Minimizing quasi-self-concordant functions by gradient regularization of Newton method

Nikita Doikov

EPFL, Switzerland

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Outline

I. Introduction: Quasi-Self-Concordance

II. Gradient Regularization of Newton Method

III. Dual and Accelerated Newton

IV. Applications and Conclusions

Problem

Two black-box convex functions:

$$\min_{x} \Big[F(x) = f(x) + \psi(x) \Big] \qquad (*)$$

- ► f is differentiable (sufficiently smooth)
- $\psi: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper closed convex function

In this talk: we show that the main cost of solving (*) is in ψ .

Assume we can solve problems with a quadratic smooth part:

$$\min_{x} \left[\frac{1}{2} \langle Ax, x \rangle - \langle b, x \rangle + \psi(x) \right]$$

Main Theorem. For solving (*), it is enough to solve the quadratic problem

$$\mathcal{O}\left(\mathsf{MD}\cdot \mathsf{ln}\, \frac{1}{\varepsilon}\right)$$
 times.

NB: No strong/uniform convexity needed!

Problem Classes

Complexity of the gradient methods:

Bounds on the second derivative

For example, Lipschitz gradient:

$$0 \leq \nabla^2 f(x) \leq L_1 I, \quad \forall x$$

or, Relative smoothness:

$$\alpha \nabla^2 d(x) \leq \nabla^2 f(x) \leq \beta \nabla^2 d(x), \quad \forall x$$

[Bauschke-Bolte-Teboulle, 2016; Van Nguyen, 2017; Lu-Freud-Nesterov, 2018]

Complexity of the second-order methods:

▶ Bounds on the third derivative!

Self-Concordant functions [Nesterov-Nemirovski, 1994]:

$$\nabla^3 f(x)[u,u,u] \leq M_{\mathfrak{sc}} \langle \nabla^2 f(x)u,u \rangle^{3/2}, \quad \forall x,u$$

- Affine-invariant
- Efficiency of the damped Newton method for logarithmic barriers, e.g. $f(x) = -\ln x$

Lipschitz Hessian and Lipschitz Third Derivative

Functions with Lipschitz Hessian:

$$\nabla^3 f(x)[u,u,u] \leq L_2 ||u||^3, \quad \forall x, u$$

- ► Fixed global norm (no affine-invariance)
- ▶ Efficiency of the Cubic regularization of Newton's method

[Nesterov-Polyak, 2006; Cartis-Gould-Toint 11; Grapiglia-Nesterov, 2017]

Functions with Lipschitz third derivative:

$$\nabla^3 f(x)[u,u,v] \leq \sqrt{2L_3} \langle \nabla^2 f(x)u,u \rangle^{1/2} \|u\| \|v\|, \qquad \forall x,u,v$$

► Faster rates for second-order schemes

[Nesterov, 2018; 2021; Kamzolov-Gasnikov-Dvurechensky, 2021; D-Mishchenko-Nesterov, 2022]

Quasi-Self-Concordant Functions

The standard Euclidean norm for some fixed operator $B = B^{\top} \succ 0$:

$$||u|| := \langle Bu, u \rangle^{1/2}, \qquad ||s||_* := \langle s, B^{-1}s \rangle^{1/2},$$

and denote the local norm:

$$||u||_{x} := \langle \nabla^2 f(x)u, u \rangle^{1/2}.$$

In this talk, we assume that f is quasi-self-concordant with constant $M \ge 0$:

$$\nabla^3 f(x)[u,u,v] \leq M||u||_x^2||v||, \qquad \forall u,v$$

► Combination of the Lipschitzness and classic Self-Concordance

[Bach, 2010; Sun-Tran-Dinh, 2019; Karimireddy-Stich-Jaggi, 2018]

Examples

$$\nabla^3 f(x)[u,u,v] \leq M||u||_x^2||v||$$

Example 0: f is quadratic. Then M = 0.

Example 1:
$$f(x) = e^x$$
. Then $f'''(x) = f''(x) = e^x \Rightarrow M = 1$.

Example 2:
$$f(x) = \ln(1 + e^x)$$
. Then

$$f'(x) = \frac{1}{1+e^{-x}}, \qquad f''(x) = f'(x) \cdot (1-f'(x)),$$

$$f'''(x) = f''(x) \cdot (1 - 2f'(x)).$$

Thus

$$|f'''(x)| = f''(x) \cdot |1 - \frac{2}{1 + e^{-x}}| \le f''(x) \Rightarrow M = 1.$$

Examples

Example 3: (Generalized Linear Models):

$$f(x) = \frac{1}{m} \sum_{i=1}^{m} \phi(\langle a_i, x \rangle),$$

and $\phi: \mathbb{R} \to \mathbb{R}$ is quasi-SC loss function $\Rightarrow f(x)$ is quasi-SC.

