How to improve first-order optimization methods

Geometry, block structure, and randomization

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Deep Learning seminar @ KRAFTON AI

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Block Optimization
Riemannian Optimization

William Powell
(3rd year Ph.D.)

Stochastic Optimization
Reinforcement Learning

Danny Duan
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Quasi-Newton Methods

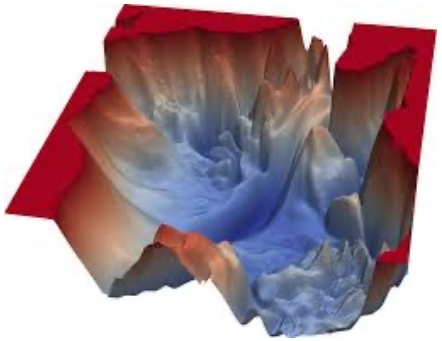
Joowon Lee
(UW Stats)

Causal Inference
Matrix Factorization

Introduction

$$\boldsymbol{\theta}^* \in \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta} \subseteq \mathbb{R}^p}{\arg\min} f(\boldsymbol{\theta})$$

- f: Objective function
  - Nonconvex, smooth (for this talk)
  - Often represents model fitness to training data
    - e.g., DNN, LLM



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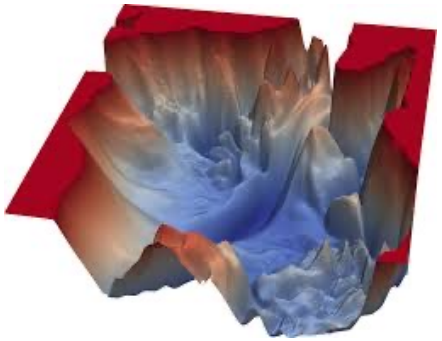
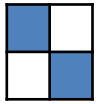
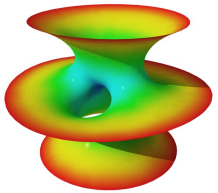
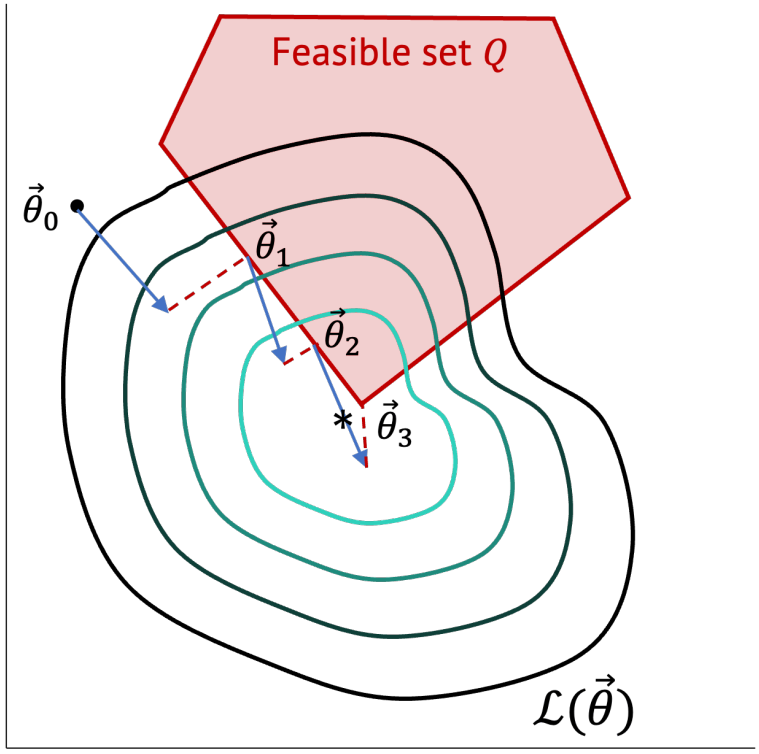


- $\boldsymbol{\Theta}$: Parameter space with various structures:
  - Convex 
  - block structure: $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_m)$ 
  - Riemannian manifold (e.g., $\boldsymbol{\Theta}$=set of orthogonal matrices)



The simplest yet commonly used method

(PGD) $$\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\boldsymbol{\Theta}} \left(\boldsymbol{\theta}_n - \alpha_n \nabla f(\boldsymbol{\theta}_n) \right)$$



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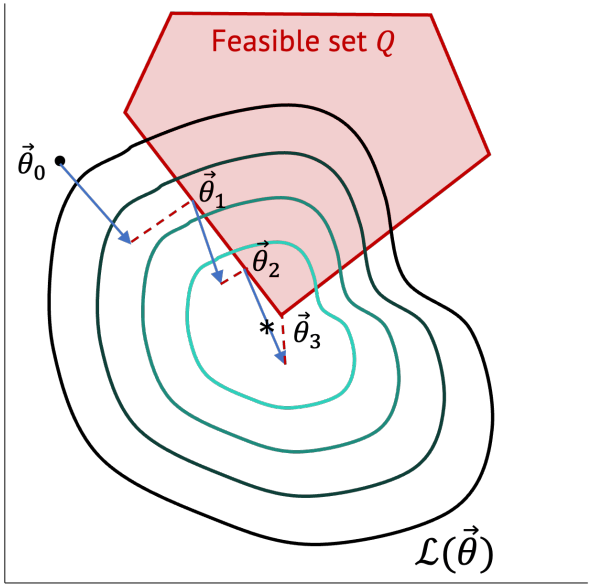
(PGD) $$\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta}_n - \alpha_n \nabla f(\boldsymbol{\theta}_n)\right)$$

- Projected Gradient Descent (PGD)
  - Widely used in ML, Statistics, Scientific Computing
  - Reduces to Gradient Descent for unconstrained problems
  - Easy to implement, cheap to run
  - Several of modifications (e.g., momentum, adaptive stepsizes)



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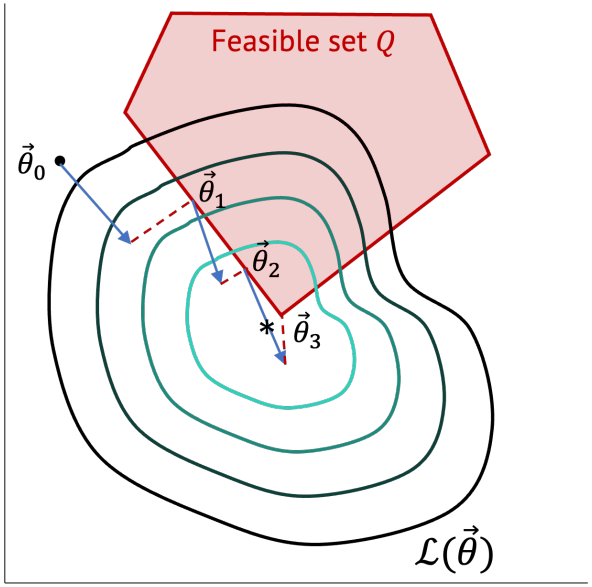

(PSGD) $$\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\boldsymbol{\Theta}} \left(\boldsymbol{\theta}_n - \alpha_n \widehat{\nabla} f(\boldsymbol{\theta}_n) \right)$$

Stochastic gradient $\approx \nabla$

$$\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta}_n - \mathbf{H}_n \nabla f(\boldsymbol{\theta}_n)\right)$$

- $\Pi_{\boldsymbol{\Theta}}$: Projection onto $\boldsymbol{\Theta}$
  - Simple for nonnegativity or norm constraints
- $\nabla f(\boldsymbol{\theta}_n)$: Gradient of the objective at current parameter θ_n
  - Assume it is cheap to compute; Requires $O(p)$ storage
- $\mathbf{H}_n$: $p \times p$ Preconditioning matrix
  - $\mathbf{H}_n = \alpha_n \mathbf{I}_p$ → Gradient Descent with stepsize α_n
  - $\mathbf{H}_n = \nabla^2 f(\boldsymbol{\theta}_n)^{-1}$ → Newton's Method
  - $\mathbf{H}_n \approx \nabla^2 f(\boldsymbol{\theta}_n)^{-1}$ → Quasi-Newton Method

Plan of the talk

- Classical 1st-order methods like P(S)GD has some limitations
  - Difficult/expensive to project onto the constrained set
  - Still expensive with high dimensionality ($p \gg 1$)
    - e.g., overparametrization
  - Slow convergence for ill-conditioned problems
  - Mathematical guarantees are too pessimistic vs. practice
    - e.g., Usually assumes the worst-case, requires very small stepsizes, i.i.d. data sampling,

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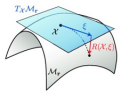
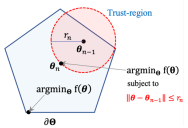
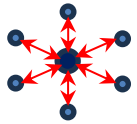
- We will propose several techniques to improve them, each based on some mathematical principles
  - Riemannian OPT
  - Adaptive BCD
  - Non-adaptive TR





  - Rand. Hessian Approx.
  - Gradient Consensus



A Math Warm-up:

Basic Ideas behind nonconvex optimization algorithms

Taylor expansion!

