabla f(x_k) - \nabla f(x_{k-1}))}_{\text{gradient correction}}$$

Polyak's heavy-ball method

$$x_{k+1} = x_k + \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}} (x_k - x_{k-1}) - s\nabla f(x_k)$$

- Only differ in *gradient correction*

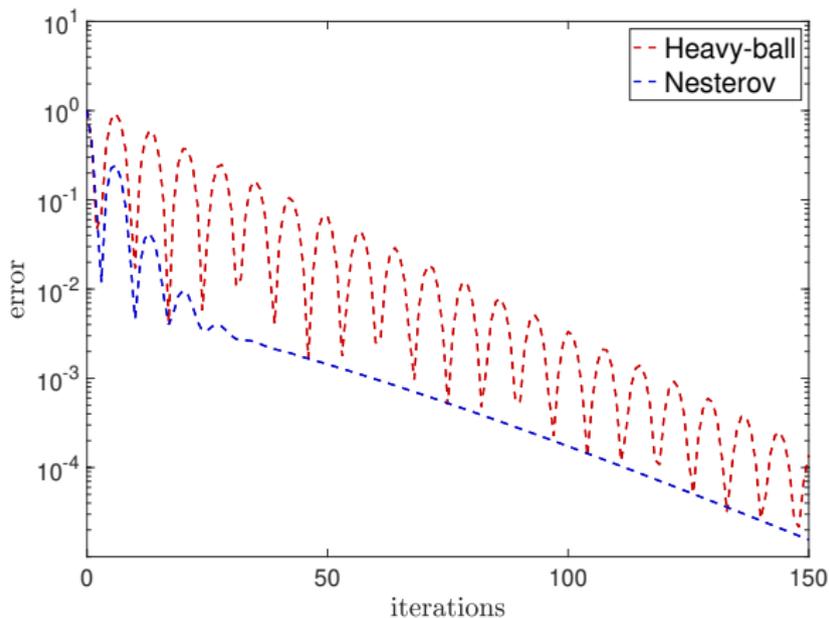
They have the same ODE

Nesterov's and Polyak's share the same ODE (Wilson et al '16)

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + \nabla f(X(t)) = 0$$

- The gradient correction $\frac{1-\sqrt{\mu s}}{1+\sqrt{\mu s}} s (\nabla f(x_k) - \nabla f(x_{k-1}))$ is not reflected due to *low resolution*

But they are very different!



$f(x_1, x_2) = x_1^2 + 5 \times 10^{-3} x_2^2$, $x_0 = (1, 1)$ and step size $s = 0.09$.

- Polyak's: oscillations

Need new ODEs to capture fine-grained behaviors

High-resolution ODEs

Let s be small but non-vanishing

High-resolution ODEs

- Polyak's

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + (1 + \sqrt{\mu s})\nabla f(X(t)) = 0$$

- Nesterov's

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + \sqrt{s}\nabla^2 f(X(t))\dot{X}(t) + (1 + \sqrt{\mu s})\nabla f(X(t)) = 0$$

High-resolution ODEs

Let s be small but non-vanishing

High-resolution ODEs

- Polyak's

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- $X(0) = x_0$ and $\dot{X}(0) = -\frac{2\sqrt{s}\nabla f(x_0)}{1+\sqrt{\mu s}}$
- $\sqrt{s}\nabla^2 f(X)\dot{X}(t)$ results from $\frac{1-\sqrt{\mu s}}{1+\sqrt{\mu s}}s(\nabla f(x_k) - \nabla f(x_{k-1}))$
- Derivation: carefully Taylor expand $\frac{1-\sqrt{\mu s}}{1+\sqrt{\mu s}}s(\nabla f(x_k) - \nabla f(x_{k-1}))$

High-resolution ODEs

Let s be small but non-vanishing

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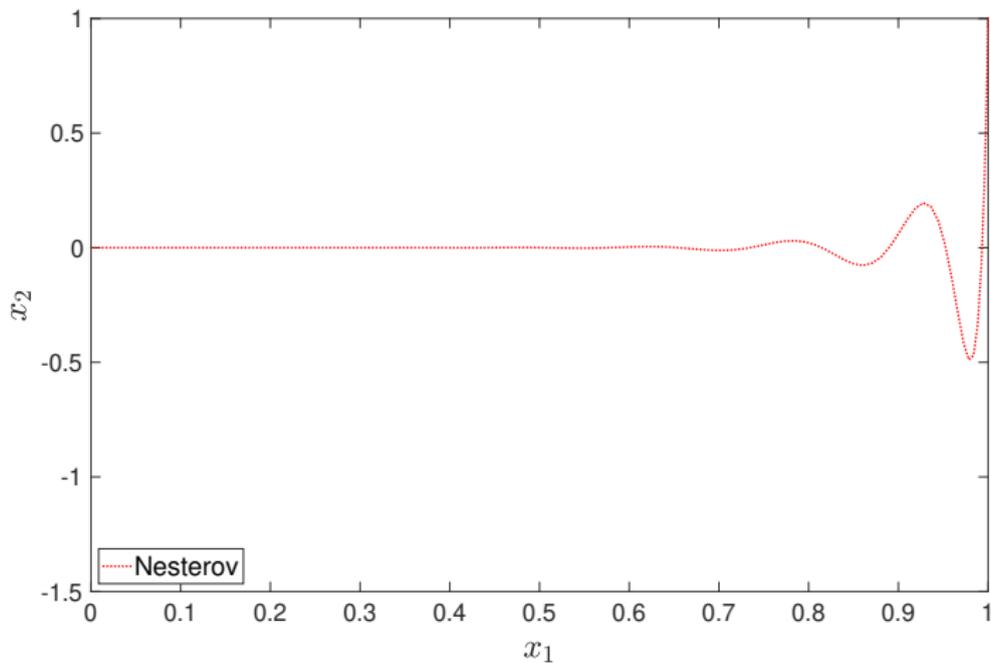
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- If $s = 0$, high-resolution ODEs reduce to low-resolution ODE
- Modified differential equations