Example 4: (Soft Maximum):

$$\min_{x} f(x) := \mu \ln \left(\sum_{i=1}^{m} \exp\left(\frac{\langle a_{i}, x \rangle - b_{i}}{\mu}\right) \right) \approx \max_{1 \leq i \leq m} \left[\langle a_{i}, x \rangle - b_{i}\right].$$

$$f(x)$$
 is quasi-SC with $M = \frac{2}{\mu}$ for $B := \sum_{i=1}^{m} a_i a_i^{\top}$.

Example 5: (Matrix Scaling, $A \in \mathbb{R}_+^{n \times n}$):

$$f(x,y) = \sum_{1 \le i, i \le n} A_{ij} e^{x_i - x_j}, \quad x, y \in \mathbb{R}^n$$

is quasi-SC with $M = \sqrt{2}$ for B := I.

Basic Operations

- 1. $f(\cdot) = f_1(\cdot) + f_2(\cdot)$ is quasi-SC with $M = \max\{M_1, M_2\}$
- 2. Adding to f an <u>arbitrary</u> convex quadratic function does not change M
- 3. Scale-invariance: $f(\cdot) \mapsto cf(\cdot)$, c > 0, does not change M
- 4. For an affine substitution, f(x) = g(Ax + b), we need to update the global norm:

$$B_f = A^{\top} B_g A$$

(no affine invariance)

Main Bounds

Lemma. for quasi-SC f we have, for any x, y:

$$\nabla^2 f(x) e^{-M\|x-y\|} \quad \leq \quad \nabla^2 f(y) \quad \leq \quad \nabla^2 f(x) e^{M\|x-y\|}$$

 \Rightarrow the Hessian is stable: For any x,y s.t. $||x-y|| \le r := \frac{1}{M}$ it holds

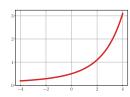
$$\frac{1}{e}\nabla^2 f(x) \leq f(y) \leq e\nabla^2 f(x).$$

[Cohen-Madry-Tsipras-Vladu, 2017; Karimireddy-Stich-Jaggi, 2018]

The gradient approximation:

$$\|\nabla f(y) - \nabla f(x) - \nabla^2 f(x)(y - x)\|_* \le M \|y - x\|_x^2 \cdot \varphi(M \|y - x\|),$$

where $\varphi(t) := \frac{e^t - t - 1}{t^2} \ge 0$ is a convex and monotone function:



Bounds on the Function

Using our previous function $\varphi(t):=\frac{e^t-t-1}{t^2}\geq 0$, we have global upper and lower second-order models:

$$\begin{split} f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle + ||\boldsymbol{y} - \boldsymbol{x}||_{\boldsymbol{x}}^2 \cdot \varphi(M||\boldsymbol{y} - \boldsymbol{x}||) \\ f(\boldsymbol{y}) \\ f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle + ||\boldsymbol{y} - \boldsymbol{x}||_{\boldsymbol{x}}^2 \cdot \varphi(-M||\boldsymbol{y} - \boldsymbol{x}||) \end{split}$$

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Gradient Regularization

Problem: $\min_{x} \left[F(x) = f(x) + \psi(x) \right]$, where f is quasi-SC.

Consider one regularized Newton step, for $\beta \geq 0$:

$$x^{+} = \underset{y}{\operatorname{argmin}} \left[\langle \nabla f(x), y - x \rangle + \frac{1}{2} ||y - x||_{x}^{2} + \frac{\beta}{2} ||y - x||^{2} + \psi(y) \right]$$

$$\Leftrightarrow \quad \nabla f(x) + [\nabla^2 f(x) + \beta B](x^+ - x) \in -\partial \psi(x^+).$$

Lemma. Set $\beta := \sigma \|\nabla f(x) + s\|_*$ for any $s \in \partial \psi(x)$ and $\sigma \geq M$. Then,

- 1. $||x^+ x|| \le \frac{1}{M}$
- 2. $||x^+ x||_x^2 \le \frac{||\nabla f(x) + s||_*}{M}$

[Polyak, 2009; Ueda-Yamashita, 2009; Mishchenko, 2021; D-Nesterov, 2021]

Progress of One Step

Main Lemma. Let $\beta := \sigma \|F'(x)\|_*$ for $F'(x) \in \partial F(x)$ and $\sigma \geq M$.

