Second-order methods with global convergence in Convex Optimization

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The Goal: efficient **second-order** optimization methods with global convergence guarantees.

- The rate should be better than that of the **first-order** methods
- We analyse the complexity of the methods alongside suitable problem classes
- Implementable algorithms

Plan of the Talk

I. Intro

- Gradient methods
- Newton's method, classical approach

II. Modern techniques

- Cubic regularization
- Contracting-point methods
- Acceleration

III. Conclusions

$$\min_x f(x), \qquad x \in \mathbb{R}^n$$

f is *differentiable*; $\nabla f(x) \in \mathbb{R}^n$ — gradient of the function,

$$\left[\nabla f(x)\right]^{(i)} = \frac{\partial f(x)}{\partial x^{(i)}}, \qquad 1 \le i \le n$$

The Gradient Method

Iterate, for $k \ge 0$:

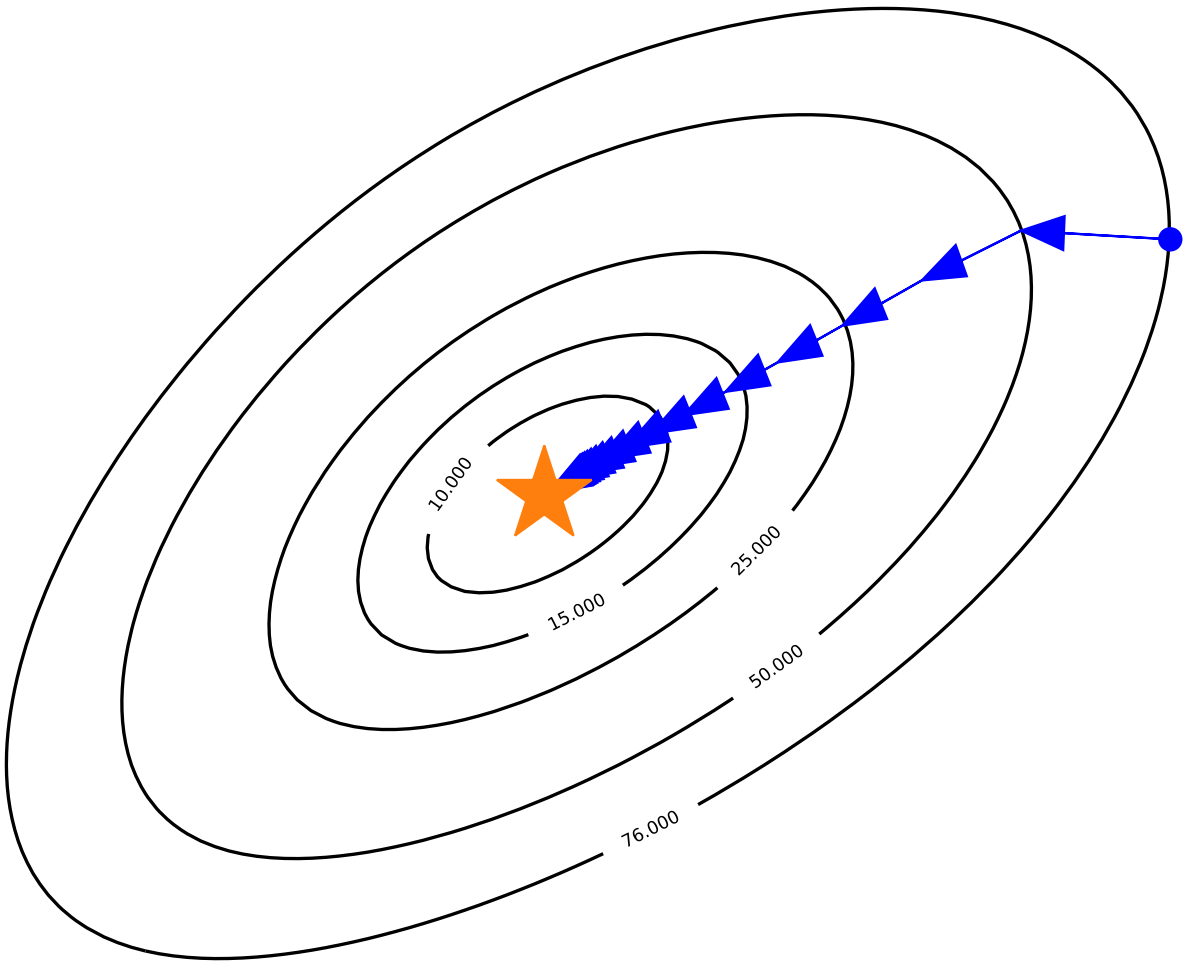
$$x_{k+1} := x_k - \alpha_k \nabla f(x_k), \quad \text{for some} \quad \alpha_k > 0$$

[Cauchy, 1847]

- \+ **Cheap iterations:** $\mathcal{O}(n)$
- \+ **Global convergence**
- – **Slow rate:** $f(x_k) - f^* \le \mathcal{O}(1/k)$

The Gradient Method: Trajectory

$$x_{k+1} \quad := \quad x_k - \alpha_k \nabla f(x_k)$$



$$\boxed{\min_{x \in \mathbb{R}^n} f(x)} \qquad (*)$$

f is convex and differentiable; the gradient is Lipschitz continuous; dimension n is big.

