Spectral Preconditioning for Gradient Methods on Graded Non-convex Functions

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Workshop on Algorithmic Optimization (ALGOPT2024) Louvain-la-Neuve August 27, 2024

Outline

- I. Motivation
- II. Grade of non-convexity
- III. Spectral preconditioning
- IV. Quasi-self-concordant functions
- V. Experiments and conclusions

Optimization Problem

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

 $ightharpoonup f: \mathbb{R}^n \to \mathbb{R}$ is differentiable; can be non-convex

The goal: find \bar{x} s.t. $\|\nabla f(\bar{x})\| \le \varepsilon$, for a small given $\varepsilon > 0$

Gradient Method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla f(\mathbf{x}_k), \qquad k \geq 0$$

- + cheap iterations
- slow convergence rates

This work. Improve the convergence by a special $P_k = P_k^{\top} \succ 0$ called *Spectral Preconditioning*:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{P}_k \nabla f(\mathbf{x}_k), \qquad k \geq 0$$

Main Complexity Parameters

The Hessian of the objective $\nabla^2 f(\mathbf{x}) \in \mathbb{R}^{n \times n}$ is a symmetric matrix \Rightarrow all eigenvalues are real. The spectrum:

$$\lambda_1(\mathbf{x}) \geq \lambda_2(\mathbf{x}) \geq \ldots \geq \lambda_n(\mathbf{x})$$

describes the complexity of our problem.

1. Non-convex problems. Define $L_1 := \max_{\mathbf{x}} \lambda_1(\mathbf{x})$. Then the GM needs to do

$$k = \frac{2L_1(f(x_0) - f^*)}{\varepsilon^2}$$
 iterations

to find $\|\nabla f(\bar{\boldsymbol{x}}_k)\| \leq \varepsilon$.

2. Convex problems: $\lambda_n(\mathbf{x}) \geq 0$.

Strongly convex: $\lambda_n(\mathbf{x}) \ge \mu > 0$.

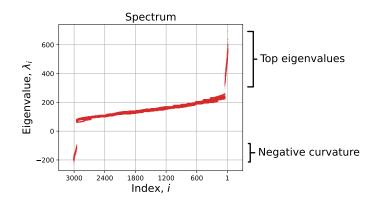
$$\Rightarrow$$
 Better rates, e.g.: $k = \frac{L_1}{\mu} \log \frac{2L(f(x_0) - f^*)}{\varepsilon^2}$.

Example: Matrix Factorization

$$f(\boldsymbol{X}, \boldsymbol{Y}) = \frac{1}{2} \|\boldsymbol{X}\boldsymbol{Y} - \boldsymbol{C}\|^2, \quad \boldsymbol{X} \in \mathbb{R}^{n \times r}, \boldsymbol{Y} \in \mathbb{R}^{r \times m},$$

where $C \in \mathbb{R}^{n \times m}$ is a given data matrix.

Thus, $f: \mathbb{R}^{(n+m)r} \to \mathbb{R}$, $\nabla^2 f(\boldsymbol{X}, \boldsymbol{Y}) \in \mathbb{R}^{(n+m)r \times (n+m)r}$.

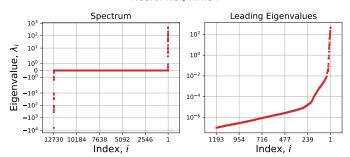


Example: 2-layer NN

$$f(\mathbf{W}_1, \mathbf{b}_1, \mathbf{w}_2, b_2) = \frac{1}{m} \sum_{i=1}^{m} \ell_i(\langle \mathbf{w}_2, \sigma(\mathbf{W}_1 \mathbf{a}_i + \mathbf{b}_1) \rangle + b_2),$$

where $\{a_i\}_{i=1}^m$ is a given dataset of features, $\sigma(\cdot)$ is an activation function, $\ell_i(\cdot)$ are losses.

Neural Net, MNIST



Newton's Method

Let the Hessian be Lipschitz, $\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \le L \|\mathbf{x} - \mathbf{y}\|$.