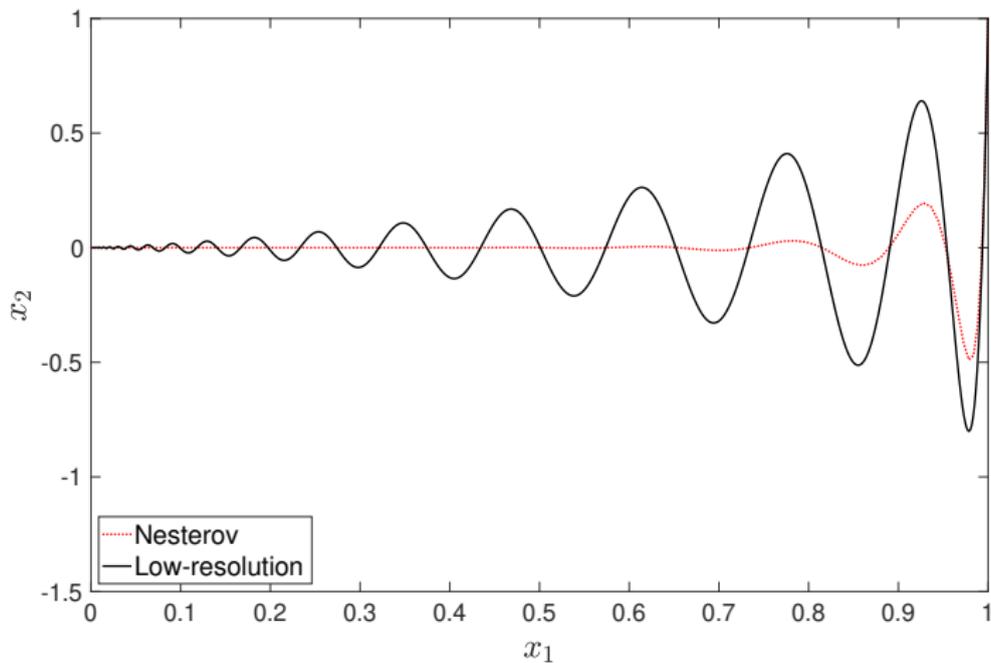
High-resolution ODEs are better surrogates

$$f(x_1, x_2) = x_1^2 + 5 \times 10^{-3} x_2^2, \quad x_0 = (1, 1)$$



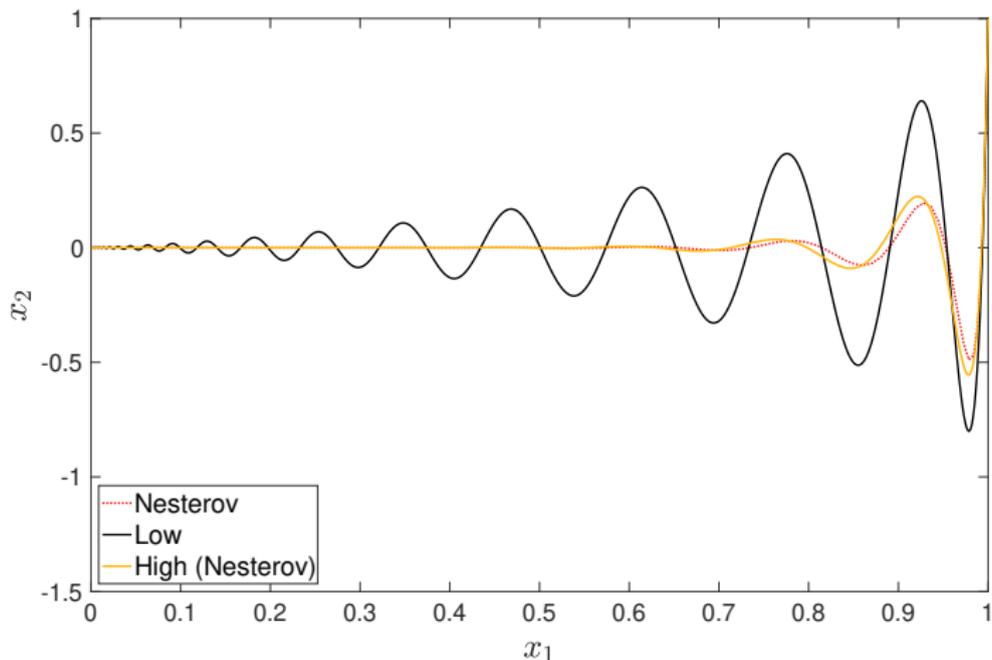
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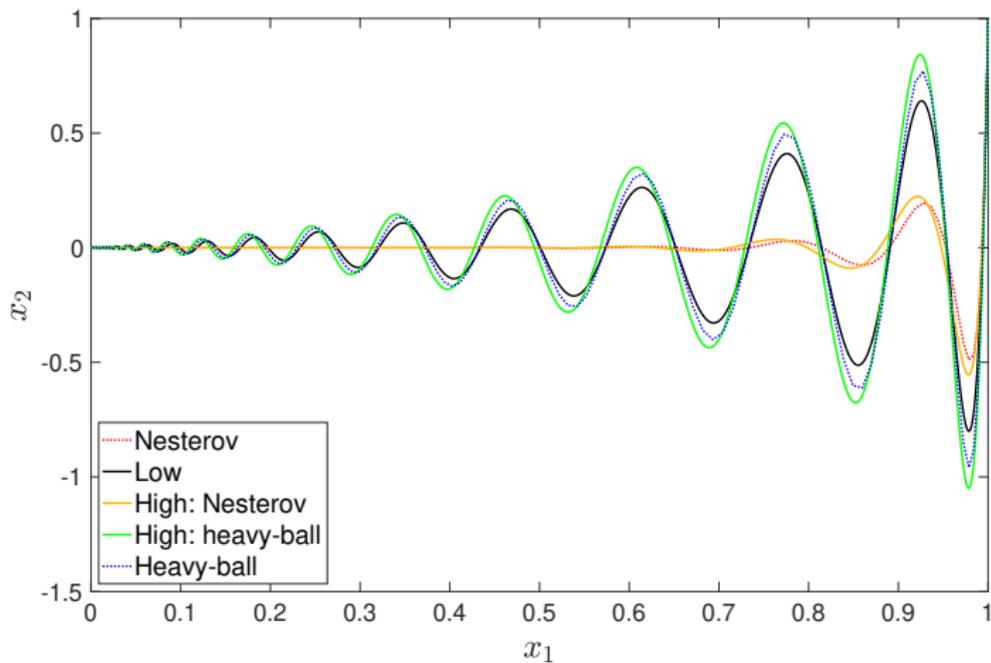
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High-resolution ODEs are better surrogates