[Nemirovski-Yudin, 1979]: Any first-order method solving $(*)$ needs at least $\mathcal{O}(\frac{1}{\sqrt{\varepsilon}})$ iterations to solve the problem with ε accuracy:

$$f(\bar{x}) - f^* \quad \leq \quad \varepsilon.$$

- The Gradient Method: $\mathcal{O}(\frac{1}{\varepsilon})$ — not optimal
- The Fast Gradient Method: $\mathcal{O}(\frac{1}{\sqrt{\varepsilon}})$ [Nesterov, 1983] — optimal
- Better rates? — impossible for the first-order methods

Newton's Method

$$\boxed{\min_{x \in \mathbb{R}^n} f(x)}$$

The Hessian $\nabla^2 f(x) \in \mathbb{R}^{n \times n}$ is the second-order information about the objective,

$$[\nabla^2 f(x)]^{(i,j)} \quad = \quad \frac{\partial^2 f(x)}{\partial x^{(i)} \partial x^{(j)}}, \qquad 1 \leq i, j \leq n$$

A full quadratic model of the objective, $f(y) \approx \Omega_2(x; y)$, where

$$\Omega_2(x; y) \quad \stackrel{\text{def}}{=} \quad f(x) + \langle \nabla f(x), y - x \rangle + \tfrac{1}{2} \langle \nabla^2 f(x)(y - x), y - x \rangle.$$

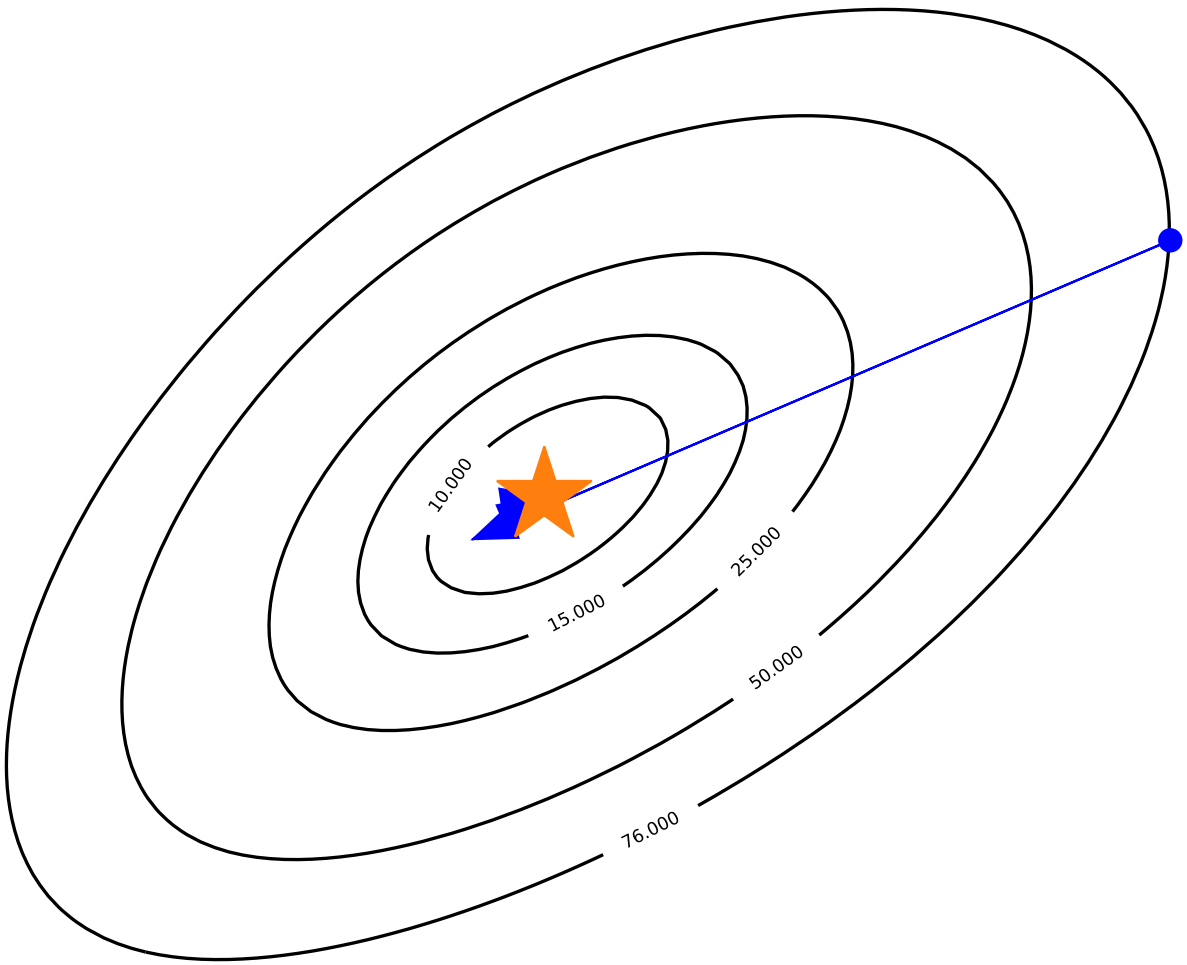
Newton's Method. Iterate, for $k \geq 0$:

$$\boxed{\begin{array}{rcl} x_{k+1} & := & \operatorname*{argmin}_{y \in \mathbb{R}^n} \Omega_2(x_k; y) \\ & = & x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k) \end{array}}$$

[Newton, 1669; Raphson, 1690; Fine-Bennett, 1916; Kantorovich, 1948]

Newton's Method: Trajectory

$$x_{k+1} := x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k)$$



Newton's Method: Analysis

$$x_{k+1} \quad := \quad x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k)$$

- Solving a linear system requires $\mathcal{O}(n^3)$ per iteration
- Fast **local** convergence:

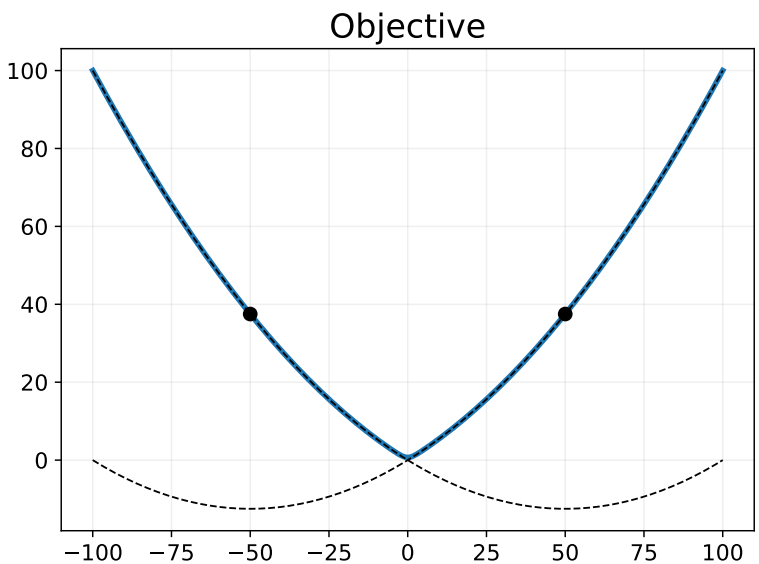
  $$\mathcal{O}(\log \log \tfrac{1}{\varepsilon})$$