Frank-Wolfe (1956)

- **Taylor expand the objective f near θ_n:**

$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle$$

- **Minimize the 1st-order Taylor approximation**

$$\boldsymbol{\theta}'_n = \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle$$

$$\boldsymbol{\theta}_{n+1} = \text{Convex combination of } \boldsymbol{\theta}_n \text{ and } \boldsymbol{\theta}'_n$$

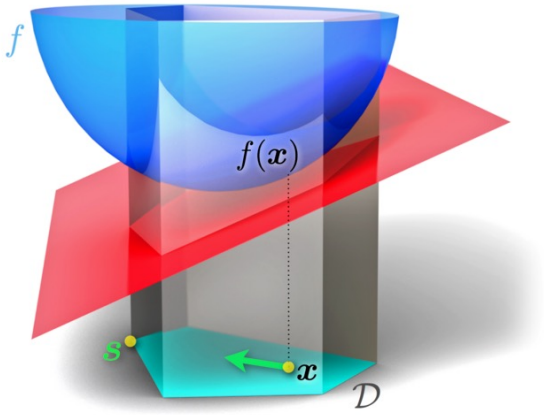


Image credit: Wikipedia

Newton's Method (1690)

(Assume $\Theta = \mathbb{R}^p$)

- **Taylor expand the objective f near θ_n:**

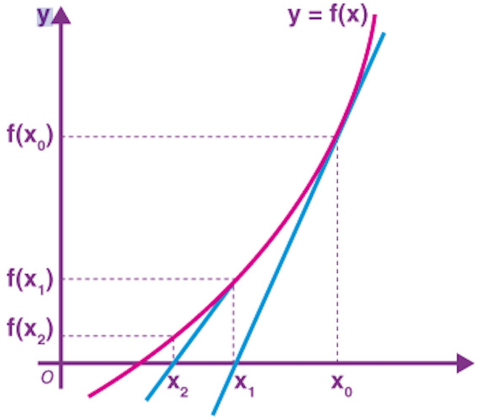
$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \left\langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \nabla f^2(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \right\rangle$$

- **Minimize the 2nd-order Taylor expansion**

$$\begin{aligned} \boldsymbol{\theta}_{n+1} &= \arg\min_{\boldsymbol{\theta} \in \mathbb{R}^p} f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \left\langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \nabla f^2(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \right\rangle \\ &= \boldsymbol{\theta}_n - \left(\nabla^2 f(\boldsymbol{\theta}_n) \right)^{-1} \nabla f(\boldsymbol{\theta}_n) \end{aligned}$$

- Undefined if the Hessian is not PD
- Inverting the Hessian is expensive

Super-fast, quadratic convergence if works ☺



A Quasi-Newton Method

(Assume $\Theta = \mathbb{R}^p$)

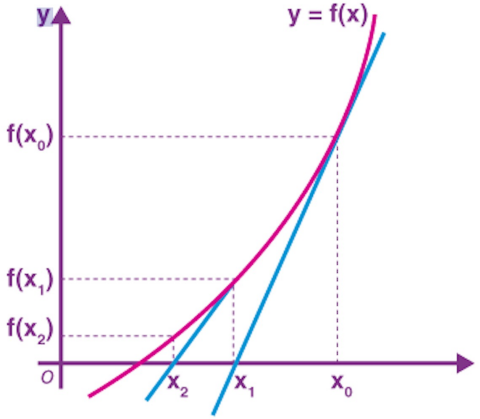
- **Taylor expand the objective f near θ_n:**

$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \left\langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \nabla f^2(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \right\rangle$$

- **Minimize the 2nd-order Taylor expansion with regularization**

$$\begin{aligned} \boldsymbol{\theta}_{n+1} &= \arg\min_{\boldsymbol{\theta} \in \mathbb{R}^p} \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \left\langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \nabla f^2(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \right\rangle + \frac{\gamma_n}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}_n\|^2 \\ &= \boldsymbol{\theta}_n - \left(\nabla^2 f(\boldsymbol{\theta}_n) + \gamma_n \mathbf{I}_p \right)^{-1} \nabla f(\boldsymbol{\theta}_n) \end{aligned}$$

  - Levenberg-Marquardt regularization ('44 '63)
  - Can make the regularized Hessian PD
  - Matrix inversion still expensive



Trust-Region (1970's)

- **Taylor expand the objective f near θ_n:**

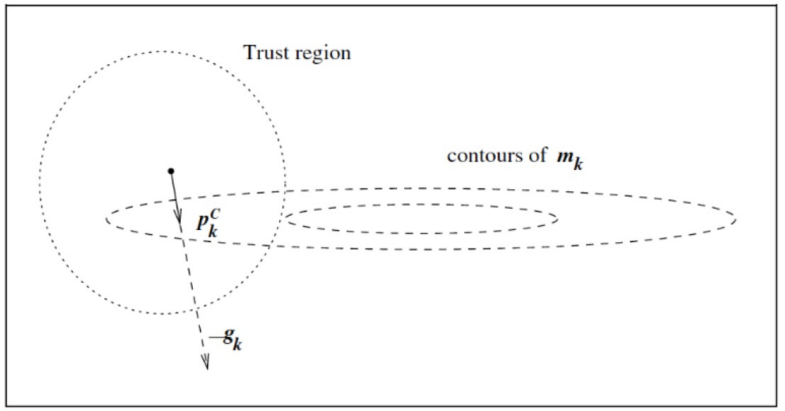
$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \nabla f^2(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \rangle$$

- **Minimize a "quadratic model" within a trust-region**

$$\boldsymbol{\theta}_{n+1} = \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta},\, \|\boldsymbol{\theta} - \boldsymbol{\theta}_n\| \le r_n}{\arg\min} \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{1}{2} \langle \boldsymbol{\theta} - \boldsymbol{\theta}_n, \mathbf{B}_n(\boldsymbol{\theta} - \boldsymbol{\theta}_n) \rangle$$

- Trust-region with radius r_n
- Next radius r_{n+1} is computed adaptively based on the performance of the previous update

- PD, and no need to be close to the Hessian



PGD (Late 1950s)

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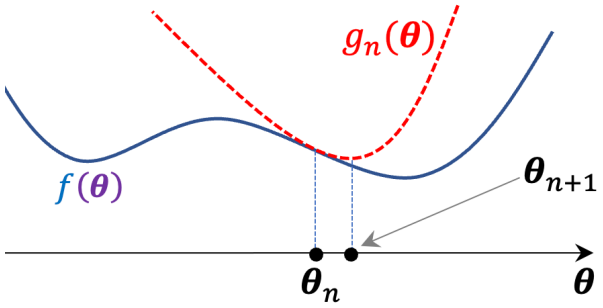
- **Replace the Hessian with L times the identity**

$$f(\boldsymbol{\theta}) \le f(\boldsymbol{\theta}_n) + \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{L}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}_n\|^2$$

L = largest absolute eigenvalue of $\nabla^2 f(\boldsymbol{\theta})$ over all $\boldsymbol{\theta}$

- **Minimize the quadratic surrogate**

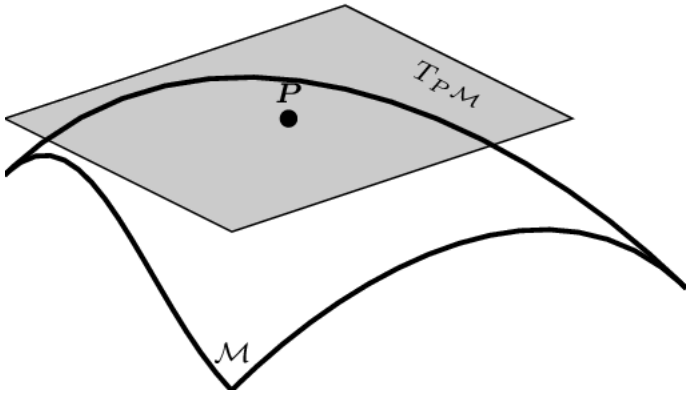
$$\begin{aligned} \boldsymbol{\theta}_{n+1} &= \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \ \langle \nabla f(\boldsymbol{\theta}_n), \boldsymbol{\theta} - \boldsymbol{\theta}_n \rangle + \frac{L}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}_n\|^2 \\ &= \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \ \left\| \boldsymbol{\theta} - \left(\boldsymbol{\theta}_n - \frac{1}{L} \nabla f(\boldsymbol{\theta}_n) \right) \right\|^2 \\ &= \Pi_{\boldsymbol{\Theta}} \left(\boldsymbol{\theta}_n - \frac{1}{L} \nabla f(\boldsymbol{\theta}_n) \right) \end{aligned}$$



A geometric approach:

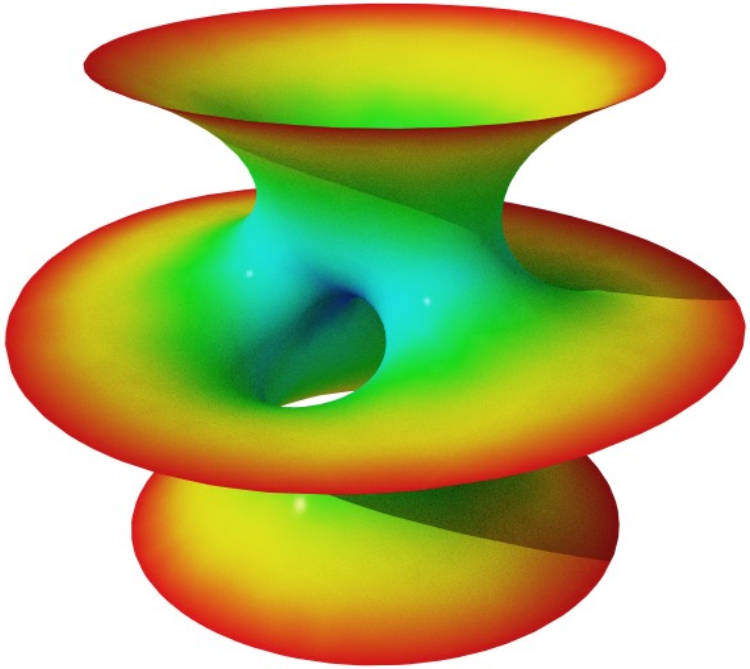
Riemannian Optimization

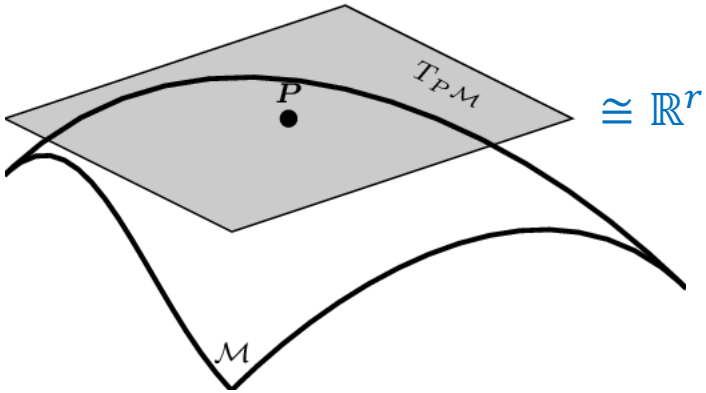
Tangent planes!