⇒ Cubic regularization of Newton's method:

$$\mathcal{O}\left(\frac{L^{1/2}(f(x_0)-f^*)}{\varepsilon^{3/2}}\right)$$

second-order oracle calls to find $\|\nabla f(\bar{x}_k)\| \leq \varepsilon$.

[Griewank, 1981; Nesterov-Polyak, 2006; Cartis-Gould-Toint, 2011]

- ▶ Computing $\nabla^2 f(\mathbf{x}_k)$ at every iteration
- ► Solving the cubic subproblem

Instead, we can use the Gradient Regularization technique:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \left(\nabla^2 f(\mathbf{x}_k) + \sqrt{L \|\nabla f(\mathbf{x}_k)\|} \mathbf{I}\right)^{-1} \nabla f(\mathbf{x}_k)$$

[Polyak, 2019; Ueda-Yamashita, 2014; Mishchenko, 2023; D-Nesterov, 2023]

- + one linear system
- + fast global rates as for the Cubic Newton
- requires $\nabla^2 f(\mathbf{x}_k) \succeq 0$ (see [Gratton-Jerad-Toint, 2023] for employing negative curvature)

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Problem Classes

Spectral decomposition of the Hessian:

$$\nabla^2 f(\mathbf{x}) \equiv \sum_{i=1}^n \lambda_i(\mathbf{x}) \mathbf{u}_i(\mathbf{x}) \mathbf{u}_i(\mathbf{x})^{\top},$$

where $\lambda_1(\mathbf{x}) \geq \ldots \geq \lambda_n(\mathbf{x})$ and $\mathbf{u}_1(\mathbf{x}), \ldots, \mathbf{u}_n(\mathbf{x}) \in \mathbb{R}^n$ are orthonormal eigenvectors (NB: several decompositions are possible, we can use any).

For a fixed $1 \le \tau \le n$, denote the Hessian of spectral order τ :

$$abla^2_{\tau}f(\mathbf{x}) := \sum_{i=1}^{\tau} \lambda_i(\mathbf{x})\mathbf{u}_i(\mathbf{x})\mathbf{u}_i(\mathbf{x})^{\top} \in \mathbb{R}^{n \times n}$$

Definition. f is non-convex of grade τ if

$$\nabla_{\tau}^{2} f(\mathbf{x}) \succeq 0, \quad \forall \mathbf{x}$$

 \Leftrightarrow top τ eigenvalues are non-negative everywhere:

$$\lambda_{\tau}(\mathbf{x}) \geq 0.$$

Main Properties

$$f \in \mathcal{F}_{ au} \stackrel{\mathsf{def}}{\Leftrightarrow} \nabla^2_{ au} f(\mathbf{x}) \succeq 0.$$

Nested family of functional cones:

- ▶ If $f \in \mathcal{F}_{\tau}$ then $\alpha f \in \mathcal{F}_{\tau}$ for any $\alpha \geq 0$.
- ▶ If $f \in \mathcal{F}_i$ and $g \in \mathcal{F}_i$ then

$$f+g \in \mathcal{F}_{i+j-n},$$

 $\operatorname{smax}(f,g) \in \mathcal{F}_{i+j-n},$

where smax
$$(f,g)(x) \stackrel{\text{def}}{=} \ln(e^{f(x)} + e^{g(x)})$$
.

- ⇒ summation with a convex function cannot decrease the grade.
 - ▶ If $f \in \mathcal{F}_{\tau}(\mathbb{R}^n)$ and $g(\mathbf{x}) = f(\mathbf{A}\mathbf{x} + \mathbf{b})$ for $\mathbf{A} \in \mathbb{R}^{n \times m}$, $\mathbf{b} \in \mathbb{R}^n$,

$$g \in \mathcal{F}_{m-n+\tau}(\mathbb{R}^m).$$

Geometric Interpretation

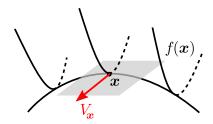
▶ $f \in \mathcal{F}_{\tau}$ cannot have strict local maxima for $\tau \geq 1$:

$$\max_{\mathbf{x} \in K} f(\mathbf{x}) = \max_{\mathbf{x} \in \partial K} f(\mathbf{x}).$$