$$f(x_1, x_2) = x_1^2 + 5 \times 10^{-3} x_2^2, \quad x_0 = (1, 1)$$



*Do the high-resolution ODEs distinguish acceleration
and non-acceleration?*

The answer is in the *gradient correction*

The difference is in $\sqrt{s}\nabla^2 f(X(t))\dot{X}(t)$

- Polyak's

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + (1 + \sqrt{\mu s})\nabla f(X(t)) = 0$$

- Nesterov's

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + \sqrt{s}\nabla^2 f(X(t))\dot{X}(t) + (1 + \sqrt{\mu s})\nabla f(X(t)) = 0$$

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- $\sqrt{s}\nabla^2 f(X(t))\dot{X}(t)$ (gradient correction) gently adjusts the “friction”

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- $\sqrt{s}\nabla^2 f(X(t))\dot{X}(t)$ (gradient correction) gently adjusts the “friction”
- Fundamental to the acceleration of Nesterov's method

Energy functional for Nesterov's ODE

$$\ddot{X}(t) + 2\sqrt{\mu}\dot{X}(t) + \sqrt{s}\nabla^2 f(X(t))\dot{X}(t) + (1 + \sqrt{\mu s})\nabla f(X(t)) = 0$$

Energy functional

$$\mathcal{E}(t) = \underbrace{(1 + \sqrt{\mu s})(f(X) - f^*)}_{\text{potential}} + \underbrace{\frac{1}{4}\|\dot{X}\|^2}_{\text{kinetic}} + \frac{1}{4}\|\dot{X} + 2\sqrt{\mu}(X - x^*) + \sqrt{s}\nabla f(X)\|^2$$

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- $\dot{X} + 2\sqrt{\mu}(X - x^*) + \sqrt{s}\nabla f(X)$ results from integrating $\ddot{X} + 2\sqrt{\mu}\dot{X} + \sqrt{s}\nabla^2 f(X)\dot{X}$
- $\sqrt{s}\nabla f(X)$ arises from gradient correction

Convergence of Nesterov's ODE

Energy functional

$$\mathcal{E}(t) = (1 + \sqrt{\mu s}) (f(X) - f^*) + \frac{1}{4} \|\dot{X}\|^2 + \frac{1}{4} \|\dot{X} + 2\sqrt{\mu}(X - x^*) + \sqrt{s}\nabla f(X)\|^2$$

Lemma

$$\frac{d\mathcal{E}}{dt} \leq -\frac{\sqrt{\mu}}{4}\mathcal{E} - \frac{\sqrt{s}}{2} \left[\|\nabla f(X)\|^2 + \dot{X}^\top \nabla^2 f(X) \dot{X} \right] \leq -\frac{\sqrt{\mu}}{4}\mathcal{E}$$

Convergence of Nesterov's ODE

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- $\frac{\sqrt{s}}{2} (\|\nabla f(X)\|^2 + \dot{X}^\top \nabla^2 f(X) \dot{X}) \geq 0$ arises from gradient correction
- For $s \leq 1/L$

$$f(X(t)) - f^* \leq \frac{2 \|x_0 - x^*\|^2}{s} e^{-\frac{\sqrt{\mu}t}{4}}$$

Convergence of Polyak's ODE

Energy functional

$$\mathcal{E}(t) = (1 + \sqrt{\mu s}) (f(X) - f^*) + \frac{1}{4} \|\dot{X}\|^2 + \frac{1}{4} \|\dot{X} + 2\sqrt{\mu}(X - x^*)\|^2$$