- Parameter spaces often has some intrinsic, ***low-dimensional geometric structures***
- **(r-dim) Riemannian manifold**

  = Smooth surface in $\mathbb{R}^p$ where every point has r-dim tangent spaces





e.g.,
- Low-rank matrix manifolds
- Orthogonal frames
- PSD matrices
- DNNs with spectrum-constrained matrix weights

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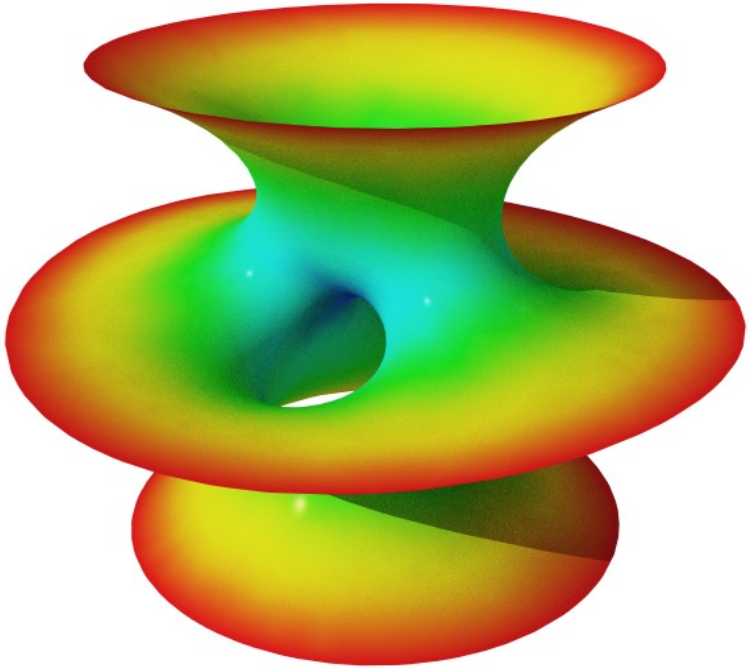

Riemann
(1826-1866)

Gauss
(1777-1855)

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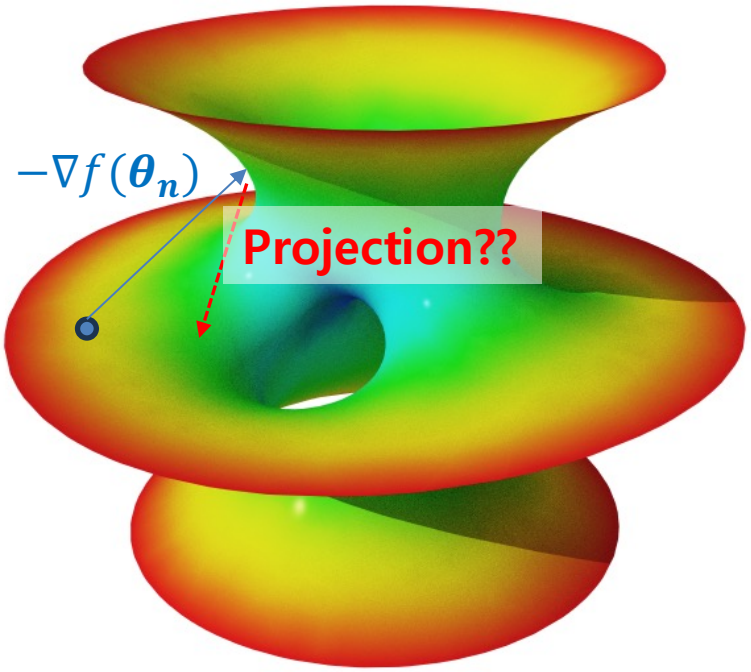

- $\Pi_{\boldsymbol{\Theta}}$: Projection onto $\boldsymbol{\Theta}$:
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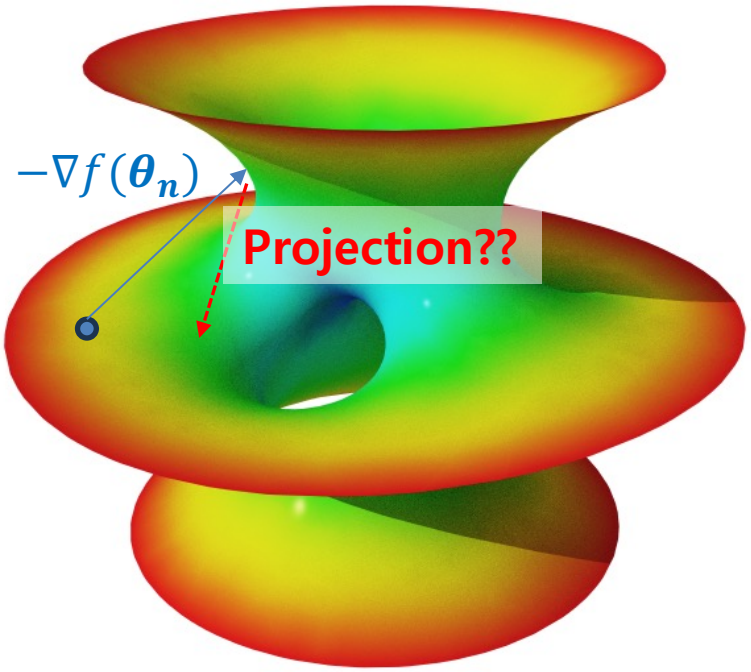

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  - Work only with r-dim stuffs?

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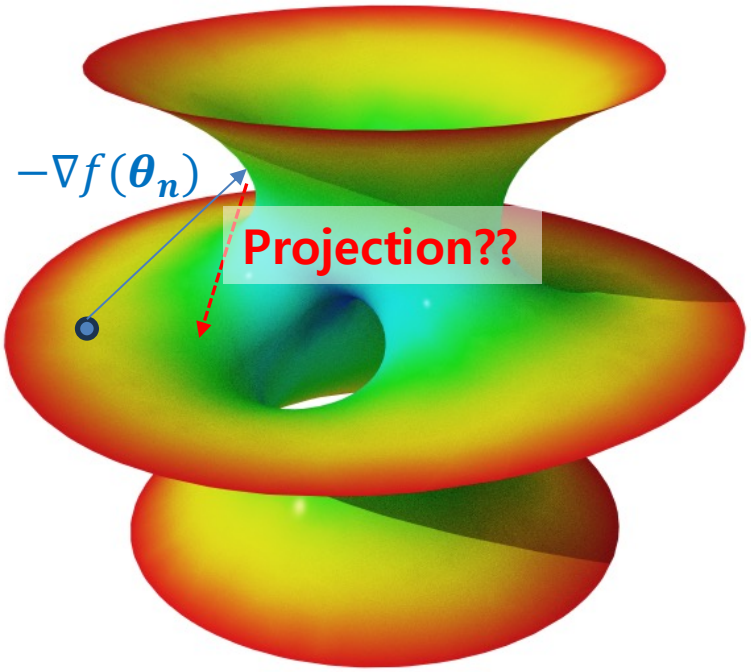

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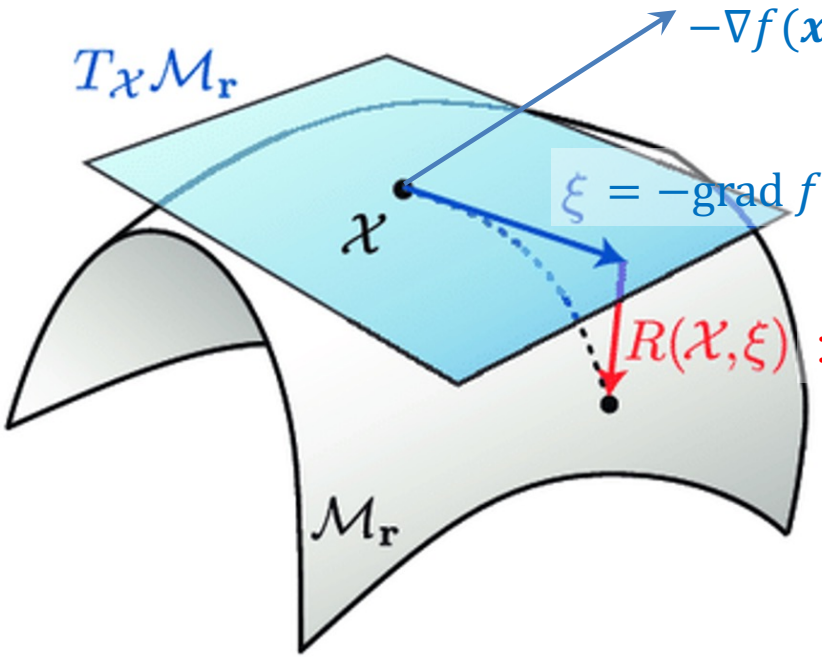
- If $\boldsymbol{\Theta}$ is low-dim (say $r \ll p$)
  - Work only with r-dim stuffs?
- *For certain low-rank matrix factorization problems, PGD with rSVD as projection can be useful*