Sufficient condition for grade τ : Let for any x there exists a vector subspace $V_x \subseteq \mathbb{R}^n$ with $\dim(V_x) \ge \tau$ s.t.

$$f(\mathbf{x} + \mathbf{h}) \geq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{h} \rangle, \quad \forall \mathbf{h} \in V_{\mathbf{x}}.$$

Then $f \in \mathcal{F}_{\tau}$.



Example: Quadratics

Example. Let $f(\mathbf{x}) = \frac{1}{2} \langle \mathbf{A} \mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{b}, \mathbf{x} \rangle$, for some $\mathbf{A} = \mathbf{A}^{\top} \in \mathbb{R}^{n \times n}$ with the top τ positive eigenvalues:

$$\lambda_1(\mathbf{A}) \geq \ldots \geq \lambda_{\tau}(\mathbf{A}) \geq 0.$$

Then $f \in \mathcal{F}_{\tau}$.

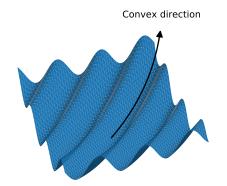
Example. Take
$$f(\mathbf{x}) = \frac{1}{2} \langle \mathbf{A} \mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{b}, \mathbf{x} \rangle + \frac{\sigma}{\rho} \|\mathbf{x}\|^{\rho}$$
. Then $f \in \mathcal{F}_{\tau}$.

- For p > 2, a global solution $x^* = \underset{x}{\operatorname{argmin}} f(x)$ always exists.
- Important in applications to regularized second-order and high-order methods.

Example: Low-rank Vector Fields

Example. Let $f(\mathbf{x}) = \varphi(\langle \mathbf{u}(\mathbf{x}), \mathbf{x} \rangle)$, where $\varphi : \mathbb{R} \to \mathbb{R}$ is arbitrary, and $\mathbf{u} : \mathbb{R}^n \to \mathbb{R}^n$ is a low-rank differential mapping.

E.g., a constant vector field: $f(\mathbf{x}) = \varphi(\langle \mathbf{u}, \mathbf{x} \rangle)$ is non-convex of grade n-1.



Function $f(x, y) = \sin(x + y) + q(x, y)$, where q is convex.

Example: Partial Convexity

▶ Let $f(\pmb{x}, \pmb{y}) : \mathbb{R}^{n+m} \to \mathbb{R}$ is such that for any fixed $\pmb{y} \in \mathbb{R}^m$

$$f(\cdot, \mathbf{y}) : \mathbb{R}^n \to \mathbb{R}$$

is convex. Then f is non-convex of grade n.

Example. Diagonal NN: $f(\mathbf{x}, \mathbf{y}) = \frac{1}{2} ||\mathbf{x} \circ \mathbf{y} - \mathbf{c}||^2 : \mathbb{R}^{2n} \to \mathbb{R}$ is non-convex of grade n.

Example. Matrix factorizations:

$$f(\boldsymbol{X}_1,\ldots \boldsymbol{X}_d) = \frac{1}{2} \| \boldsymbol{X}_1 \boldsymbol{X}_2 \cdots \boldsymbol{X}_d - \boldsymbol{C} \|_F^2, \quad \boldsymbol{X}_i \in \mathbb{R}^{n_i \times m_i},$$

is non-convex of grade $\tau = \max_{1 \le i \le d} [n_i \times m_i]$.

Example. Any deep model with convex losses. $\tau = \text{size}$ of last layer.

Open question: better estimates of τ when the deepness is increasing?

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Spectral Preconditioning

Problem:
$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$$
.

Preconditioned Gradient Method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{P}_k \nabla f(\mathbf{x}_k), \quad k \geq 0.$$

Main idea. Use $P_k := (H_k + \alpha_k I)^{-1}$ where $H_k \approx \nabla_{\tau}^2 f(\mathbf{x}_k)$.