Lemma

$$\frac{d\mathcal{E}}{dt} \leq -\frac{\sqrt{\mu}}{4} \mathcal{E}$$

- $\frac{\sqrt{s}}{2} (\|\nabla f(X)\|^2 + \dot{X}^\top \nabla^2 f(X) \dot{X})$ is not found
- For $s \leq 1/L$

$$f(X(t)) - f^* \leq \frac{7 \|x_0 - x^*\|^2}{2s} e^{-\frac{\sqrt{\mu}t}{4}}$$

Returning to the discrete world

Discrete energy functional for Nesterov's

Continuous-time

$$\mathcal{E}(t) = (1 + \sqrt{\mu s}) (f(X) - f^*) + \frac{1}{4} \|\dot{X}\|^2 + \frac{1}{4} \|\dot{X} + 2\sqrt{\mu}(X - x^*) + \sqrt{s}\nabla f(X)\|^2$$

Discrete energy functional for Nesterov's

Continuous-time

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Discrete-time

$$\begin{aligned} \mathcal{E}(k) = & \frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} (f(x_k) - f^*) + \frac{1}{4} \|v_k\|^2 \\ & + \frac{1}{4} \left\| v_k + \frac{2\sqrt{\mu}}{1 - \sqrt{\mu s}} (x_{k+1} - x^*) + \sqrt{s}\nabla f(x_k) \right\|^2 - \frac{s \|\nabla f(x_k)\|^2}{2(1 - \sqrt{\mu s})} \end{aligned}$$

- Phase variable $v_k = \frac{x_{k+1} - x_k}{\sqrt{s}}$
- Seamless transform via phase space representation

Discrete energy functional for Nesterov's

$$\begin{aligned}\mathcal{E}(k) &= \frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} (f(x_k) - f^*) + \frac{1}{4} \|v_k\|^2 \\ &\quad + \frac{1}{4} \left\| v_k + \frac{2\sqrt{\mu}}{1 - \sqrt{\mu s}} (x_{k+1} - x^*) + \sqrt{s} \nabla f(x_k) \right\|^2 - \frac{s \|\nabla f(x_k)\|^2}{2(1 - \sqrt{\mu s})}\end{aligned}$$

Lemma

If $0 < s \leq 1/(4L)$, then $\mathcal{E}(k+1) - \mathcal{E}(k) \leq -\frac{\sqrt{\mu s}}{6} \mathcal{E}(k+1)$

Discrete energy functional for Nesterov's

$$\begin{aligned}\mathcal{E}(k) &= \frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} (f(x_k) - f^*) + \frac{1}{4} \|v_k\|^2 \\ &\quad + \frac{1}{4} \left\| v_k + \frac{2\sqrt{\mu}}{1 - \sqrt{\mu s}} (x_{k+1} - x^*) + \sqrt{s} \nabla f(x_k) \right\|^2 - \frac{s \|\nabla f(x_k)\|^2}{2(1 - \sqrt{\mu s})}\end{aligned}$$

Lemma

If $0 < s \leq 1/(4L)$, then $\mathcal{E}(k+1) - \mathcal{E}(k) \leq -\frac{\sqrt{\mu s}}{6} \mathcal{E}(k+1)$

- Implies

$$f(x_k) - f^* \leq \frac{5L \|x_0 - x^*\|^2}{\left(1 + \frac{1}{12} \sqrt{\mu/L}\right)^k}$$

- $\log(f(x_k) - f^*) \leq -O(k\sqrt{\mu/L})$ matches the optimal bound (Nesterov '13)

Discrete energy functional for Polyak's

$$\mathcal{E}(k) = \frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} (f(x_k) - f^*) + \frac{1}{4} \|v_k\|^2 + \frac{1}{4} \left\| v_k + \frac{2\sqrt{\mu}}{1 - \sqrt{\mu s}} (x_{k+1} - x^*) \right\|^2$$

Lemma

$$\begin{aligned} \mathcal{E}(k+1) - \mathcal{E}(k) &\leq -\sqrt{\mu s} \min \left\{ \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}}, \frac{1}{4} \right\} \mathcal{E}(k+1) \\ &\quad - \left[\frac{3\sqrt{\mu s}}{4} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right) (f(x_{k+1}) - f^*) - \frac{s}{2} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right)^2 \|\nabla f(x_{k+1})\|^2 \right] \end{aligned}$$

- Need to ensure the “annoying” term

$$\frac{3\sqrt{\mu s}}{4} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right) (f(x_{k+1}) - f^*) - \frac{s}{2} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right)^2 \|\nabla f(x_{k+1})\|^2 \geq 0$$

Where is this “annoying” term from?

The continuous energy functional for Nesterov's

$$\frac{d\mathcal{E}}{dt} \leq -\frac{\sqrt{\mu}}{4}\mathcal{E} - \underbrace{\frac{\sqrt{s}}{2} \left[\|\nabla f(X)\|^2 + \dot{X}^\top \nabla^2 f(X) \dot{X} \right]}_D$$

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- In fact, the “annoying” term appears in Nesterov's, but canceled out by D
- Recall D is due to gradient correction
- Thus, the “annoying” term is due to the lack of gradient correction in Polyak's

When is the “annoying” term nonnegative?