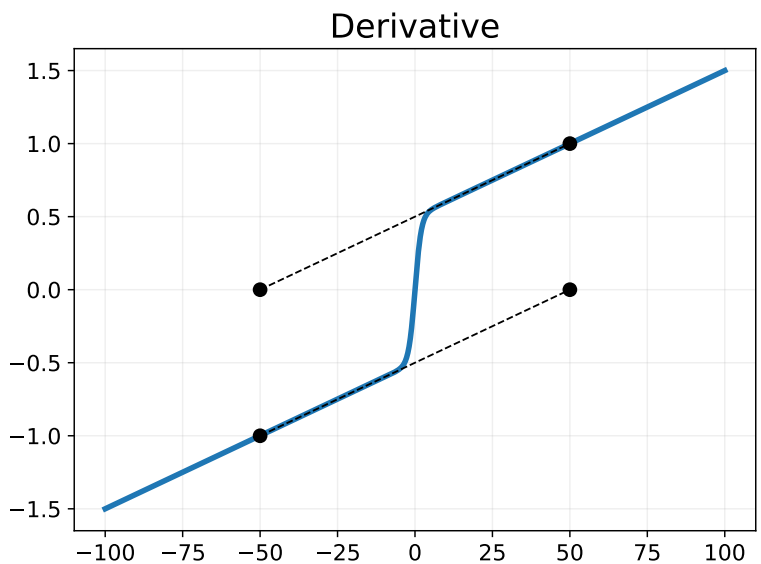
  iterations to find an ε-solution, **when in the neighbourhood of the optimum**
- Global convergence — ?

Newton's Method: Global Behaviour

$$\min_{x\in\mathbb{R}} \left\{ f(x) \;:=\; \log(1+\exp(x)) - \tfrac{1}{2}x + \tfrac{\mu}{2}x^2 \right\}, \qquad \mu \;:=\; 10^{-2}.$$

- The objective is smooth and strongly convex; $x^* = 0$.





The method oscillates between two points!

How to Fix the Newton Method?

- **Damped Newton step** [Kantorovich, 1948]

$$x_{k+1} \quad = \quad x_k - \alpha_k \nabla^2 f(x_k)^{-1} \nabla f(x_k), \qquad \alpha_k \in (0, 1]$$

- **Quadratic regularization**
  [Levenberg, 1944; Marquardt, 1963]

$$x_{k+1} \quad = \quad x_k - \left(\nabla^2 f(x_k) + \alpha_k I\right)^{-1} \nabla f(x_k)$$

- **Trust-region approach**
  [Goldfeld-Quandt-Trotter, 1966; Conn-Gould-Toint, 2000]

$$x_{k+1} \quad = \quad \underset{\|y - x_k\| \leq \Delta_k}{\operatorname{argmin}} \ \Omega_2(x_k; y)$$

Works well in practice. Difficult to establish good global rates

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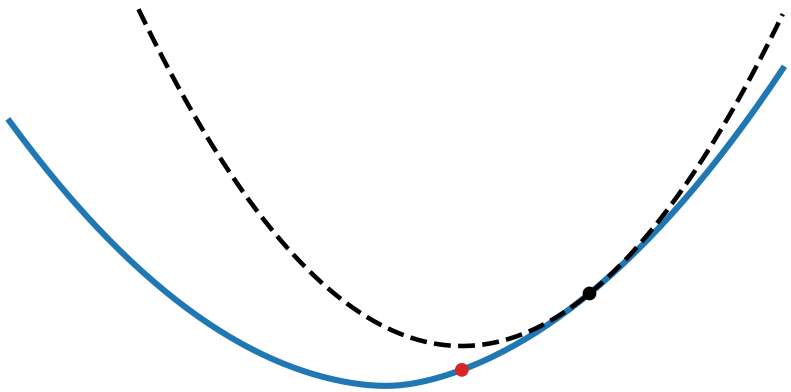
The Gradient Method: a Modern View

$\min_{x \in \mathbb{R}^n} f(x)$

Assumption: gradient is Lipschitz continuous

$$\|\nabla f(y) - \nabla f(x)\| \leq L_1 \|y - x\|, \qquad \forall x, y \in \mathbb{R}^n$$

$$\Rightarrow \qquad f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L_1}{2} \|y - x\|^2$$



The Gradient Step minimizes **the model of the objective**:

$$\begin{aligned} x_{k+1} &= \operatorname*{argmin}_{y \in \mathbb{R}^n} \left[f(x_k) + \langle \nabla f(x_k), y - x_k \rangle + \frac{L_1}{2} \|y - x_k\|^2 \right] \\ &= x_k - \frac{1}{L_1} \nabla f(x_k) \end{aligned}$$

Cubic Regularization of Newton's Method

$\boxed{\min_{x\in\mathbb{R}^n} f(x)}$ **New assumption:** Hessian is Lipschitz continuous

$$\|\nabla^2 f(y) - \nabla^2 f(x)\| \;\leq\; L_2\|y-x\|, \qquad \forall x, y \in \mathbb{R}^n$$

$$\Rightarrow \qquad f(y) \;\leq\; \Omega_2(x;y) + \tfrac{L_2}{6}\|y-x\|^3,$$

where Ω_2 is the second-order Taylor approximation of f.