- $ightharpoonup \alpha_k \ge 0$ is a regularization parameter (stepsize)
- $\tau = 0$: $\mathbf{H}_k = 0 \Rightarrow$ the gradient descent
- au = n: $\mathbf{H}_k = \nabla^2 f(\mathbf{x}_k) \Rightarrow \text{regularized Newton}$
- Let $\tau = 1$. Take

$$\mathbf{H}_k = \lambda_1(\mathbf{x}_k)\mathbf{u}_1(\mathbf{x}_k)\mathbf{u}_1(\mathbf{x}_k)^{\top}$$

is a rank-1 matrix where u_1 is the top eigenvector of $\nabla^2 f(x_k)$.

ightharpoonup au = 2: top 2 eigenvectors, . . .

Gradient Method with Spectral Preconditioning

Choose $\mathbf{x}_0 \in \mathbb{R}^n$ and $0 \le \tau \le n$.

For k > 0 iterate:

- 1. Estimate $\boldsymbol{H}_k \approx \nabla_{\tau}^2 f(\boldsymbol{x}_k) \in \mathbb{R}^{n \times n}$
- 2. Perform the gradient step, for some $\alpha_k \geq 0$:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\mathbf{H}_k + \alpha_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$$

Implementation

Computing eigenvectors is difficult. For us, it is enough to use inexact approximation

$$\mathbf{H}_k \approx \nabla^2 f(\mathbf{x}_k)$$
.

Power Method. Fast linear rate of convergence. The arithmetic complexity of each step is $\mathcal{O}(\tau^2 n)$

More advanced: Oja's and Lanczos iterations.

Low-rank representation $\boldsymbol{H}_k = \boldsymbol{V}_k \mathrm{Diag}(\boldsymbol{a}_k) \boldsymbol{V}_k^{\top}$, where $\boldsymbol{V}_k \in \mathbb{R}^{n \times \tau}$ has orthonormal columns. Then

$$(\boldsymbol{H}_k + \alpha_k \boldsymbol{I})^{-1} = \frac{1}{\alpha_k} [\boldsymbol{I} - \boldsymbol{V}_k (\boldsymbol{I} + \alpha_k \operatorname{Diag}(\boldsymbol{a}_k)^{-1})^{-1} \boldsymbol{V}_k^{\top}].$$

The Woodbury matrix identity: $\mathcal{O}(\tau n)$ cost.

Global Rate

Let the Hessian be Lipschitz continuous,

$$\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \le \mathbf{L} \|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y}$$

- ▶ Denote $\sigma_{\tau} \ge \max\{\lambda_{\tau+1}(\mathbf{x}), -\lambda_n(\mathbf{x})\}$
- ▶ Let $\delta \ge \|\boldsymbol{H}_k \nabla_{\tau}^2 f(\boldsymbol{x}_k)\|$

Theorem. Let $f \in \mathcal{F}_{\tau}$ for some fixed $0 \le \tau \le n$. Set

$$\alpha_k := \sqrt{\frac{L\|\nabla f(\mathbf{x}_k)\|}{2}} + \sigma_{\tau} + \delta.$$

Then, to ensure $\min_{1 \le i \le k} \|\nabla f(\mathbf{x}_i)\| \le \varepsilon$ it is enough to choose

$$k = \left\lceil 8(f(\mathbf{x}_0) - f^*) \cdot \left(\sqrt{\frac{L}{2}} \frac{1}{\varepsilon^{3/2}} + \frac{\sigma_{\tau} + \delta}{\varepsilon^2} \right) + 2 \ln \frac{\|\nabla f(\mathbf{x}_0)\|}{\varepsilon} \right\rceil$$

- Increasing τ we improve the parameter σ_{τ} . E.g. for $\tau := 1$ the method does not depend on λ_1 .
- ightharpoonup au := n gives the global rate of the Cubic Newton

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Convex Problems

Let $\nabla^2 f(\mathbf{x}) \succeq 0$ (i.e. $f \in \mathcal{F}_n$).