Lemma (Polyak's)

$$\mathcal{E}(k+1) - \mathcal{E}(k) \leq -\sqrt{\mu s} \min \left\{ \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}}, \frac{1}{4} \right\} \mathcal{E}(k+1) - \left[\frac{3\sqrt{\mu s}}{4} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right) (f(x_{k+1}) - f^*) - \frac{s}{2} \left(\frac{1 + \sqrt{\mu s}}{1 - \sqrt{\mu s}} \right)^2 \|\nabla f(x_{k+1})\|^2 \right]$$

- It is nonnegative if $s = O\left(\frac{\mu}{L^2}\right)$ in Polyak's
- $\mathcal{E}(k+1) - \mathcal{E}(k) \leq -\sqrt{\mu s} \min \left\{ \frac{1 - \sqrt{\mu s}}{1 + \sqrt{\mu s}}, \frac{1}{4} \right\} \mathcal{E}(k+1)$
- Take $s = \mu/(16L^2)$, Polyak's convergence

$$f(x_k) - f(x_0) \leq \frac{5L \|x_0 - x^*\|^2}{\left(1 + \frac{\mu}{16L}\right)^k}$$

It is the gradient correction that matters

Nesterov's

- Contains gradient correction
- Step size $s = O\left(\frac{1}{L}\right)$
- $\log(f(x_k) - f^*) \leq -O(k\sqrt{\mu/L})$
- Achieves acceleration

Polyak's

- No gradient correction
- Step size $s = O\left(\frac{\mu}{L^2}\right)$
- $\log(f(x_k) - f^*) \leq -O(k\mu/L)$
- No (global) acceleration

- For ill-conditioned $\mu \ll L$ cases, $O\left(\frac{1}{L}\right) \gg O\left(\frac{\mu}{L^2}\right)$

Numerical stability

Forward Euler scheme on Nesterov's

$$\frac{X(t+\sqrt{s})-2X(t)+X(t-\sqrt{s})}{s} + (2\sqrt{\mu} + \sqrt{s}\nabla^2 f(X(t-\sqrt{s}))) \cdot \frac{X(t)-X(t-\sqrt{s})}{\sqrt{s}} + (1 + \sqrt{\mu s})\nabla f(X(t-\sqrt{s})) = 0$$

Stable step sizes for solving Nesterov's

$$s \leq O\left(\frac{1}{L}\right)$$

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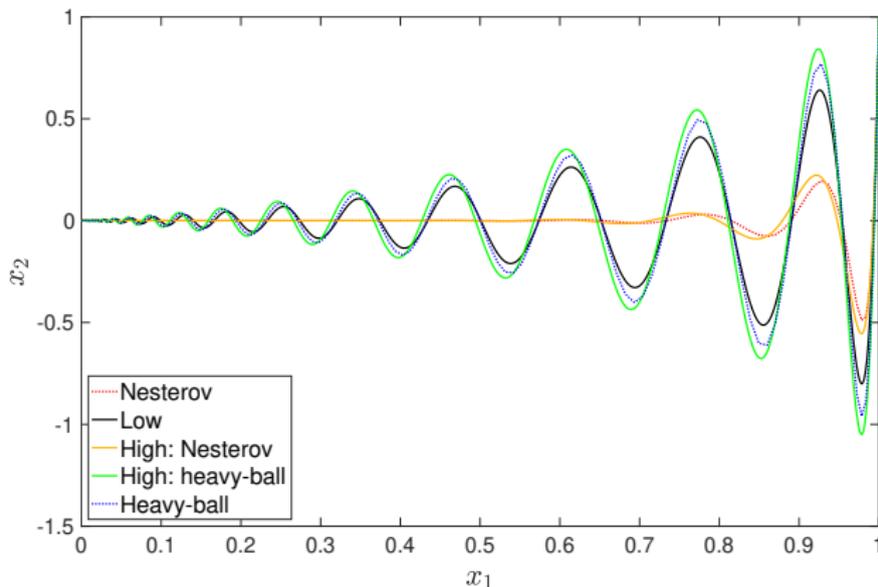
$$\frac{X(t+\sqrt{s})-2X(t)+X(t-\sqrt{s})}{s} + 2\sqrt{\mu}\frac{X(t)-X(t-\sqrt{s})}{\sqrt{s}} + (1 + \sqrt{\mu s})\nabla f(X(t-\sqrt{s})) = 0$$

Stable step sizes for solving Polyak's

$$s \leq O\left(\frac{\mu}{L^2}\right)$$

A straight or winding road?

Why Nesterov's allows a larger step size than Polyak's?



- Gradient correction in Nesterov's "smooths out" bumps

All roads lead to Rome, but...



Yet another application of high-resolution ODEs

Make gradient small

Let f be L -smooth (non-strongly) convex

How to minimize $\|\nabla f(x)\|^2$ efficiently?

Make gradient small

Let f be L -smooth (non-strongly) convex

How to minimize $\|\nabla f(x)\|^2$ efficiently?

