

Spectral Preconditioning for Gradient Methods on Graded Non-convex Functions

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Outline

- I. Motivation
- II. Grade of non-convexity
- III. Spectral preconditioning
- IV. Experiments and conclusions

Optimization Problem

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

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is differentiable; can be **non-convex**

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

Gradient Method:

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

+ cheap iterations

– slow convergence rates

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

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

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**:

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

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

$$k = \frac{2L_1(f(\mathbf{x}_0) - f^*)}{\varepsilon^2} \text{ iterations}$$

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

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

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

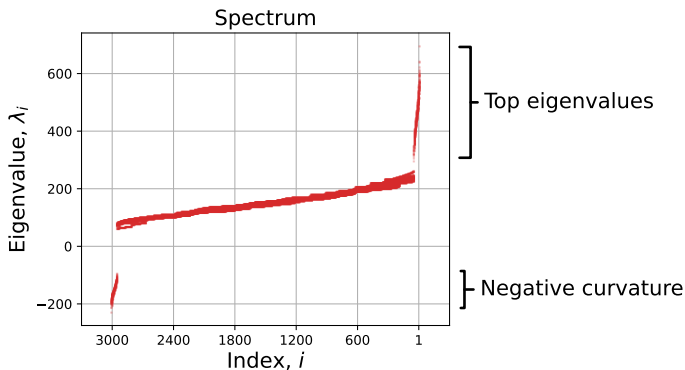
\Rightarrow Better rates, e.g.: $k = \frac{L_1}{\mu} \log \frac{2L(f(\mathbf{x}_0) - f^*)}{\varepsilon^2}$.

Example: Matrix Factorization

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

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

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

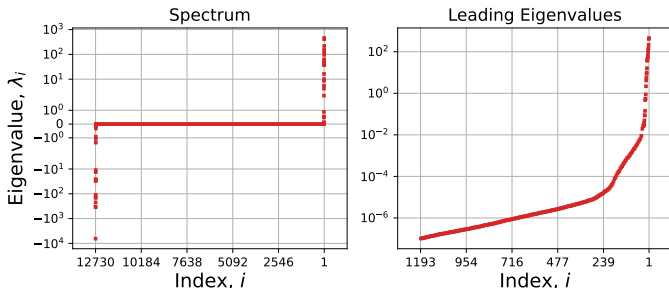


Example: 2-layer NN

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

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

Neural Net, MNIST



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

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

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

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

$$f \in \mathcal{F}_\tau \stackrel{\text{def}}{\iff} \nabla^2 f_\tau(\mathbf{x}) \succeq 0.$$

Nested family of functional cones:

$$\underbrace{\mathcal{F}_0}_{\text{all functions}} \supset \mathcal{F}_1 \supset \dots \supset \mathcal{F}_{n-1} \supset \underbrace{\mathcal{F}_n}_{\text{convex functions}}$$

- ▶ 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 $g \in \mathcal{F}_j$ then

$$\begin{aligned} f + g &\in \mathcal{F}_{i+j-n}, \\ \text{smax}(f, g) &\in \mathcal{F}_{i+j-n}, \end{aligned}$$

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

\Rightarrow 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

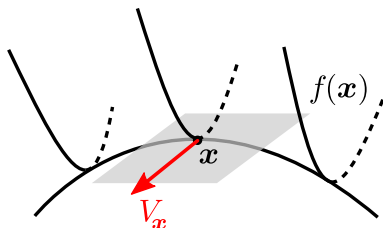
- ▶ $f \in \mathcal{F}_\tau$ cannot have strict local maxima for $\tau \geq 1$:

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

- ▶ **Sufficient condition for grade τ** : Let for any \mathbf{x} there exists a vector subspace $V_{\mathbf{x}} \subseteq \mathbb{R}^n$ with $\dim(V_{\mathbf{x}}) \geq \tau$ 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:

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

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

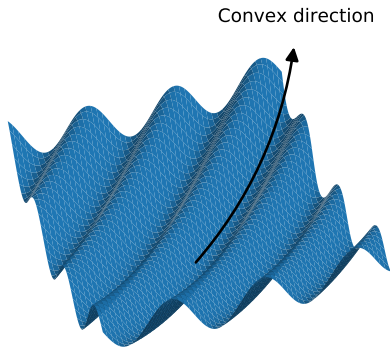
Example. Take $f(\mathbf{x}) = \frac{1}{2}\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{b}, \mathbf{x} \rangle + \frac{\sigma}{p}\|\mathbf{x}\|^p$. Then $f \in \mathcal{F}_\tau$.