  [Lee, Lyu, Yao NeurIPS '23]

(Riemannian GD) $\boldsymbol{\theta}_{n+1} \leftarrow \mathrm{Rtr}_{\boldsymbol{\theta}_n}\left(-\alpha_n \operatorname{grad} f(\boldsymbol{\theta}_n)\right)$



$\xi = -\operatorname{grad} f(x)$: Rimannian gradient

$R(\mathcal{X},\xi)$: Retraction at x

(Proj from $T_x \to \mathcal{M}$)

- RGD = gradient descent within the tangent space + Retraction

(RGD) $$\boldsymbol{\theta}_{n+1} \leftarrow \mathrm{Rtr}_{\boldsymbol{\theta}_n}\left(-\alpha_n \operatorname{grad} f(\boldsymbol{\theta}_n)\right)$$

- Limitation: ***grad*** and ***Retraction*** *can be expensive to compute*

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[Li, Lyu, Balzano, Needell ICML '24]

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- ***It's OK to use approximate grad* and *Retraction***

  (Both mathematically and practically)

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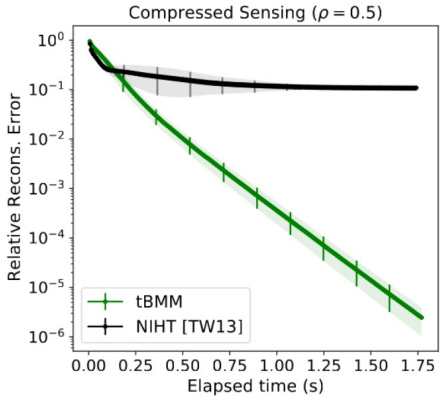
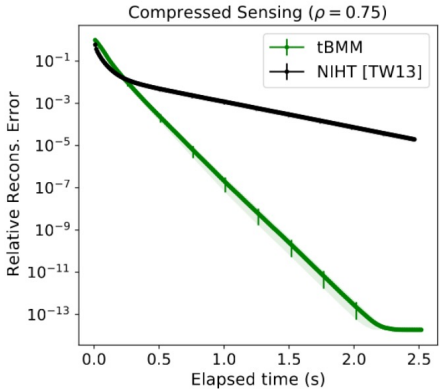
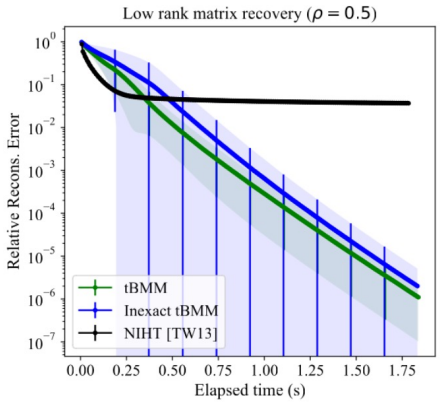
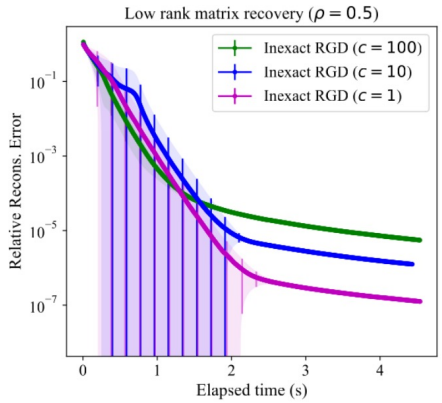




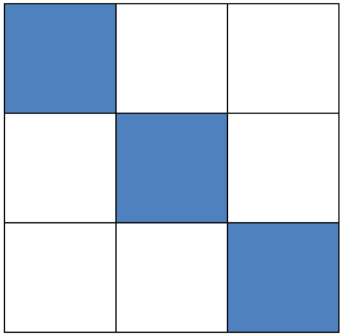




A coordinate-wise approach:

Adaptive Block Coordinate Descent

Optimize one block at a time!



Stepsizes in PGD

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- α_n: Stepsizes. How to choose them?

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- α_n: Stepsizes. How to choose them?
  - "*Small enough stepsize*": $\alpha_n \leq 1/L$, where
    - L = **Lipschitz constant for ∇f over Θ**
      $\approx$ **Largest absolute eigenvalue of $\nabla^2 f$ over Θ**

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  - "*Small enough stepsize*": $\alpha_n \leq 1/L$, where
    - $\boldsymbol{L}$ = **Lipschitz constant for ∇f over $\boldsymbol{\Theta}$**
      $\approx$ **Largest absolute eigenvalue of $\nabla^2 f$ over $\boldsymbol{\Theta}$**
  - But $\alpha_n = 1/L$ is TOO SMALL!
    - In practice use "line search" to find larger α_n that works
    - L might be unknown and hard to estimate

(PGD) $$\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\Theta}\left(\boldsymbol{\theta}_n - \alpha_n \nabla f(\boldsymbol{\theta}_n)\right)$$

- α_n: Stepsizes. How to choose them?
  - "*Small enough stepsize*": $\alpha_n \leq 1/L$, where
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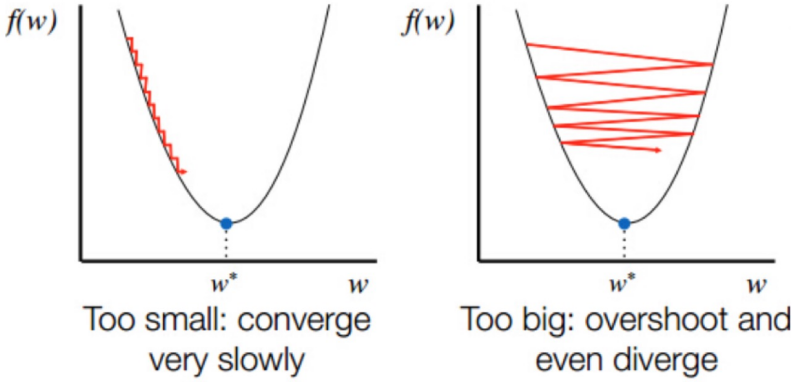
In practice, performance of P(S)GD depends very sensitively on α_ns



Block PGD = BCD

Two-Block structure : $\boldsymbol{\theta} = (A, B)$, $\boldsymbol{\Theta} = \Theta_A \times \Theta_B$

(Block PGD)
(or BCD)

$$A_{n+1} \leftarrow \Pi_{\Theta_A}\left(A_n - \alpha_n \nabla_A f(A_n, B_n)\right)$$
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  - e.g., low-rank matrix factorization, dictionary learning, tensor factorization, kernel learning, linear tranceiver design

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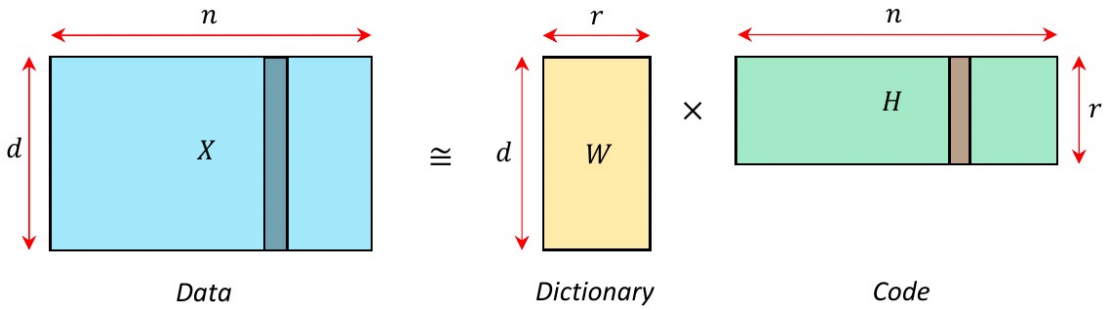
  → **Sensitive dependence on stepsize**

- **Exploiting block structure → The "effective L" is reduced**

Motivating example : **Nonnegative Matrix Factorization (Lee & Seung, Nature '99)**



$$\begin{cases} \text{minimize} & f(W,H) = \|X - WH\|_F^2 & \text{(Reconstruction error)} \\ \text{subject to} & W \in \mathbb{R}^{p\times r}_{\geq 0},\ H \in \mathbb{R}^{r\times n}_{\geq 0} & \text{(Constraints)} \end{cases}$$