- A centerpiece in non-convex optimization
- Nesterov's achieves

$$\|\nabla f(x_k)\|^2 \leq O\left(\frac{1}{k^2}\right)$$

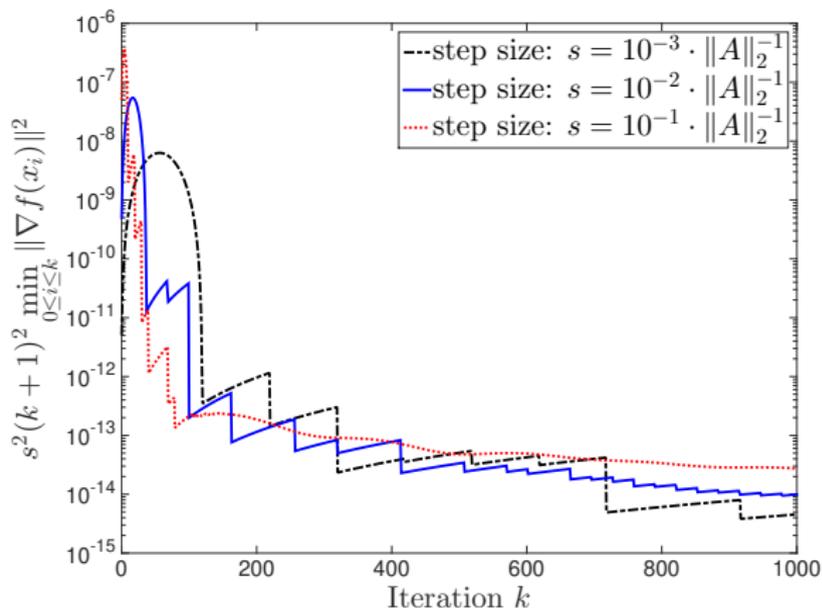
because $\|\nabla f(x_k)\|^2 \leq 2L(f(x_k) - f^*)$ and $f(x_k) - f^* \leq O(1/k^2)$. Recall

$$x_k = y_{k-1} - s\nabla f(y_{k-1})$$

$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$

Is $O(1/k^2)$ the right rate?

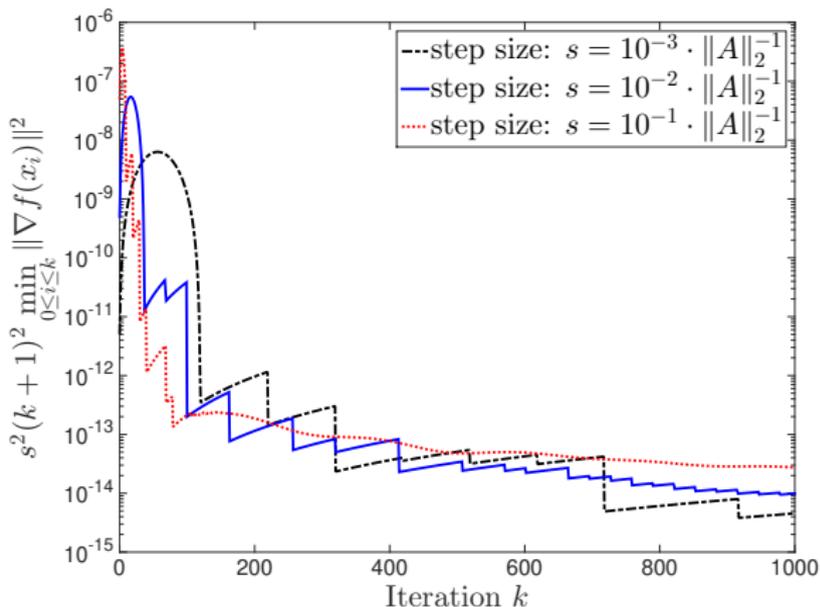
Scaled squared gradient norm $s^2(k+1)^2 \min_{0 \leq i \leq k} \|\nabla f(x_i)\|^2$



$f(x) = \frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle$, where A is 500×500

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$f(x) = \frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle$, where A is 500×500

- Unfortunately, the low-resolution ODE *cannot* explain

Yet another high-resolution ODE

High-resolution ODE for non-strongly convex objectives

$$\ddot{X}(t) + \frac{3}{t}\dot{X}(t) + \sqrt{s}\nabla^2 f(X(t))\dot{X}(t) + \left(1 + \frac{3\sqrt{s}}{2t}\right)\nabla f(X(t)) = 0$$

for $t \geq 3\sqrt{s}/2$, with $X(3\sqrt{s}/2) = x_0$ and $\dot{X}(3\sqrt{s}/2) = -\sqrt{s}\nabla f(x_0)$

- Reduces to the low-resolution ODE if $s = 0$
- Contains gradient correction $\sqrt{s}\nabla^2 f(X)\dot{X}$

High-resolution energy functional of Nesterov's method

$$\mathcal{E}(t) = t \left(t + \frac{\sqrt{s}}{2} \right) (f(X) - f^*) + \frac{1}{2} \|t\dot{X} + 2(X - x^*) + t\sqrt{s}\nabla f(X)\|^2$$

Lemma

$$\frac{d\mathcal{E}(t)}{dt} \leq - \left[\sqrt{s}t^2 + \left(\frac{1}{L} + \frac{s}{2} \right) t + \frac{\sqrt{s}}{2L} \right] \|\nabla f(X)\|^2$$

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- $\|\nabla f(X)\|^2$ arises from gradient correction. Thus does *not* apply to low-resolution ODE
- Observe

$$\begin{aligned} & \inf_{t_0 \leq u \leq t} \|\nabla f(X(u))\|^2 \int_{t_0}^t \left[\sqrt{s}u^2 + \left(\frac{1}{L} + \frac{s}{2} \right) u + \frac{\sqrt{s}}{2L} \right] du \\ & \leq \int_{t_0}^t \left[\sqrt{s}u^2 + \left(\frac{1}{L} + \frac{s}{2} \right) u + \frac{\sqrt{s}}{2L} \right] \|\nabla f(X(u))\|^2 du \end{aligned}$$

An improved rate in continuous case

Theorem

Let $s = 1/L$. The squared gradient norm in the high-resolution ODE satisfies

$$\inf_{t_0 \leq u \leq t} \|\nabla f(X(u))\|^2 = O\left(\frac{\sqrt{L}}{t^3}\right)$$

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- Improved from $O(1/t^2)$ to $O(1/t^3)$
- Possible to extend the result to discrete cases?