- ▶ For $p > 2$, a global solution $\mathbf{x}^* = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x})$ 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 $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ is arbitrary, and $\mathbf{u} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ 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 $f(\mathbf{x}, \mathbf{y}) : \mathbb{R}^{n+m} \rightarrow \mathbb{R}$ is such that for any fixed $\mathbf{y} \in \mathbb{R}^m$

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

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

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

Example. Matrix factorizations:

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

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

Example. Any deep model with convex losses.
 $\tau =$ 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 $\mathbf{P}_k := (\mathbf{H}_k + \alpha_k \mathbf{I})^{-1}$ where $\mathbf{H}_k \approx \nabla_{\tau}^2 f(\mathbf{x}_k)$.

- ▶ $\alpha_k \geq 0$ is a regularization parameter (stepsize)
- ▶ $\tau = 0$: $\mathbf{H}_k = 0 \Rightarrow$ the gradient descent
- ▶ $\tau = n$: $\mathbf{H}_k = \nabla^2 f(\mathbf{x}_k) \Rightarrow$ 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 \mathbf{u}_1 is the top eigenvector of $\nabla^2 f(\mathbf{x}_k)$.

- ▶ $\tau = 2$: top 2 eigenvectors, ...

Gradient Method with Spectral Preconditioning

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

For $k \geq 0$ iterate:

1. Estimate $\mathbf{H}_k \approx \nabla_{\tau}^2 f(\mathbf{x}_k) \in \mathbb{R}^{n \times n}$
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 is $\mathcal{O}(\tau^2 n)$ – linear with respect to n .

More advanced: *Oja's* and *Lanczos iterations*.

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

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

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

Global Rate

- ▶ Let the Hessian be Lipschitz continuous,

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

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

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

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

Then, to ensure $\min_{1 \leq i \leq k} \|\nabla f(\mathbf{x}_i)\| \leq \varepsilon$ 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 .
- ▶ $\tau := n$ gives the global rate of the Cubic regularization of Newton's method [Nesterov-Polyak, 2006]

Cutting the Negative Spectrum

- ▶ $\sigma_\tau \geq \max\{\lambda_{\tau+1}(\mathbf{x}), -\lambda_n(\mathbf{x})\}$ depends on the negative part of the spectrum.

Instead of σ_τ we can have

$$\sigma_\tau^+ \geq \max\{\lambda_{\tau+1}(\mathbf{x}), 0\}$$

- ▶ For that, we need a modification of the stepsize rule:

$$\alpha_k := \arg \max_{\alpha > 0} \left[-\frac{1}{2} \langle (\mathbf{H}_k + (\alpha + \eta)\mathbf{I})^{-1} \mathbf{g}_k, \mathbf{g}_k \rangle - \frac{2\alpha^3}{3L_2} \right] + \eta,$$

where $\eta > 0$ is a fixed constant

- ▶ The same rate, substituting $\sigma_\tau \mapsto \sigma_\tau^+$

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:

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

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

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

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], $\forall \mathbf{x}, \mathbf{y}$:

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

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

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

Convergence on Convex Problems

Theorem. Let f be strongly convex and quasi-SC with parameter $M > 0$. Choose

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

Then, to ensure $f(\mathbf{x}_k) - f^* \leq \varepsilon$ it is enough to choose

$$k = 4 \left[\left(MD + \frac{\lambda_{\tau+1} + \delta}{2\lambda_n} \right) \ln \frac{f(\mathbf{x}_0) - f^*}{\varepsilon} + \ln \frac{\|\nabla f(\mathbf{x}_0)\|D}{\varepsilon} \right]$$