Can we improve convergence rate? Yes.

▶ Previous smoothness condition – the Hessian is Lipschitz:

$$abla^3 f(\mathbf{x})[\mathbf{u}, \mathbf{u}, \mathbf{v}] \leq L \|\mathbf{u}\|^2 \|\mathbf{v}\|, \quad \forall \mathbf{x}, \mathbf{u}, \mathbf{v} \in \mathbb{R}^n.$$

► Refined smoothness condition. Assume that f is quasi-self-concordant [Bach, 2010]:

$$abla^3 f(\mathbf{x})[\mathbf{u},\mathbf{u},\mathbf{v}] \leq M \|\mathbf{u}\|_{\mathbf{x}}^2 \|\mathbf{v}\|, \quad \forall \mathbf{x},\mathbf{u},\mathbf{v} \in \mathbb{R}^n,$$
 where $\|\mathbf{u}\|_{\mathbf{x}}^2 := \langle \nabla^2 f(\mathbf{x})\mathbf{u},\mathbf{u} \rangle$ is the local norm.

A direct consequence – the Hessian is stable [Karimireddy-Stich-Jaggi, 2018], $\forall x, y$:

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

Examples

Example 0. Quadratic functions: M = 0.

Example 1.
$$\varphi(x) = e^x$$
. Then $\varphi^{(p)}(x) = e^x$. Hence, $M = 1$.

Example 2.
$$\varphi(x) = \ln(1 + e^x)$$
, we have $M = 1$.

Therefore, the logistic and exponential regressions

$$f(\mathbf{x}) = \frac{1}{m} \sum_{i=1}^{m} \varphi(\langle \mathbf{a}_i, \mathbf{x} \rangle)$$

are quasi-SC.

Example 3. Soft maximum: $f(\mathbf{x}) = \mu \ln \left(\sum_{i=1}^{m} \exp \left(\frac{\langle \mathbf{a}_i, \mathbf{x} \rangle - b_i}{\mu} \right) \right)$ is

quasi-SC with
$$M = \frac{2}{\mu}$$
.

Example 4. Matrix scaling, $\mathbf{A} \in \mathbb{R}_+^{n \times n}$: $f(\mathbf{x}, \mathbf{y}) = \sum_{1 \le i, j \le n} A_{ij} e^{x_i - x_j}$ is

quasi-SC with
$$M = \sqrt{2}$$
.

Gradient Regularization of Newton's Method

Consider the following full Newton method with regularization:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k) + \alpha_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$$

Theorem. [D, 2023] Set

$$\alpha_k := M \|\nabla f(\mathbf{x}_k)\|$$

Then, we have the global linear rate:

$$f(\boldsymbol{x}_k) - f^* \leq \exp\left(-\frac{k}{8MD}\right) \left(f(\boldsymbol{x}_0) - f^*\right) + \exp\left(-\frac{k}{4}\right) \|\nabla f(\boldsymbol{x}_0)\| D,$$

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 $f(x_k) - f^* \leq \varepsilon$

NB: compare with

- ▶ The Gradient Method: $\mathcal{O}(\frac{\lambda_1 D^2}{\varepsilon})$
- ► The Cubic Newton: $\mathcal{O}(\sqrt{\frac{LD^3}{\varepsilon}})$

Convergence on Convex Problems

Spectral Preconditioning:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\mathbf{H}_k + \alpha_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k), \quad \mathbf{H}_k \approx \nabla_{\tau}^2 f(\mathbf{x}_k)$$

Theorem. Let f be strongly convex and quasi-SC with M > 0. Set

$$\alpha_k := M \|\nabla f(\mathbf{x}_k)\| + \lambda_{\tau+1} + \delta.$$

Then, to ensure $f(x_k) - f^* \le \varepsilon$ it is enough to choose

$$k = 4 \left[\left(\frac{MD + \frac{\lambda_{\tau+1} + \delta}{2\lambda_n}}{2\lambda_n} \right) \ln \frac{f(x_0) - f^*}{\varepsilon} + \ln \frac{\|\nabla f(x_0)\|D}{\varepsilon} \right]$$