Newton method with cubic regularization:

$$\begin{aligned} x_{k+1} &= \operatorname*{argmin}_{y\in\mathbb{R}^n}\left[M_H(x_k;y) \overset{\text{def}}{=} \Omega_2(x_k;y) + \tfrac{H}{6}\|y-x_k\|^3\right] \\ &= x_k - \left(\nabla^2 f(x_k) + \tfrac{H\|x_{k+1}-x_k\|I}{2}\right)^{-1}\nabla f(x_k) \end{aligned}$$

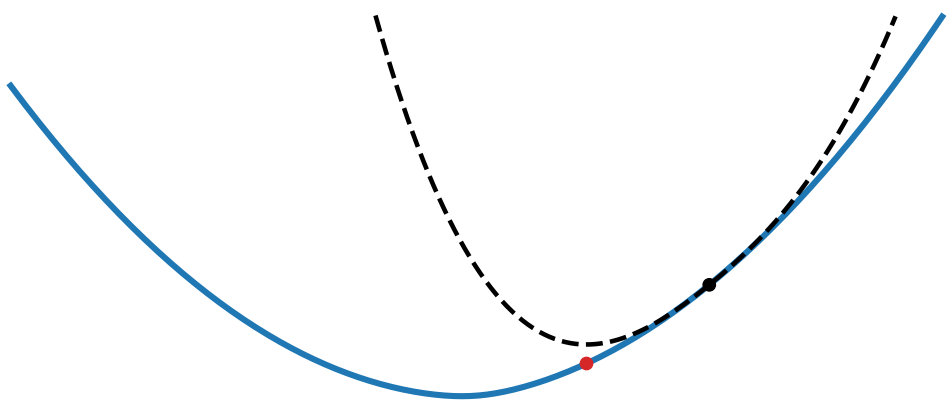
Theorem. Set $H := L_2$. Then, $f(x_k) - f^* \leq \mathcal{O}(1/k^2)$
[Nesterov-Polyak, 2006]

Adaptive Cubic Newton

Iterate, for $k \geq 0$:

$$\boxed{\begin{array}{rcl} x_{k+1} & := & \operatorname*{argmin}_{y \in \mathbb{R}^n} \left[M_H(x_k; y) \right] \\ & & \\ & = & x_k - \left(\nabla^2 f(x_k) + \frac{H r_k}{2} I \right)^{-1} \nabla f(x_k) \end{array}}$$

- $H := 0 \quad \Rightarrow \quad$ the classical Newton's Method
- **Constant choice** $H := L_2$
- **Adaptive strategy** [Nesterov-Polyak, 2006; Cartis-Gould-Toint, 2011; Grapiglia-Nesterov, 2017] ensures $f(x_{k+1}) \leq M_H(x_k; x_{k+1})$

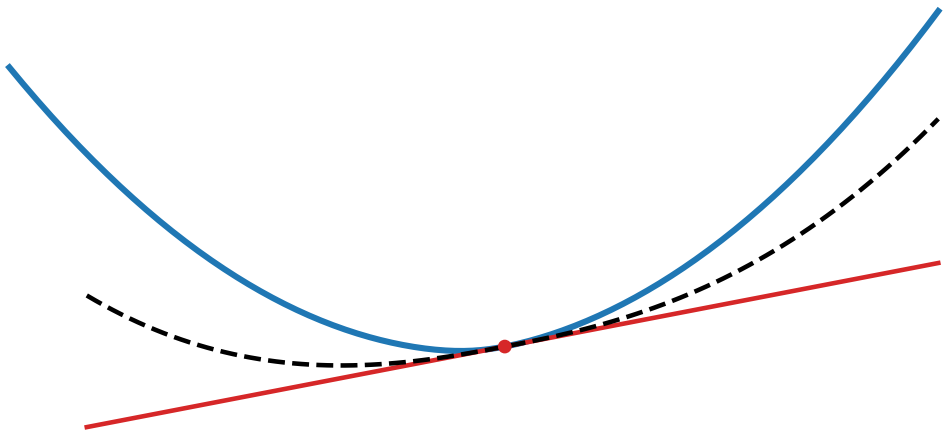


H = 0.1

Global Linear Rates

f is called **uniformly convex** of degree $q \geq 2$ with $\sigma > 0$ iff

$$f(y) \quad \geq \quad f(x) + \langle \nabla f(x), y - x \rangle + \frac{\sigma}{q} \|y - x\|^q, \qquad \forall x, y \in \mathbb{R}^n$$



$q = 2$: strongly convex functions. **GM:** global linear rate.
Second-order methods — ?

Theorem. [D-Nesterov, 2019]:
The global complexity of the adaptive Cubic Newton for $q \in [2, 3]$ is

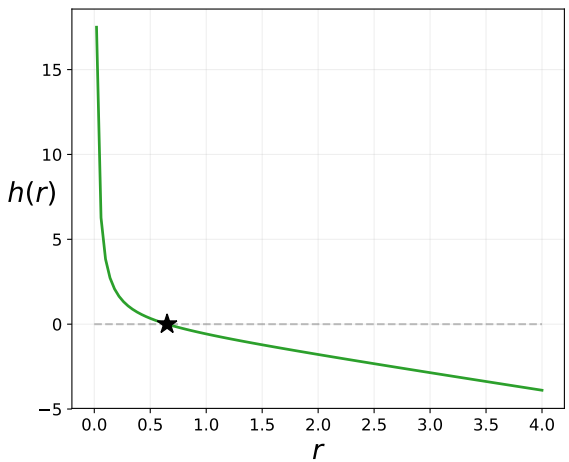
$$\mathcal{O}\Big(\inf_{q \in [2,3]} \omega_q \log \frac{f(x_0) - f^*}{\varepsilon} \Big),$$

ω_q is a second-order condition number $\Rightarrow$ **Cubic Newton** is better than the **Gradient Method**

How to Compute Iteration?

$$\text{Cubic step:} \quad x^+ = x - \left(\nabla^2 f(x) + \frac{Hr^+}{2} I\right)^{-1} \nabla f(x),$$

where $r^+ = \|x^+ - x\|$ is the root of 1-D equation $h(r) = 0$:



We can apply any one-dimensional method (bisection, Newton, ...)