Returning to the discrete world (which we care about)

Theorem

Let $s \leq 1/(3L)$, the Nesterov's method (non-strongly convex) satisfies

$$\min_{0 \leq i \leq k} \|\nabla f(x_i)\|^2 \leq \frac{8568 \|x_0 - x^*\|^2}{s^2(k+1)^3}$$

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- Improved from $O(1/k^2)$ to $O(1/k^3)$
- Based on the discrete energy functional

$$\begin{aligned} \mathcal{E}(k) = & s(k+3)(k+1)(f(x_k) - f^*) \\ & + \frac{1}{2} \left\| (k+1)\sqrt{s}v_k + 2(x_{k+1} - x^*) + (k+1)s\nabla f(x_k) \right\|^2, \end{aligned}$$

which satisfies $\mathcal{E}(k+1) - \mathcal{E}(k) \leq -Cs^2k^2 \|\nabla f(x_{k+1})\|^2$

- $s^2k^2 \|\nabla f(x_{k+1})\|^2$ due to gradient correction

More comments on the improved rate

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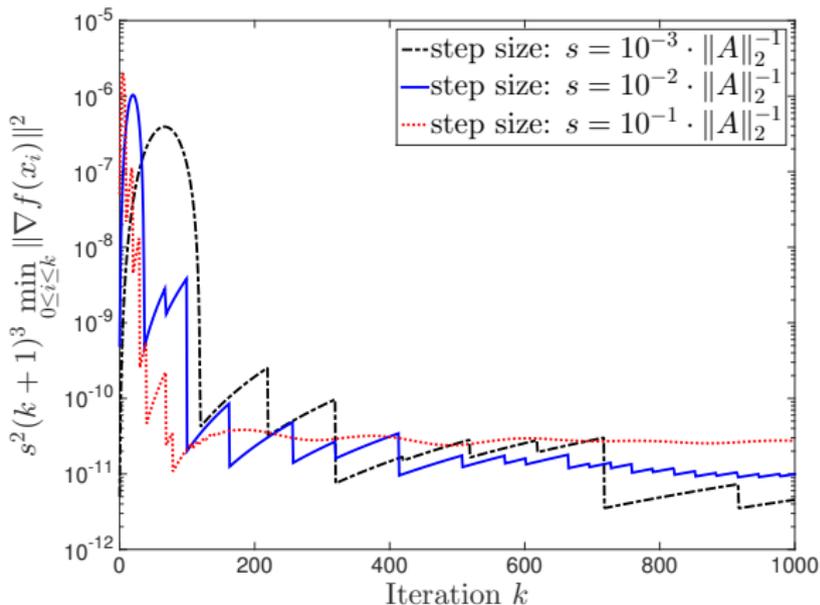
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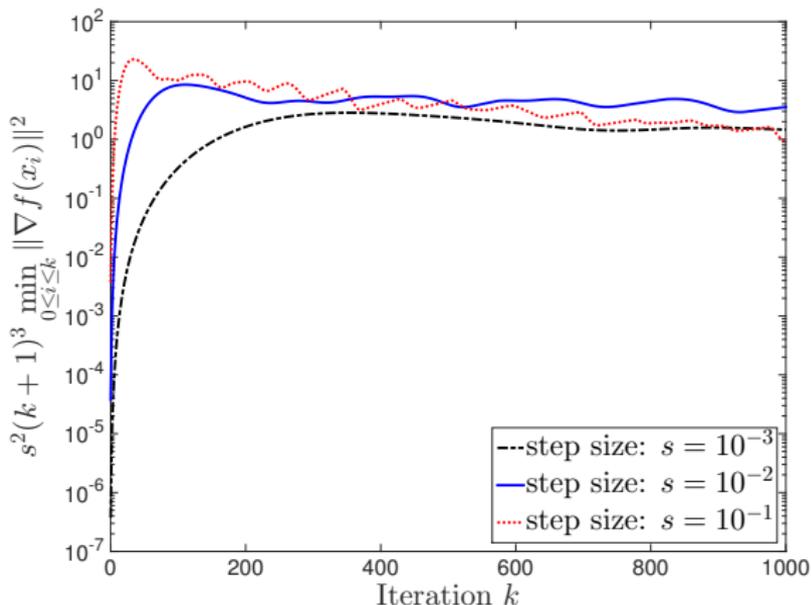
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- Why minimization of gradient is easier?

Simulations I



Scaled squared gradient norm $s^2(k+1)^3 \min_{0 \leq i \leq k} \|\nabla f(x_i)\|^2$.
 $f(x) = \frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle$, where A is 500×500

Simulations II



Scaled squared gradient norm $s^2(k+1)^3 \min_{0 \leq i \leq k} \|\nabla f(x_i)\|^2$.

$$f(x) = \rho \log \left\{ \sum_{i=1}^{200} \exp [(\langle a_i, x \rangle - b_i) / \rho] \right\}, \text{ where } A = [a_1, \dots, a_{200}]' \text{ is } 200 \times 50$$

and $\rho = 20$

Can the high-resolution ODEs suggest new methods?