Then, for the specific subgradient

$$F'(x^+) := \nabla f(x^+) - \nabla f(x) - [\nabla^2 f(x) + \beta B](x^+ - x) \in \partial F(x^+),$$

we have

$$\langle F'(x^+), x - x^+ \rangle \geq \frac{1}{2\beta} \|F'(x^+)\|_*^2.$$

Note: by convexity, we conclude

$$F(x) - F(x^+) \ge \langle F'(x^+), x - x^+ \rangle \ge \frac{1}{2\beta} \|F'(x^+)\|_*^2.$$

Gradient Regularization of Newton Method

Init: $x_0 \in \text{dom } \psi \text{ and } g_0 = \|F'(x_0)\|_* \text{ for any } F'(x_0) \in \partial F(x_0).$

Iteration, $k \ge 0$:

▶ For some $\sigma_k \ge 0$, compute x_{k+1} s.t.

$$\nabla f(x_k) + [\nabla^2 f(x_k) + \sigma_k g_k B](x_{k+1} - x_k) \in -\partial \psi(x_{k+1})$$

▶ Update $g_{k+1} = \|\nabla f(x_{k+1}) - \nabla f(x_k) - [\nabla^2 f(x_k) + \sigma_k g_k B](x_{k+1} - x_k)\|_*$

Theorem. Set $\sigma_k := M$. Then, we have the global linear rate:

$$F(x_k) - F^* \le \exp\left(-\frac{k}{8MD}\right) \left(F(x_0) - F^*\right) + \exp\left(-\frac{k}{4}\right) g_0 D,$$

where $D := \max\{\|x - x^*\| : F(x) \le F(x_0)\}.$

$$\Rightarrow$$
 the global complexity: $\mathcal{O}\left(MD \ln \frac{1}{\varepsilon}\right)$ to find $F(x_k) - F^* \leq \varepsilon$

Super-Universal Newton Method

In our method, we set $\sigma_k := M$

▶ Instead, we can use a simple adaptive search:

Init: Choose $x_0 \in \text{dom } \psi$, $g_0 = ||F'(x_0)||_*$, and $\sigma_0 > 0$. Iteration, $k \ge 0$:

1. Find smallest $j_k \geq 0$ s.t. for $\beta_k := 4^{j_k} \sigma_k g_k$ and x^+ : $\nabla f(x_k) + \left[\nabla^2 f(x_k) + \beta_k B\right](x^+ - x_k) \in -\partial \psi(x^+)$ it holds

$$\langle F'(x^+), x_k - x^+ \rangle \geq \frac{1}{2\beta_k} ||F'(x^+)||_*^2.$$

2. Set
$$x_{k+1} = x^+$$
, $g_{k+1} = ||F'(x^+)||_*$, and $\sigma_{k+1} = \frac{4^{j_k} \sigma_k}{4}$.

[D-Mishchenko-Nesterov, 2022]

- ▶ The method does not need to know any parameters
- ► Automatic adjustment to the right problem class
- In average: one extra oracle call per iteration

Local Analysis

The classic Newton's method has a local quadratic convergence, when close to the solution [Fine, 1916; Bennett, 1916; Kantorovich, 1948]

▶ We have the same local rate for our method!

Theorem. Let $\nabla^2 f(x) \succeq \mu I, \forall x$. Let

$$||F'(x_0)||_* \le \frac{\mu}{2M}$$
 (a neighborhood of the solution)

Then,

$$||F'(x_k)||_* \leq \frac{\mu}{2M} \cdot \left(\frac{1}{e}\right)^{2^k}.$$

P Quadratic convergence: to find $||F'(x_k)||_* \le \varepsilon$ it is enough to perform $k = \mathcal{O}(\ln \ln \frac{\mu}{M\varepsilon})$ steps.

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Proximal Viewpoint

Proximal-Point Method:

$$x_{k+1} \approx \underset{y}{\operatorname{argmin}} \left[h_k(y) = F(y) + \frac{1}{2a_{k+1}} ||y - x_k||^2 \right]$$

[Moreau, 1965; Rockafellar, 1976; Martinet, 1978; Solodov-Svaiter, 2002]

Note: the subproblem $h_k(\cdot)$ is **strongly convex** with constant $\mu = \frac{1}{2k+1}$. We have

$$h'_k(y) = F'(y) + \frac{1}{a_{k+1}}B(y-x_k).$$

The neighborhood of local quadratic convergence:

$$||h'_k(x_k)||_* = ||F'(x_k)||_* \stackrel{(?)}{\leq} \frac{\mu}{2M} = \frac{1}{2a_{k+1}M}.$$