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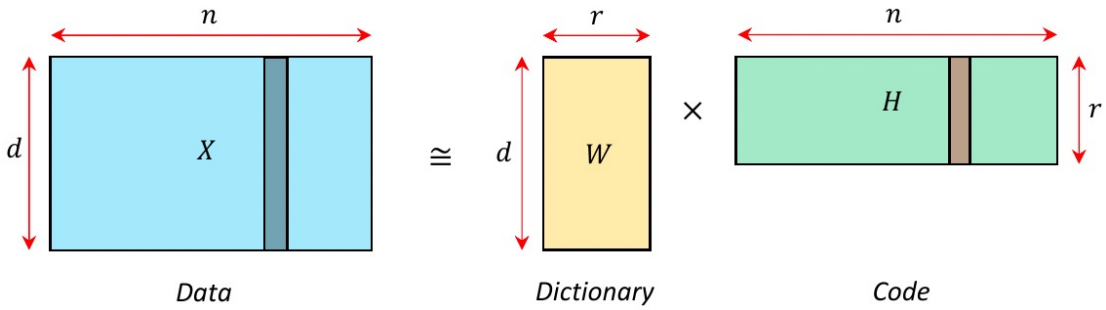

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(Almost no one uses this ☺)

- $f(W,H)$ = Bi-convex
- $\nabla_W f(W,H) = (WH-X)H^T$
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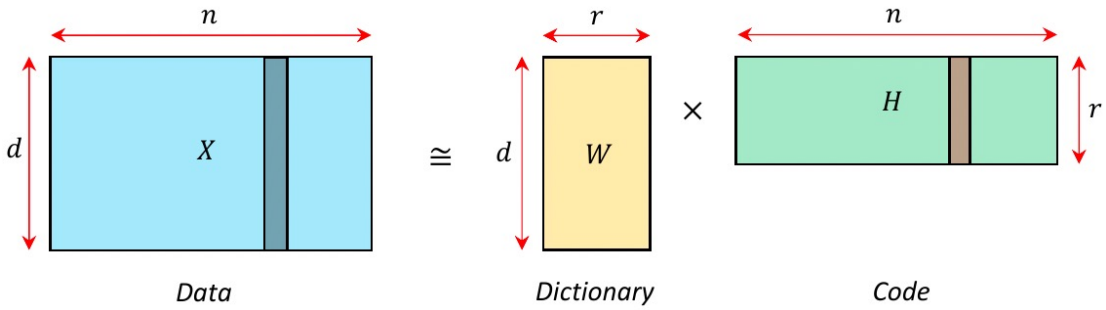

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$$A_{12} = [(\mathbf{H}\otimes\mathbf{W}) + \mathbf{I}_r \otimes (\mathbf{W}\mathbf{H} - \mathbf{X})]\,\mathbf{C}^{(r,n)}$$

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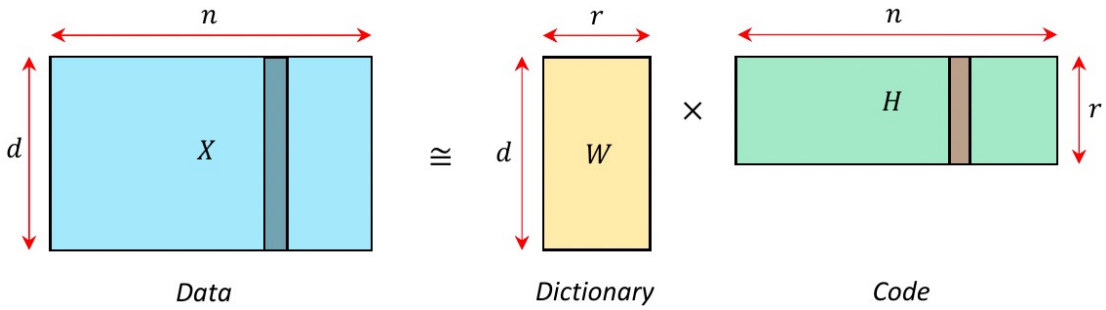

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L = Max eval over all (W,H)

= *Unbounded!*

Case study: **Supervised Matrix Factorization (Lee, Lyu, Yao ICML '24)**

Adaptive BCD:

$$\mathbf{W} \leftarrow \Pi\left(\mathbf{W} - \frac{1}{\lambda_{\max}(\mathbf{H}\mathbf{H}^T) + \varepsilon}(\mathbf{W}\mathbf{H} - \mathbf{X})\mathbf{H}^T\right),$$
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$\nabla^2_W f(\cdot, \mathbf{H})$ $\quad$ $\nabla^2_H f(\mathbf{W}, \cdot)$

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$\nabla^2_W f(\cdot, \mathbf{H})$ $\qquad$ $\nabla^2_H f(\mathbf{W}, \cdot)$

Largest Eval of *diagonal blocks* of the Hessian

$\ll$ Largest Eval of the entire Hessian

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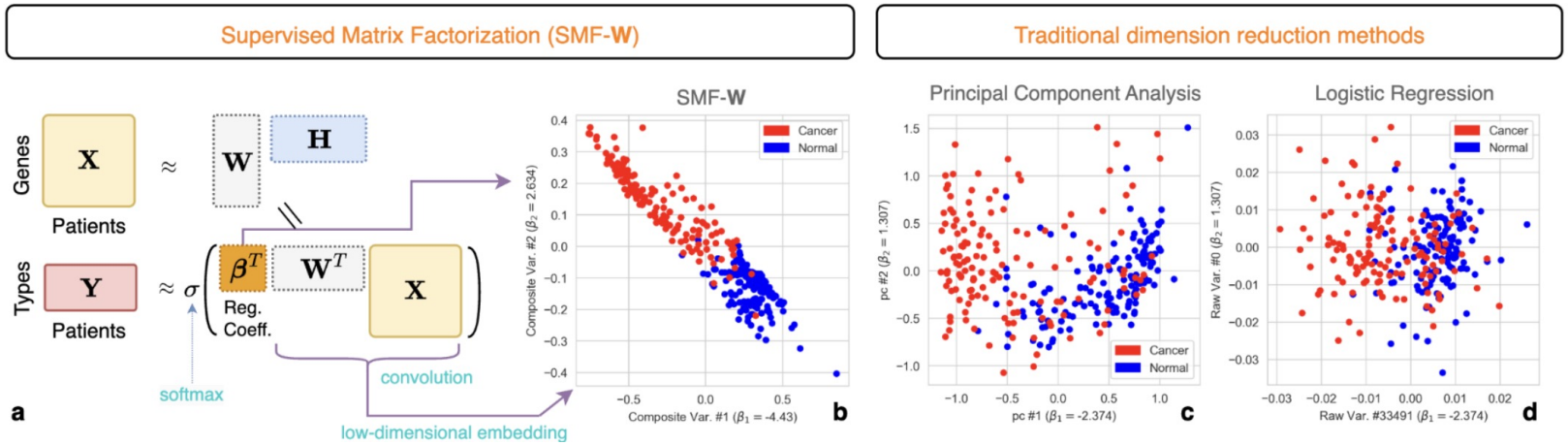
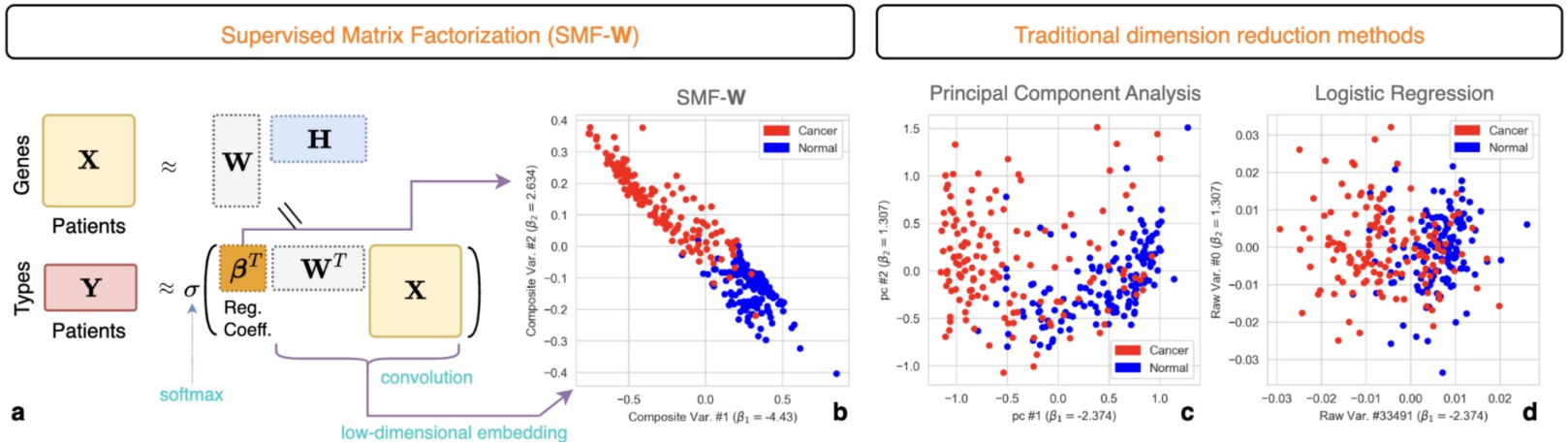


Simultaneous dimension reduction and classification

Case study: **Supervised Matrix Factorization (Lee, Lyu, Yao ICML '24)**



Simultaneous dimension reduction and classification

Classification loss Dimension reduction loss

$$\min_{\mathbf{W},\mathbf{H},\boldsymbol{\beta}} f(\mathbf{W},\mathbf{H},\boldsymbol{\beta}) := \sum_{i=1}^{n} \ell(y_i, \boldsymbol{\beta}^T \mathbf{W}^T \mathbf{x}_i) + \xi \|\mathbf{X} - \mathbf{W}\mathbf{H}\|_F^2$$