- ▶ The rate is linear and the condition number is $\frac{\lambda_{\tau+1}}{\lambda_n}$
- ▶ Increasing τ we cut off the top τ eigenvalues of the spectrum
- ▶ For convex functions ($\lambda_n = 0$), we have sublinear rate:

$$k = \mathcal{O} \left(\frac{(\lambda_{\tau+1} + \delta)D^2}{\varepsilon} + MD \ln \frac{f(\mathbf{x}_0) - f^*}{\varepsilon} + \ln \frac{\|\nabla f(\mathbf{x}_0)\|D}{\varepsilon} \right)$$

- ▶ $\tau := n$ gives the global linear rate of the Gradient regularization of Newton's method [D, 2023]

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):

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

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:

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

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

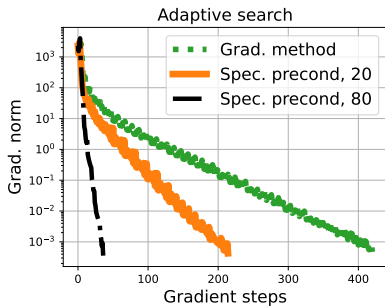
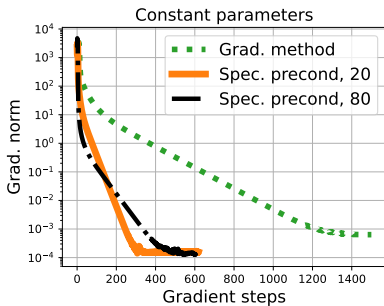
$$\tilde{\mathcal{O}}\left(\frac{\lambda_1}{\lambda_n} \cdot \frac{\lambda_2}{\lambda_1 - \lambda_2}\right)$$

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

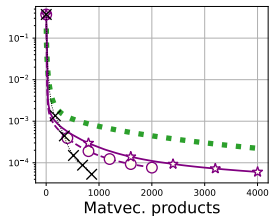
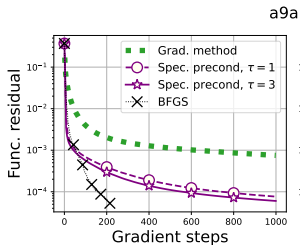
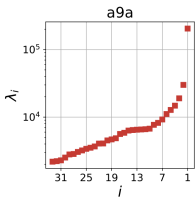
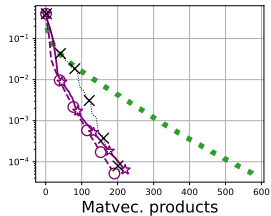
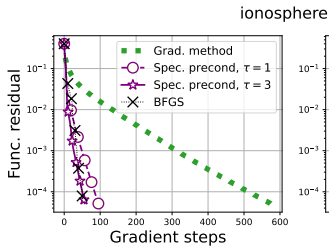
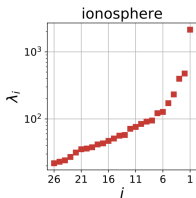
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Matrix Factorization



Logistic Regression



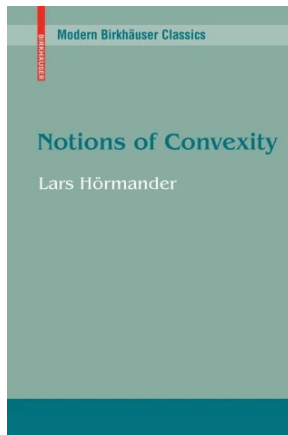
Conclusions

- ▶ 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**

- ▶ Other **Notions of Convexity** (weak, plurisubharmonic functions, convexity with respect to a linear group, ...)



Lars Hörmander (24 Jan 1931, Mjällby — 25 Nov 2012, Lund)

Open problems

- ▶ 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]
 - **Heavy-ball method** [Scieur-Pedregosa, 2020]
 - **Polynomial preconditioning** [D-Rodomanov, 2023]
- ▶ Local superlinear convergence \Rightarrow a bridge to quasi-Newton methods

Thank you for your attention!