Set:
$$\left|a_{k+1} := \frac{1}{2M\|F'(x_k)\|_*}\right| \Rightarrow \text{ we can minimize } h_k(\cdot) \text{ up to any}$$

accuracy by Newton's method

Dual Newton Scheme

Init: $x_0 \in \text{dom } \psi \text{ and } g_0 = ||F'(x_0)||_* \text{ for } F'(x_0) \in \partial F(x_0), \ \delta > 0.$

Iteration, k > 0:

- 1. Set $z_0 = x_k$
- **2.** For t > 0 iterate:
 - ▶ Compute z_{t+1} s.t.

$$\nabla f(z_t) + \left[\nabla^2 f(z_t) + Mg_k B\right](z_{t+1} - z_t) \in -\partial \psi(z_{t+1})$$

▶ Until $||s_{t+1}||_* \leq \frac{2Mg_k\delta}{(k+1)^2}$, where

$$s_{t+1} := \nabla f(z_{t+1}) - \nabla f(z_t) - \nabla^2 f(z_t)(z_{t+1} - z_t).$$

- 3. Set $x_{k+1} = z_{t+1}$ and $g_{k+1} = ||s_{t+1} 2Mg_kB(x_{k+1} x_k)||_*$
- **4**. If $g_{k+1} \leq \delta$ then **return** x_{k+1}

Convergence of the Dual Newton

Theorem. We have the global linear rate for the gradient norm:

$$\|F'(x_k)\|_* \le \exp\left(2M^2(\|x_0 - x^*\|^2 + 2\delta)^2 - \frac{k}{2}\right)\|F'(x_0)\|_*$$

The total number N_k of second-order oracle calls is bounded as

$$N_k \leq k \cdot \left(1 + \frac{1}{\ln 2} \ln \ln \frac{(k+1)^2}{2M\delta}\right).$$

- \Rightarrow the method stops after $\mathcal{O}(M^2||x_0 x^*||^2)$ iterations.
 - + Possibility of restarts
 - + Convergence in terms of the (sub)gradient norm
 - The condition number is worse: $(MD)^2$ vs. MD

Acceleration

Idea. Contraction + regularization, for $\gamma \in (0,1)$:

$$\min_{y} \left[h_{k}(y) = A_{k+1} f(\gamma y + (1-\gamma)x_{k}) + a_{k+1} \psi(y) + \frac{1}{2} \|y - v_{k}\|^{2} \right]$$

where $A_k := A_0(1-\gamma)^{-k}$, $a_k := A_k - A_{k-1}$.

Contracting Proximal Method. Iteration, $k \ge 0$:

$$v_{k+1} \approx \underset{y}{\operatorname{argmin}} h_k(y)$$

 $x_{k+1} = \gamma v_{k+1} + (1 - \gamma)x_k$

[Nesterov, 1983; Güler, 1991; Lin-Mairal-Harchaoui, 2018; D-Nesterov, 2020]

Theorem.
$$A_k(F(x_k) - F^*) + \frac{1}{2} \sum_{i=1}^k ||v_i - v_{i-1}||^2 \le \mathcal{O}(||x_0 - x^*||^2)$$

- ► Global linear rate by design: $F(x_k) F^* \leq \mathcal{O}\left(\frac{\|x_0 x^*\|^2}{\exp(\gamma k)}\right)$
- ► Control over $||v_i v_{i-1}||$

Choice of γ

How to minimize $v_{k+1} \approx \underset{v}{\operatorname{argmin}} h_k(y)$?

Consider
$$\varphi(y) = f(\gamma y + (1 - \gamma)x_k), \quad \gamma \in (0, 1)$$

- $ightharpoonup \gamma = 0$, we have $\varphi(y) \equiv f(x_k)$
- $ightharpoonup \gamma = 1$, we have $\varphi(y) = f(y)$

The parameter of quasi-SC is $M_{\varphi} = \gamma M$.

Hence, the **Dual Newton Method** needs the following number of iterations at step $k \ge 0$, to approximate $v_k^* = \operatorname{argmin} h_k(y)$:

$$I_k \le \mathcal{O}\left(M_{\varphi}^2 \|v_k - v_k^{\star}\|^2\right) = \mathcal{O}\left(\gamma^2 M^2 \|v_k - v_{k+1}\|^2\right)$$