Negative log-likelihood under logistic model

$$\ell(y, a) = \log(1 + \exp(a)) - \mathbf{1}_{\{y=1\}} a$$

Parameters = Three factor matrices $\boldsymbol{W}, \boldsymbol{H}, \boldsymbol{\beta}$

Block Coordinate Descent : **Optimize one by one, not all at once**

Case study: **Supervised Matrix Factorization (Lee, Lyu, Yao ICML '24)**

Algorithm 1 BCD for SMF-$\mathbf{W}$

Input: $\mathbf{X} \in \mathbb{R}^{p\times n}$ (Data); $\mathbf{X}_{\text{aux}} \in \mathbb{R}^{q\times n}$ (Auxiliary covariate); $\mathbf{Y}_{\text{label}} \in \{0,\dots,\kappa\}^{1\times n}$ (Label);
Constraints: Convex subsets $\mathcal{C}_1 \subseteq \mathbb{R}^{p\times r}$, $\mathcal{C}_2 \subseteq \mathbb{R}^{r\times n}$, $\mathcal{C}_3 \subseteq \mathbb{R}^{r\times\kappa}$, $\mathcal{C}_4 \subseteq \mathbb{R}^{q\times\kappa}$
Parameters: $\xi \geq 0$ (Tuning parameter); $T \in \mathbb{N}$ (number of iterations); $(\eta_{k;i})_{k\geq 1, 1\leq i\leq 4}$ (step-sizes)
Initialize $\mathbf{W} \in \mathcal{C}_1, \mathbf{H} \in \mathcal{C}_2, \boldsymbol{\beta} \in \mathcal{C}_3, \boldsymbol{\Gamma} \in \mathcal{C}_4$
For $k = 1, 2, \dots, T$ **do:** ($\triangleright$ *For* α^+ *see 4.3.*)
  (Update $\mathbf{W}$)
  Update activation $\mathbf{a}_1, \dots, \mathbf{a}_n$ and $\mathbf{K}$
  $\nabla_{\mathbf{W}} f(\mathbf{Z}) \leftarrow \mathbf{X}\mathbf{K}^T\boldsymbol{\beta}^T + 2\xi(\mathbf{W}\mathbf{H} - \mathbf{X})\mathbf{H}^T$
  Choose $\eta_{k,1}^{-1} > L_1 := \alpha^+\|\boldsymbol{\beta}\|_2^2 \cdot \|\mathbf{X}\|_2^2 + 2\xi\|\mathbf{H}\|_2^2$
  $\mathbf{W} \leftarrow \Pi_{\mathcal{C}_1}(\mathbf{W} - \eta_{k;1}\nabla_{\mathbf{W}} f(\mathbf{Z}))$
  (Update $\mathbf{H}$)
  $\nabla_{\mathbf{H}} f(\mathbf{Z}) \leftarrow 2\xi\mathbf{W}^T(\mathbf{W}\mathbf{H} - \mathbf{X})$
  Choose $\eta_{k,2}^{-1} > L_2 := 2\xi\|\mathbf{W}\|_2^2$
  $\mathbf{H} \leftarrow \Pi_{\mathcal{C}_2}(\mathbf{H} - \eta_{k;2}\nabla_{\mathbf{H}} f(\mathbf{Z}))$
  (Update $\boldsymbol{\beta}$)
  Update activation $\mathbf{a}_1, \dots, \mathbf{a}_n$ and $\mathbf{K}$
  $\nabla_{\boldsymbol{\beta}} f(\mathbf{Z}) \leftarrow \mathbf{W}^T\mathbf{X}\mathbf{K}^T$
  Choose $\eta_{k,3}^{-1} > L_3 := \alpha^+\|\mathbf{W}\|_2^2 \cdot \|\mathbf{X}\|_2^2$
  $\boldsymbol{\beta} \leftarrow \Pi_{\mathcal{C}_3}(\boldsymbol{\beta} - \eta_{k;3}\nabla_{\boldsymbol{\beta}} f(\mathbf{Z}))$
  (Update $\boldsymbol{\Gamma}$)
  Update activation $\mathbf{a}_1, \dots, \mathbf{a}_n$ and $\mathbf{K}$
  $\nabla_{\boldsymbol{\Gamma}} f(\mathbf{Z}) \leftarrow \mathbf{X}_{\text{aux}}\mathbf{K}^T$
  Choose $\eta_{k,4}^{-1} > L_4 := \alpha^+\|\mathbf{X}_{\text{aux}}\|_2^2$
  $\boldsymbol{\Gamma} \leftarrow \Pi_{\mathcal{C}_4}(\boldsymbol{\Gamma} - \eta_{k;4}\nabla_{\boldsymbol{\Gamma}} f(\mathbf{Z}))$
End for
Output: $\mathbf{Z} = (\mathbf{W}, \mathbf{H}, \boldsymbol{\beta}, \boldsymbol{\Gamma})$

- $\nabla^2 f =$

	$\text{vec}(\mathbf{W})^T$	$\text{vec}(\mathbf{H})^T$	$\text{vec}(\boldsymbol{\beta})^T$	$\text{vec}(\boldsymbol{\Gamma})^T$
$\text{vec}(\mathbf{W})$	A_{11}	A_{12}	A_{13}	O
$\text{vec}(\mathbf{H})$	A_{21}	A_{22}	O	O
$\text{vec}(\boldsymbol{\beta})$	A_{31}	O	A_{33}	A_{34}
$\text{vec}(\boldsymbol{\Gamma})$	O	O	A_{43}	A_{44}

Lemma D.2 (Derivatives of the SMF-$\mathbf{W}$ objective). *Let $f(\mathbf{Z})$ denote the objective of SMF-$\mathbf{W}$ in (40). Suppose Assumption 4.3 holds. Recall $\dot{\mathbf{h}}$ and $\ddot{\mathbf{H}}$ defined in (44). Then the gradients of $f(\mathbf{Z})$ are given by*

$$\nabla_{\mathbf{W}} f(\mathbf{Z}) = \mathbf{X}\mathbf{K}^T\boldsymbol{\beta}^T + 2\xi(\mathbf{W}\mathbf{H} - \mathbf{X})\mathbf{H}^T, \tag{68}$$
$$\nabla_{\mathbf{H}} f(\mathbf{Z}) = 2\xi\mathbf{W}^T(\mathbf{W}\mathbf{H} - \mathbf{X}), \tag{69}$$
$$\nabla_{\boldsymbol{\beta}} f(\mathbf{Z}) = \mathbf{W}^T\mathbf{X}\mathbf{K}^T, \tag{70}$$
$$\nabla_{\boldsymbol{\Gamma}} f(\mathbf{Z}) = \mathbf{X}_{\text{aux}}\mathbf{K}^T. \tag{71}$$

The block-diagonal terms in the Hessian are given by

$$\nabla_{\text{vec}(\mathbf{W})}\nabla_{\text{vec}(\mathbf{W})^T} f(\mathbf{Z}) = (\boldsymbol{\beta}\otimes\mathbf{X})\mathbf{C}^{(\kappa,n)}\mathbf{M}\mathbf{C}^{(n,\kappa)}(\boldsymbol{\beta}\otimes\mathbf{X})^T + 2\xi(\mathbf{H}\mathbf{H}^T\otimes\mathbf{I}_p), \tag{72}$$
$$\nabla_{\text{vec}(\mathbf{H})}\nabla_{\text{vec}(\mathbf{H})^T} f(\mathbf{Z}) = 2\xi(\mathbf{I}_n\otimes\mathbf{W}^T\mathbf{W}), \tag{73}$$
$$\nabla_{\text{vec}(\boldsymbol{\beta})}\nabla_{\text{vec}(\boldsymbol{\beta})^T} f(\mathbf{Z}) = (\mathbf{I}_\kappa\otimes\mathbf{W}^T\mathbf{X})\mathbf{C}^{(\kappa,n)}\mathbf{M}\mathbf{C}^{(n,\kappa)}(\mathbf{I}_\kappa\otimes\mathbf{W}^T\mathbf{X})^T, \tag{74}$$
$$\nabla_{\text{vec}(\boldsymbol{\Gamma})}\nabla_{\text{vec}(\boldsymbol{\Gamma})^T} f(\mathbf{Z}) = (\mathbf{I}_\kappa\otimes\mathbf{X}_{\text{aux}})\mathbf{C}^{(\kappa,n)}\mathbf{M}\mathbf{C}^{(n,\kappa)}(\mathbf{I}_\kappa\otimes\mathbf{X}_{\text{aux}})^T. \tag{75}$$