- $\tilde{\mathcal{O}}(1)$ matrix inversions, or one matrix factorization — $\mathcal{O}(n^3)$

Gradient regularization [Mishchenko, 2021; D-Nesterov, 2021]:

$$x^+ = x - \left(\nabla^2 f(x) + \sqrt{\frac{H\|\nabla f(x)\|}{3}} I\right)^{-1} \nabla f(x),$$

- One matrix inversion; fast global rates

Stochastic Subspace Cubic Newton

$\boxed{\min_{x \in \mathbb{R}^n} f(x)}$ where n is Huge

- even $\mathcal{O}(n)$ per iteration can be expensive

Idea: sample random coordinates $S \subset \{1, \dots, n\}$ of size $\tau = |S|$ and apply one step of the Cubic Newton along these coordinates

- The cost of each step is $\mathcal{O}(\tau^3)$

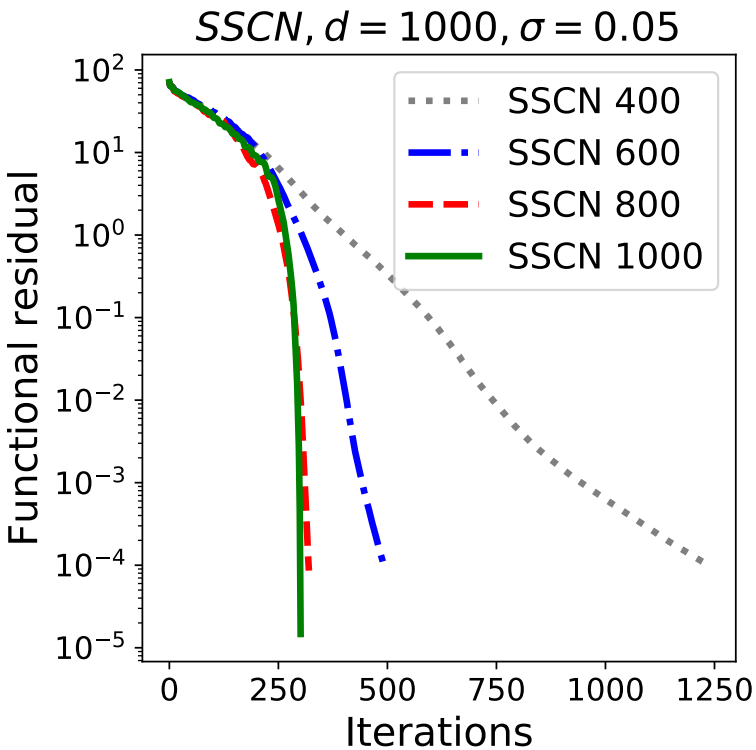
[D-Richtárik, 2018; Hanzely-D-Richtárik-Nesterov, 2020]

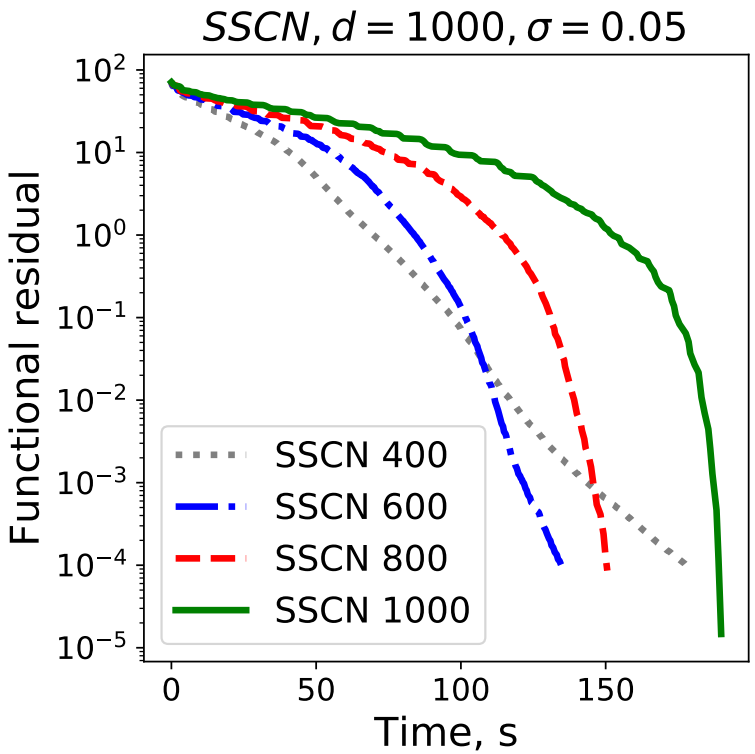
Theorem. The method converges globally, after k iterations:

$$\mathbb{E} f(x_k) - f^* \quad \leq \mathcal{O}\left(\frac{n-\tau}{\tau} \cdot \frac{1}{k} + \left(\frac{n}{\tau}\right)^2 \cdot \frac{1}{k^2} \right)$$

Experiment

$$\min_{x\in\mathbb{R}^d} f(x) \quad = \quad \sigma \log\left(\sum_{i=1}^{m} e^{(\langle a_i,x\rangle - b_i)/\sigma}\right) \quad \approx \quad \max_{i=1}^{m} \langle a_i, x\rangle - b_i$$





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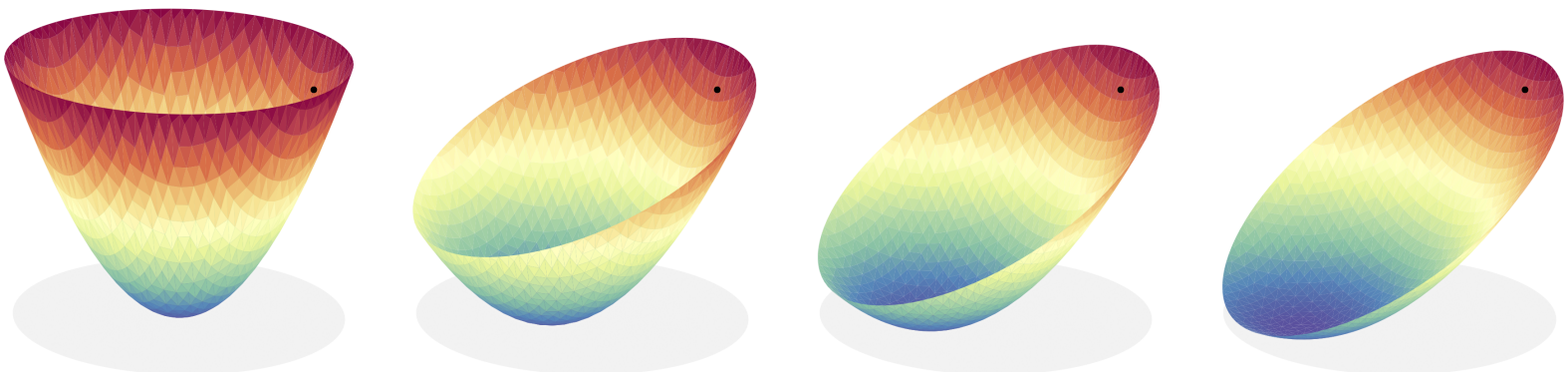
Contraction Technique