- ► The rate is linear and the condition number is $\frac{\lambda_{\tau+1}}{\lambda_n}$
- \blacktriangleright Increasing τ we cut off the top τ eigenvalues of the spectrum

Example: Quadratic Problem

- ▶ Let $f(\mathbf{x}) = \frac{1}{2} \langle \mathbf{A} \mathbf{x}, \mathbf{x} \rangle \langle \mathbf{b}, \mathbf{x} \rangle$ with $\mathbf{A} = \mathbf{A}^{\top} \succ 0$. (M = 0)
- 1. The classical gradient descent: $\mathbf{x}_{k+1} = \mathbf{x}_k \gamma \nabla f(\mathbf{x}_k)$. The number of iterations (matrix-vector products):

$$\mathcal{O}(\frac{\lambda_1}{\lambda_n}\log\frac{1}{\varepsilon})$$
 (*)

2. Our Spectral Preconditioning for $\tau = 1$:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \left(a_1 \mathbf{v}_1 \mathbf{v}_1^\top + \alpha \mathbf{I}\right)^{-1} \nabla f(\mathbf{x}_k)$$
. The number of iterations:

$$\mathcal{O}(\frac{\lambda_2}{\lambda_n}\log\frac{1}{\varepsilon}).$$

The cost of computing $\mathbf{v}_1 \approx \mathbf{u}_1(\mathbf{A})$ by the Power Method is $\tilde{\mathcal{O}}(\frac{\lambda_1}{\lambda_1 - \lambda_2})$. Hence, the total complexity

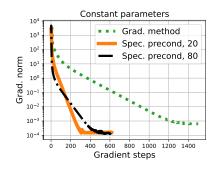
$$\tilde{\mathcal{O}}\left(\frac{\lambda_1}{\lambda_n}\cdot\frac{\lambda_2}{\lambda_1-\lambda_2}\right)$$

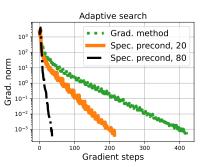
can be much better than in (*), when $\lambda_1 \gg \lambda_2$.

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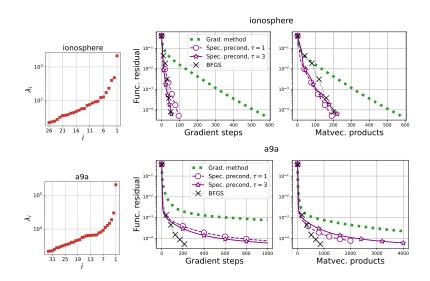
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Matrix Factorization





Logistic Regression



Conclusions

- ▶ The spectrum of the Hessian $\nabla^2 f(\mathbf{x})$ often determines the complexity of the problem.
- In practice a specific distribution of eigenvalues ⇒ refined problem classes and more advanced methods
- Graded non-convexity: most of the eigenvalues are usually positive
- ► Spectral Preconditioning: we can cut the large gaps between the top eigenvalues

Reference:

 Doikov, N., Stich, S.U., Jaggi, M., ICML 2024 (International Conference on Machine Learning) Spectral Preconditioning for Gradient Methods on Graded Non-convex Functions

Open problems

- Other Notions of Convexity (weak, plurisubharmonic functions, convexity with respect to a linear group, ...)
- Grade of non-convexity for deep models
- Practical performance (efficient implementation of Hessian-vector products)
- Refined specification of the problem / different methods
 - Kernel ridge regression [Ma-Belkin, 2017]
 - Matrix factorizations
 [Zhang-Fattahi-Zhang, 2021, 2023; Ma-Xu-Tong-Chi, 2023]
 - o Heavy-ball method [Scieur-Pedregosa, 2020]
 - Polynomial preconditioning [D-Rodomanov, 2023]
- lackbox Local superlinear convergence \Rightarrow a bridge to quasi-Newton methods

Thank you for your attention!