The block-off-diagonal terms in the Hessian are given by

$$\nabla_{\text{vec}(\mathbf{H})}\nabla_{\text{vec}(\mathbf{W})^T} f(\mathbf{Z}) = 2\xi\mathbf{C}^{(n,r)}\left[(\mathbf{H}^T\otimes\mathbf{W}^T) + \mathbf{I}_r\otimes(\mathbf{W}\mathbf{H} - \mathbf{X})^T\right], \tag{76}$$
$$\nabla_{\text{vec}(\boldsymbol{\beta})}\nabla_{\text{vec}(\mathbf{W})^T} f(\mathbf{Z}) = \mathbf{C}^{(\kappa,r)}(\mathbf{I}_r\otimes\mathbf{X}\mathbf{K}^T)^T + (\mathbf{I}_\kappa\otimes\mathbf{W}^T\mathbf{X})\mathbf{C}^{(\kappa,n)}\mathbf{M}\mathbf{C}^{(n,\kappa)}(\boldsymbol{\beta}\otimes\mathbf{X})^T, \tag{77}$$
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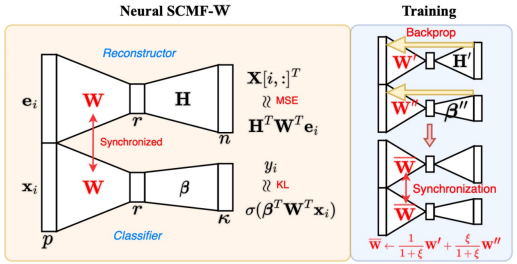
$$\nabla_{\text{vec}(\boldsymbol{\Gamma})}\nabla_{\text{vec}(\boldsymbol{\beta})^T} f(\mathbf{Z}) = (\mathbf{I}_r\otimes\mathbf{X}_{\text{aux}})\mathbf{C}^{(\kappa,n)}\mathbf{M}\mathbf{C}^{(n,\kappa)}(\mathbf{I}_\kappa\otimes\mathbf{W}^T\mathbf{X})^T. \tag{79}$$

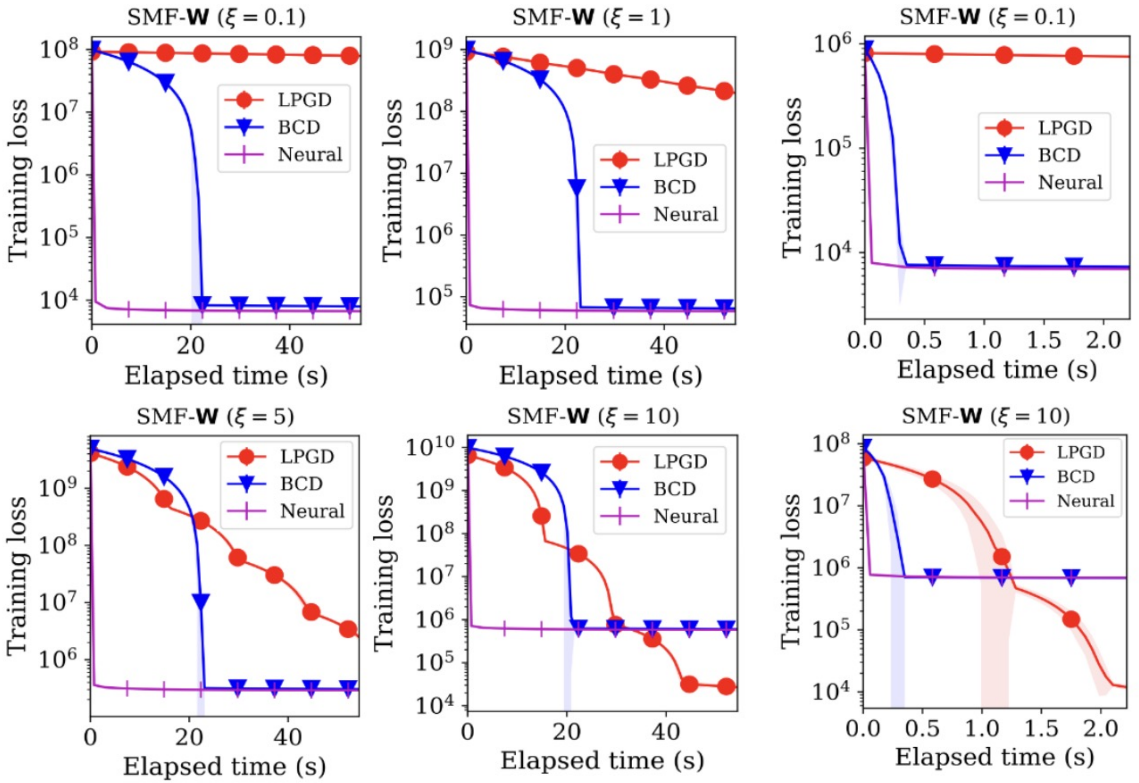
Case study: **Supervised Matrix Factorization (Lee, Lyu, Yao ICML '24)**

LPGD = Low-rank PGD [Lee, Lyu, Yao NeurIPS '23]

BCD = Adaptive BCD [Lee, Lyu, Yao ICML '24]

Neural = 2-year coupled NN implementation of BCD [Lee, Lyu, Yao ICML '24]





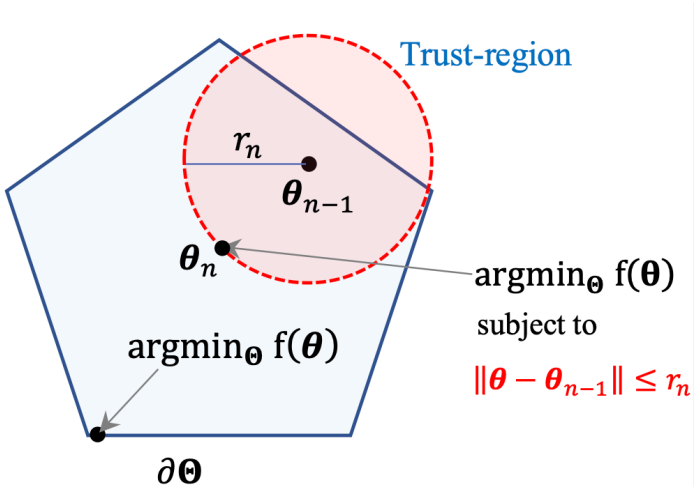
a Job postings

b Semi-synthetic MNIST data

A safeguarding approach:

Non-adaptive Trust-Region

Disciplined Agressiveness



(BCD)

$$
\begin{aligned}
A_{n+1} &\leftarrow \Pi_{\Theta_A}\left(A_n - \alpha_n \nabla_A f(A_n, B_n, C_n)\right) \\
B_{n+1} &\leftarrow \Pi_{\Theta_B}\left(B_n - \beta_n \nabla_B f(A_{n+1}, B_n, C_n)\right) \\
C_{n+1} &\leftarrow \Pi_{\Theta_C}\left(C_n - \gamma_n \nabla_C f(A_{n+1}, B_{n+1}, C_n)\right)
\end{aligned}
$$

- Pros: **Robust against stepsize choices**

(BCD)

$$
\begin{aligned}
A_{n+1} &\leftarrow \Pi_{\Theta_A}\left(A_n - \alpha_n \nabla_A f(A_n, B_n, C_n)\right)\\
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\end{aligned}
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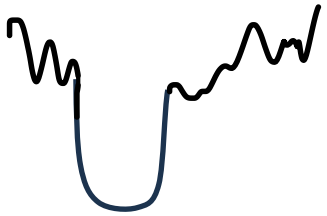

- Pros: **Robust against stepsize choices**
- Cons: **Convergence rate could be slow for FLAT landscape**
  - (# of iterations to reach an ϵ-stationary points for PGD) $= O(L\epsilon^{-2})$

$$
\text{“ } \|\nabla f(\theta_n)\| \le \epsilon \text{ ”}
$$

(BCD)

$$
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A_{n+1} &\leftarrow \Pi_{\Theta_A}\left(A_n - \alpha_n \nabla_A f(A_n, B_n, C_n)\right)\\
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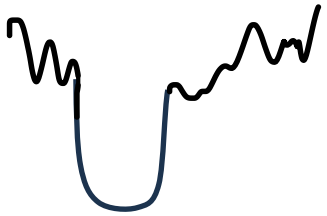
$$



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  - (# of iterations to reach an ϵ-stationary points for PGD) $= O(L\epsilon^{-2})$

$$\text{“ } \|\nabla f(\theta_n)\| \le \epsilon \text{ ”}$$

[Razaviyayn et al. ’14, Lyu, Li ’24+]

  - (# of iterations to reach an ϵ-stationary points for **BCD**) $= O(L(1+\rho^{-1})\epsilon^{-2})$

(BCD)

$$A_{n+1} \leftarrow \Pi_{\Theta_A}\left(A_n - \alpha_n \nabla_A f(A_n, B_n, C_n)\right)$$
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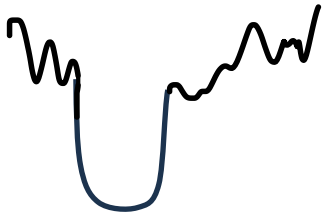

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  - (# of iterations to reach an ϵ-stationary points for **BCD**) $= O(L(1+\rho^{-1})\epsilon^{-2})$

Largest allowed stepsize

(ρ=Local smoothness parameter)

(Small ρ ⇔ Flat local landscape ⇔ Large allowed stepsize)

BCD with Diminishing Radius

(BCD-DR)

$$
\begin{aligned}
A_{n+1} &\leftarrow \Pi_{\Theta_A \cap \{A : \|A - A_n\| \le r_n\}} \left(A_n - \alpha_n \nabla_A f(A_n, B_n, C_n)\right) \\
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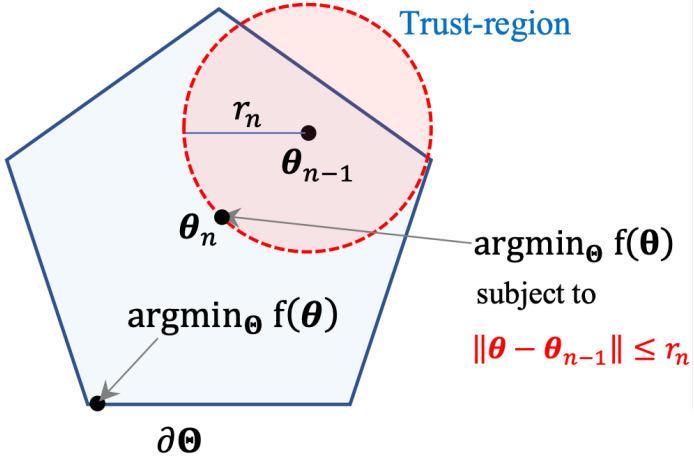