Extensions for non-strongly convex functions

Generalized high-resolution ODE

$$\ddot{X} + \frac{\alpha}{t}\dot{X} + \beta\sqrt{s}\nabla^2 f(X)\dot{X} + \left(1 + \frac{\alpha\sqrt{s}}{2t}\right)\nabla f(X) = 0$$

for $t \geq \alpha\sqrt{s}/2$, with $X(\alpha\sqrt{s}/2) = x_0$ and $\dot{X}(\alpha\sqrt{s}/2) = -\sqrt{s}\nabla f(x_0)$

- Reduces to the original Nesterov's if $\alpha = 3, \beta = 1$

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Generalized Nesterov's method

$$y_{k+1} = x_k - \beta s \nabla f(x_k)$$

$$x_{k+1} = x_k - s \nabla f(x_k) + \frac{k}{k + \alpha} (y_{k+1} - y_k),$$

starting with $x_0 = y_0$

Accelerated rates

$$y_{k+1} = x_k - \beta s \nabla f(x_k)$$

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Theorem

If $\alpha \geq 3$ and $\beta > \frac{1}{2}$, then

$$f(x_k) - f^* \leq O\left(\frac{1}{k^2}\right), \quad \min_{0 \leq i \leq k} \|\nabla f(x_i)\|^2 \leq O\left(\frac{1}{k^3}\right)$$

In addition, if $\alpha > 3$ then

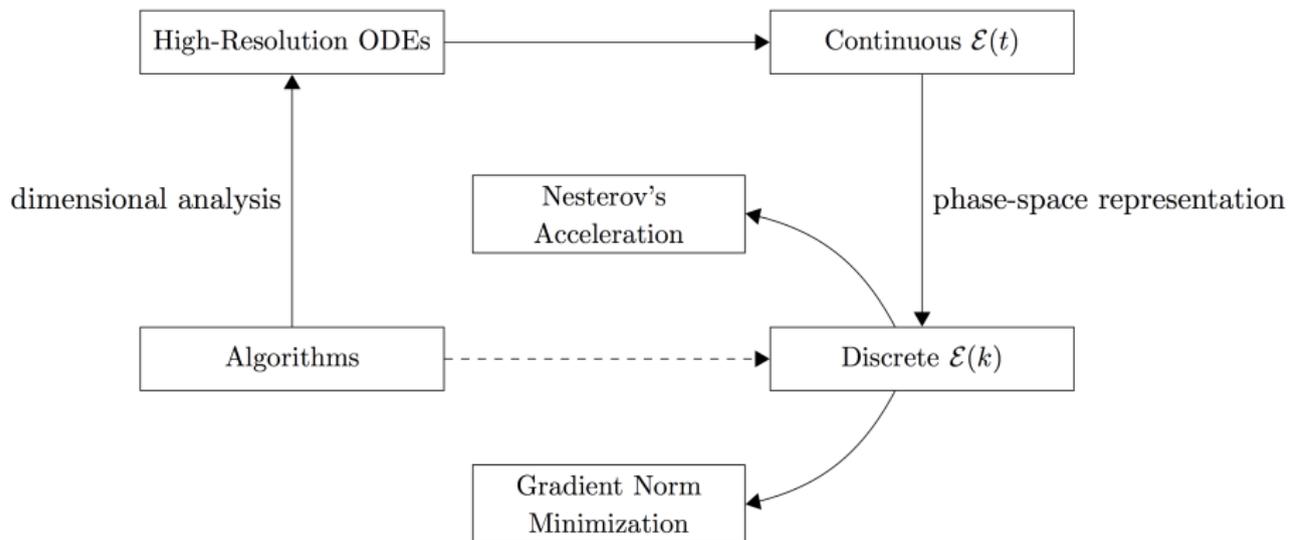
$$f(x_k) - f^* \leq o\left(\frac{1}{k^2}\right)$$

- Why $\beta > \frac{1}{2}$? A phase transition at certain β^*
- $f(x_k) - f^* \leq o\left(\frac{1}{k^2}\right)$ for $\alpha > 3$ extends Attouch and Peypouquet '16

Outline

1. A second-order ODE
2. High-resolution ODEs
3. Concluding remarks

A new framework for understanding optimization



Rambling thoughts



Hermann Weyl

*In these days the angel of topology
and the devil of abstract algebra
fight for the soul of every individual
discipline of mathematics*

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- *Algebraic topology*. What is dynamical systems + optimization?
- Gaps between discrete and continuous worlds exist
- Need more research efforts

Take home messages

- ODEs are amenable tools for analyzing gradient-based methods

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- Conceptually simple, suggest new methods

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Take home messages

- ODEs are amenable tools for analyzing gradient-based methods
- Conceptually simple, suggest new methods
- Sometimes, need to “upgrade” ODEs
- Non-convex, stochastic, constrained settings? Many research opportunities

Thank you!

- *A Differential Equation for Modeling Nesterov's Accelerated Gradient Method: Theory and Insights*
with Boyd and Candès, Journal of Machine Learning Research, 2016
- *Understanding the Acceleration Phenomenon via High-Resolution Differential Equations*
with Shi, Du, and Jordan, arXiv, 2018
- *Acceleration via Symplectic Discretization of High-Resolution Differential Equations*
with Shi, Du, and Jordan, NeurIPS, 2019
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