Let us consider contraction of the objective:

$$g(x) \quad := \quad f(\gamma x + (1-\gamma)\bar{x}), \qquad \gamma \in [0,1].$$



$\gamma = 1$ $\gamma = 0.8$ $\gamma = 0.7$ $\gamma = 0.6$

Note:

$$\nabla g(x) = \gamma \nabla f(\ldots),$$

$$\nabla^2 g(x) = \gamma^2 \nabla^2 f(\ldots),$$

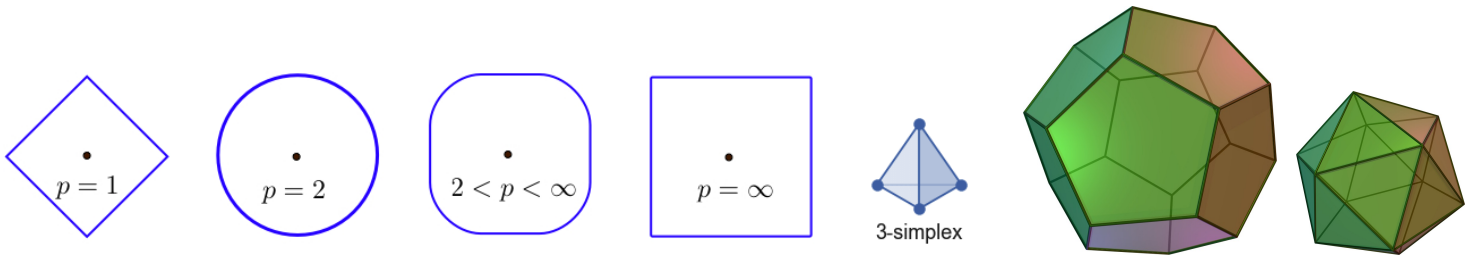
$$\ldots$$

Smoothness properties of $g(\cdot)$ are better than that of $f(\cdot)$

Idea: use γ to balance the error of $g(x) \approx f(x)$ and smoothness

Contracting-Point Methods

$\min_{x \in Q} f(x)$ where $Q \subset \mathbb{R}^n$ is a bounded convex set, e.g.:



Conceptual Contracting-Point Method. Iterate, $k \geq 0$:

$$\begin{aligned} v_{k+1} &\approx \operatorname*{argmin}_{v \in Q} f(\gamma_k v + (1-\gamma_k)x_k), \\ x_{k+1} &= \gamma_k v_{k+1} + (1-\gamma_k)x_k \end{aligned}$$

Approximate f by p-th order Taylor's polynomial.

- $p = 1$: The Conditional Gradient Method [Frank-Wolfe, 1956]
- $p = 2$: Contracting Newton [D-Nesterov, 2020]

Contracting Newton

$$\min_{x \in Q} f(x)$$

Iterate, for $k \geq 0$:

$$x_{k+1} \quad := \quad \operatorname{argmin}_y \left\{ \Omega_2(x_k; y) \ : \ y \in x_k + \gamma_k (Q - x_k) \right\}$$

where Ω_2 is the second-order approximation of f

- $\gamma_k = 1$: The classical Newton's Method
- Interpretation: regularization of quadratic model by the assymmetric trust region

Theorem. Set $\gamma_k = \frac{3}{k+3} \quad \Rightarrow \quad$ **global rate:** $f(x_k) - f^* \leq \mathcal{O}(1/k^2)$

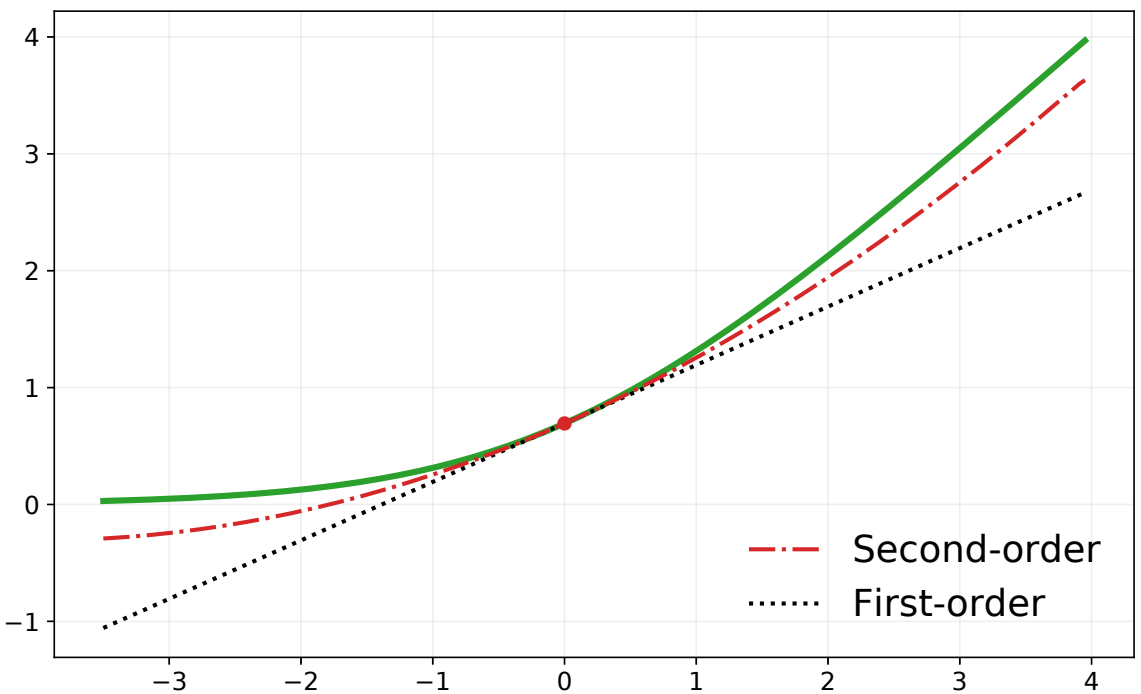
Contracting Newton: Interpretation

1. f is convex: $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$
2. $\nabla^2 f$ is Lipschitz continuous:

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \quad \leq \quad L_2 \|x - y\|$$

Convexity + Smoothness $\Rightarrow$ **tighter lower bound**: $\exists \gamma_{x,y} \in (0, 1]$

$$f(y) \quad \geq \quad f(x) + \langle \nabla f(x), y - x \rangle + \frac{\gamma_{x,y}}{2} \langle \nabla^2 f(x)(y - x), y - x \rangle$$



Cubic Newton vs. Contracting Newton

Cubic Newton, H_k	**Contracting Newton**, γ_k
global *upper* approximation	global *lower* model
fixed Euclidean norm	affine-invariant
-	bounded domain

Complexity

- Convex functions: $\mathcal{O}(\frac{1}{\sqrt{\varepsilon}})$; $\gamma_k = \frac{3}{3+k}$
- Strongly convex functions: $\mathcal{O}(\omega \log \frac{f(x_0)-f^*}{\varepsilon})$; $\gamma_k = \frac{1}{1+\omega}$
- Local quadratic convergence: $\gamma_k = 1$

Inexact Contracting Newton

$$x_{k+1} \quad = \quad \operatorname*{argmin}_{y} \Big\{ \Omega_2(x_k; y) \ : \ y \in x_k + \gamma_k(Q - x_k) \Big\}$$

How to compute the iteration?

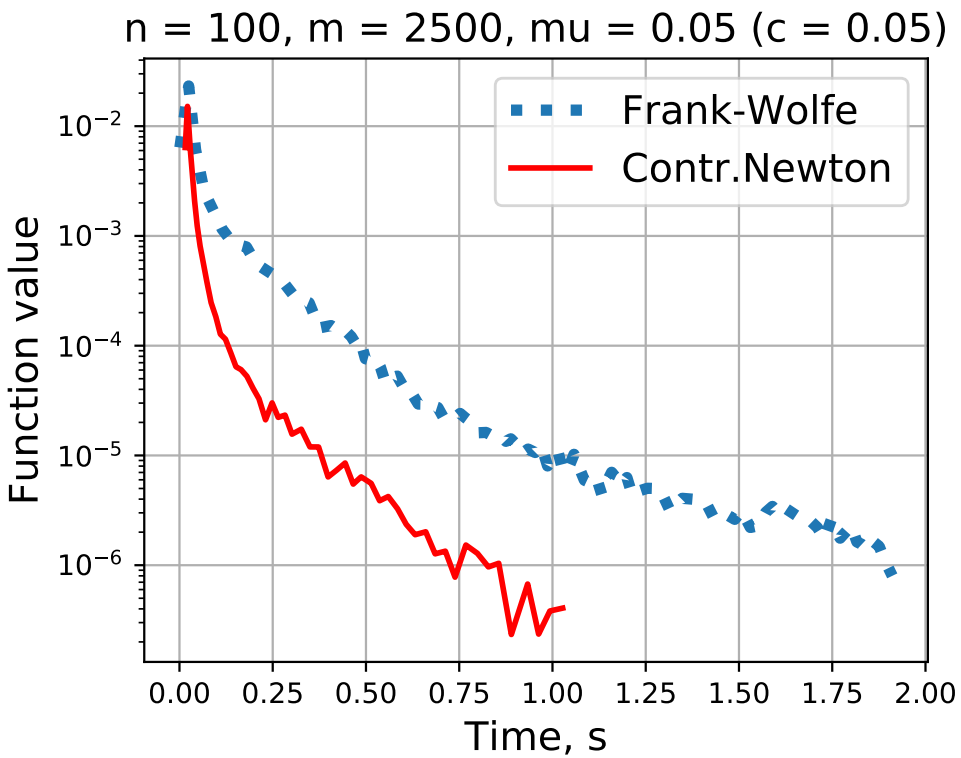
- At each step we solve the subproblem inexactly by the first-order Frank-Wolfe algorithm
- We have full control over the required accuracy

Theorem. To reach $f(x_K) - f^* \leq \varepsilon$ it needs

- $K = \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right)$ oracle calls for f
- $\mathcal{O}(\frac{1}{\varepsilon})$ linear minimization oracle calls for Q totally

Experiment: Log-sum-exp over the Simplex

$$\min_{x \in \mathbb{R}^n_+} \left\{ f(x) \quad = \quad \mu \log \left(\sum_{i=1}^{m} e^{(\langle a_i, x \rangle - b_i)/\mu} \right) \quad : \quad \sum_{i=1}^{n} x^{(i)} = 1 \right\}$$