Totally, after k steps:

$$\sum_{i=1}^{k} I_{i} \leq \mathcal{O}\left(\gamma^{2} M^{2} \sum_{i=1}^{k} \|v_{i} - v_{i-1}\|^{2}\right) \leq \mathcal{O}\left(\gamma^{2} M^{2} \|x_{0} - x^{*}\|^{2}\right) \stackrel{(?)}{=} \frac{1}{\gamma}$$

$$\Rightarrow$$
 optimal choice: $\gamma = [M||x_0 - x^*||]^{-2/3}$

Convergence Rates Summary

Problem:
$$\min_{x} \left[F(x) = f(x) + \psi(x) \right]$$

1. Primal Newton with Gradient Regularization:

$$\mathcal{O}\left(MD \ln \frac{1}{\varepsilon}\right)$$
 second-order oracle calls for f

2. Dual Newton:

$$\mathcal{O}\left(\left[\mathbf{M}\|\mathbf{x}_0 - \mathbf{x}^{\star}\|\right]^2 \ln \frac{1}{\varepsilon} \ln \ln \frac{1}{\varepsilon^2}\right)$$

3. Accelerated Newton:

$$\tilde{\mathcal{O}}\left(\left[\mathbf{M}\|\mathbf{x}_0-\mathbf{x}^{\star}\|\right]^{2/3}\right)$$

Optimal? Most probably yes!

► Matches the lower bound for the *ball minimization oracle* [Carmon-Jambulapati-Jiang-Jin-Lee-Sidford-Tian, 2020]

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Pointwise Maximum

Non-smooth problem:

$$\min_{x \in \mathbb{R}^n} \Big[f(x) = \max_{1 \le i \le m} \Big[\langle a_i, x \rangle - b_i \Big] \Big]$$

Find x_k s.t. $f(x_k) - f^* \le \varepsilon$.

- 1. Subgradient method: $\mathcal{O}(1/\varepsilon^2)$ [Shor, 1962]
- 2. Smoothing technique: $f_{\mu}(x) \leq f(x) \leq f_{\mu}(x) + \mu D^2$ where

$$f_{\mu}(x) := \mu \ln \left(\sum_{i=1}^{m} \exp \left(\frac{\langle a_i, x \rangle - b_i}{\mu} \right) \right)$$

- ▶ Need to choose $\mu = \mathcal{O}(\varepsilon)$
- Lipschitz gradient $L(f_{\mu}) = 1/\mu = \mathcal{O}(1/arepsilon)$
- Fast Gradient Method

$$\mathcal{O}\Big(\sqrt{L(f_{\mu})D^{2}\varepsilon^{-1}}\Big) = \mathcal{O}(1/\varepsilon)$$
 [Nesterov, 2003]

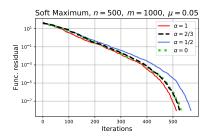
- 3. Newton's Method. f_{μ} is quasi-SC with $M=2/\mu=\mathcal{O}(1/\varepsilon)$.
 - ▶ Primal Newton Method: $\tilde{\mathcal{O}}(MD) = \tilde{\mathcal{O}}(1/\varepsilon)$
 - ► Accelerated Newton: $\tilde{\mathcal{O}}((MD)^{2/3}) = \tilde{\mathcal{O}}(1/\varepsilon^{2/3})$!

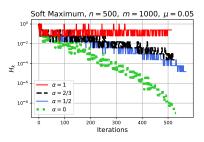
Experiment: Soft Maximum

$$\min_{x} f_{\mu}(x)$$

Iterate $k \ge 0$:

$$x_{k+1} = x_k - \left(\nabla^2 f_{\mu}(x_k) + \left(\sigma \|\nabla f_{\mu}(x_k)\|\right)^{\alpha} B\right)^{-1} \nabla f(x_k)$$





Conclusions

- ightharpoonup Quasi-SC functions pprox loss functions with exponential tails
- ► The Newton method is very efficient in this case (fast global linear rate): $\mathcal{O}\left(MD\ln\frac{1}{\varepsilon}\right)$
- We can accelerate: $\tilde{\mathcal{O}}((MD)^{2/3})$
- Solving

$$\min_{x} \Big[F(x) = f(x) + \psi(x) \Big]$$

is as difficult as

$$\min_{x} \left[\langle Ax, x \rangle - \langle b, x \rangle + \psi(x) \right]$$

References:

- 1. Doikov, N., Mishchenko, K. and Nesterov, Y., 2022. Super-universal regularized Newton method. SIAM Journal on Optimization.
- 2. Doikov, N., 2023. Minimizing quasi-self-concordant functions by gradient regularization of Newton method. arXiv:2308.14742.

Open Questions

- Lower complexity bounds
- Practical accelerated schemes (currently, no local superlinear convergence)
- Comparison with polynomial-time Interior-Point schemes
- Other problem classes? Minimizing an arbitrary convex analytic function
- ► Consequences for non-convex optimization

Thank you very much for your attention!

Happy Birthday to Prof. Boris Mordukhovich!