two times faster

Finite-sum minimization: $f(x) = \frac{1}{M} \sum_{i=1}^{M} f_i(x)$

Big $M \Rightarrow$ computing $\nabla f(x)$ and $\nabla^2 f(x)$ is **expensive**

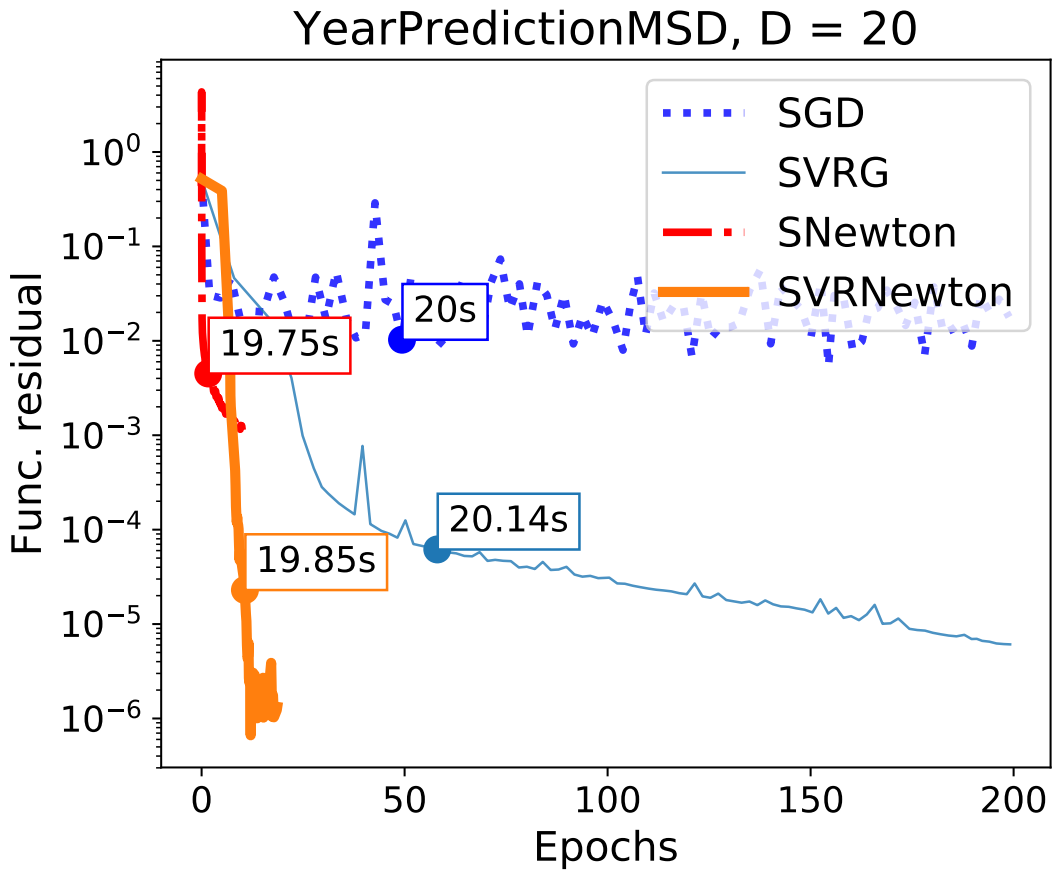
Idea: sample random batch $B \subseteq \{1, \ldots, M\}$ and approximate

$$\nabla f(x) \approx \frac{1}{|B|} \sum_{i \in B} \nabla f_i(x), \qquad \nabla^2 f(x) \approx \frac{1}{|B|} \sum_{i \in B} \nabla^2 f_i(x)$$

Idea #2: at some iterations recompute the full gradient and Hessian — *variance reduction* [Schmidt-Roux-Bach, 2011]

New algorithm: **Stochastic Contracting Newton Method** with global complexities: $\mathcal{O}(\frac{1}{\varepsilon^{1/2}})$ iterations and $\mathcal{O}(\frac{1}{\varepsilon^{3/2}})$ total random samples among all batches

Experiments: Stochastic Methods for Logistic Regression



The problem with big dataset size ($M = 463715$) and small dimension ($n = 90$)

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Problem class: convex functions with Lipschitz Hessian

Basic Cubic Newton: $f(x_k) - f^* \leq \mathcal{O}(1/k^2)$

Accelerated Cubic Newton: $\mathcal{O}(1/k^3)$ [Nesterov, 2008]

Accelerated second-order prox: $\mathcal{O}(1/k^{3.5})$ [Monteiro-Svaiter, 2013]

(extra one-dimensional search each iteration)

Optimal rate, matching the lower bound [Arjevani-Shamir-Shiff, 2019]

Problem class: convex functions with bounded second and fourth derivatives

Superfast second-order schemes: $\mathcal{O}(1/k^5)$ [Nesterov, 2020; Kamzolov-Gasnikov, 2020]

- Approximation of third derivative by finite-differences

General Accelerating Scheme

- **Contracting-Point Method:**

$$\boxed{\begin{array}{rcl} v_{k+1} & \approx & \operatorname*{argmin}_{x \in Q} f(\gamma_k x + (1-\gamma_k)x_k), \\ x_{k+1} & = & \gamma_k v_{k+1} + (1-\gamma_k)x_k. \end{array}}$$

One step of 2-order Taylor's approximation $\Rightarrow$ $\mathcal{O}(1/k^2)$-rate.

- **Contracting Proximal Method** [D-Nesterov, 2019]:

$$\boxed{\begin{array}{rcl} v_{k+1} & \approx & \operatorname*{argmin}_{x \in Q} \left\{ f(\gamma_k x + (1-\gamma_k)x_k) + \frac{1}{A_{k+1}} \beta_d(v_k; x) \right\}, \\ x_{k+1} & = & \gamma_k v_{k+1} + (1-\gamma_k)x_k. \end{array}}$$

$\beta_d(v_k; x) = d(x) - d(v_k) - \langle \nabla d(v_k), x - v_k \rangle$ is Bregman divergence

Theorem. Set $d(x) = \frac{1}{3}\|x\|^3$, $A_k = \frac{k^3}{L_2}$, $\gamma_k = 1 - \frac{A_k}{A_{k+1}}$, then

$\tilde{\mathcal{O}}(1)$ steps of the basic method $\Rightarrow$ $\mathcal{O}(1/k^3)$-rate.

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Conclusions

1. To globalize the Newton's method we need to do regularization
   - Cubic Newton — explicit regularizer, $\|\cdot\|^3$
   - Contracting Newton — implicit regularization by contraction
   - Acceleration: prox-point and contracting-point together

2. We can solve the composite problems

$$\min_x \left\{ F(x) \;:=\; f(x) + \psi(x) \right\}$$

   and

$$\min_x \left\{ F(x) \;:=\; \phi(f(x)) \right\}$$

   where f is a *smooth* component

3. In practice: we can use stochastic approximations and inexact methods with first-order subsolvers, preserving the global rates

Open Questions

- Efficient implementation: parallel and distributed systems

  Note: computation of $\nabla^2 f(x)h$ for any $h \in \mathbb{R}^n$ has the same cost as for $\nabla f(x)$

- Worst-case complexities can be too pessimistic

  $\Rightarrow$ benefits of using two-level schemes

- Theory of the Damped Newton: $x^+ = x - \alpha \nabla^2 f(x)^{-1} \nabla f(x)$

  Hint: different problem classes
  - **Self-Concordant Functions** [Nesterov-Nemirovski, 1994; Dvurechensky-Nesterov, 2018]
  - **Generalized S.C.** [Bach, 2010; Sun-Tran–Dinh, 2019]
  - **Hessian Stability** [Karimireddy-Stich-Jaggi, 2018]

- Quasi-Newton methods