DR = Diminishing Radius: $r_n \sim c/\sqrt{n}$

(In classic Trust-Region literature, r_n is chosen adaptively)

[Lyu, Strohmeier, Needell JMLR '22]

[Lyu, JMLR '24] [Powell, Lyu ICML'24]

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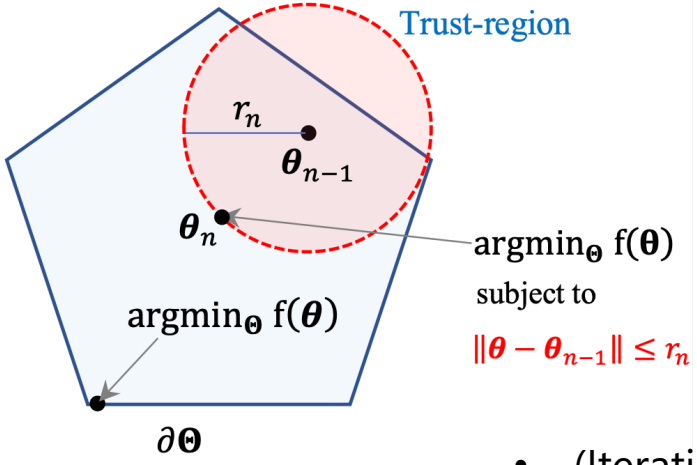

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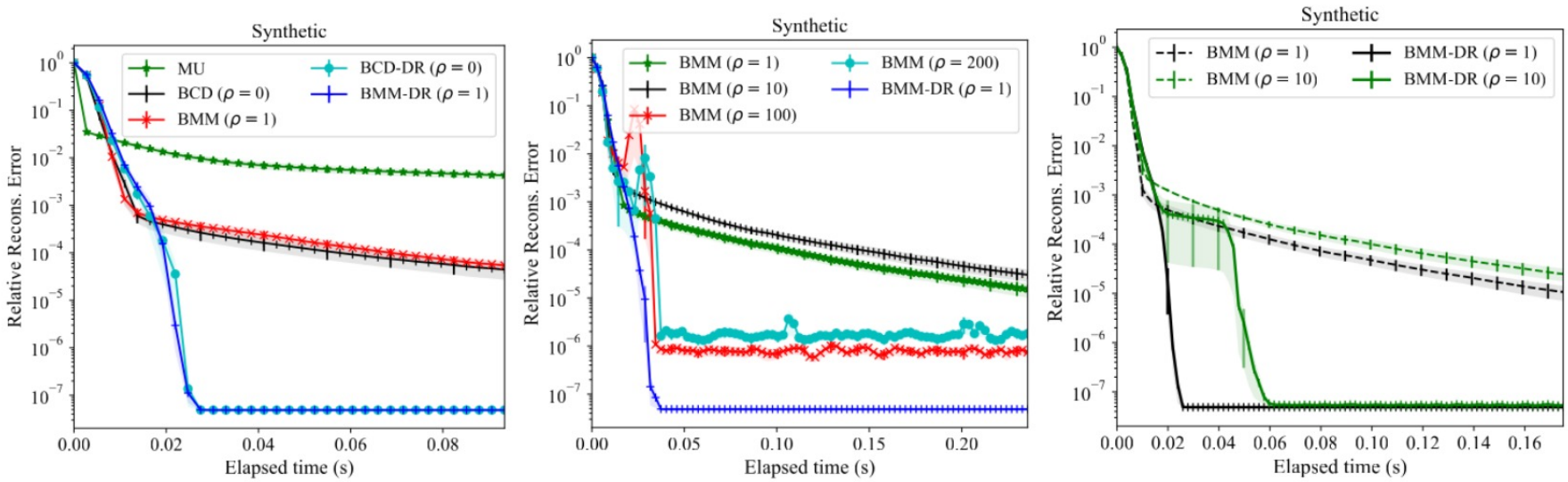
[Lyu, JMLR '24] [Powell, Lyu ICML'24]

- (Iteration complexity for PGD) $= O(L\epsilon^{-2})$
- (iteration complexity for BCD) $= O(L(1+\rho^{-1})\epsilon^{-2})$
- (Iteration complexity for **BCD-DR**) $= O(L\epsilon^{-2})$ [Li, Lyu '24+]

No dependence on ρ

A very flat nonconvex problem



MU=Multiplicative Update

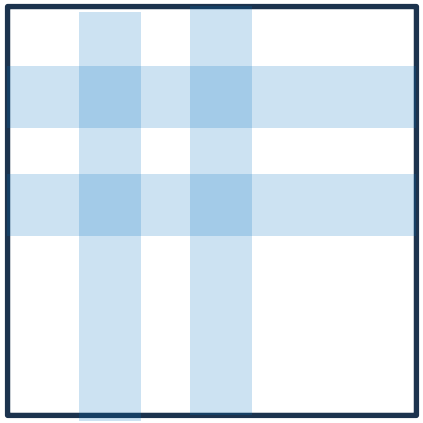
BCD = Block Coordianate Descent

BMM= Block Majorization-Minimization (in this case BCD+prox. Reg.)

A randomization approach:

Randomized Hessian Approximation

Flip the right coins!



What's known for the simplest algorithm?

(QN) $$\boldsymbol{\theta}_{n+1} \leftarrow \boldsymbol{\theta}_n - \overbrace{\left(\nabla^2 f(\boldsymbol{\theta}_n) + \gamma_n \mathbf{I}_p\right)^{-1}}^{\mathbf{H}_n} \nabla f(\boldsymbol{\theta}_n)$$

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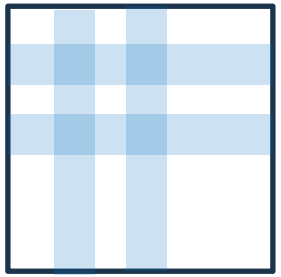
Idea: Sample rows and columns of the Hessian with prob. ∝ diag(Hessian)



Randomized Low-rank Quasi-Newton

(RLQN)
$$\begin{cases} \mathbf{F}_n\mathbf{F}_n^T \approx \nabla^2 f(\boldsymbol{\theta}_n) + \tau_n \mathbf{I}_N & (\triangleright \textit{Randomized low-rank Hessian approx.}) \\ \mathbf{H}_n \leftarrow \alpha_n \left(\mathbf{F}_n\mathbf{F}_n^T + \delta_n \mathbf{I}_N\right)^{-1} & (\triangleright \textit{Preconditioning matrix}) \\ \boldsymbol{\theta}_{n+1} \leftarrow \boldsymbol{\theta}_n - \mathbf{H}_n \nabla f(\boldsymbol{\theta}_n) & (\triangleright \textit{Parameter update}). \end{cases}$$

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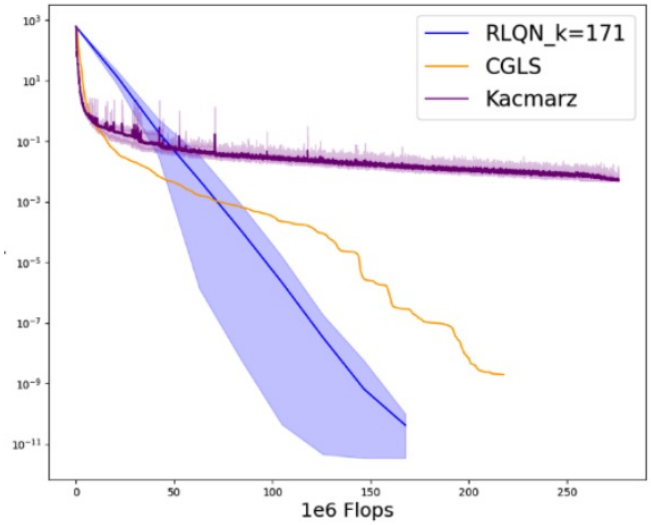
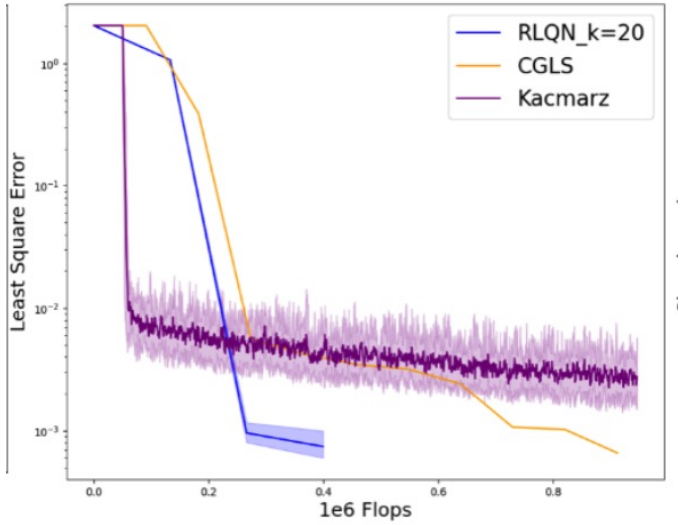
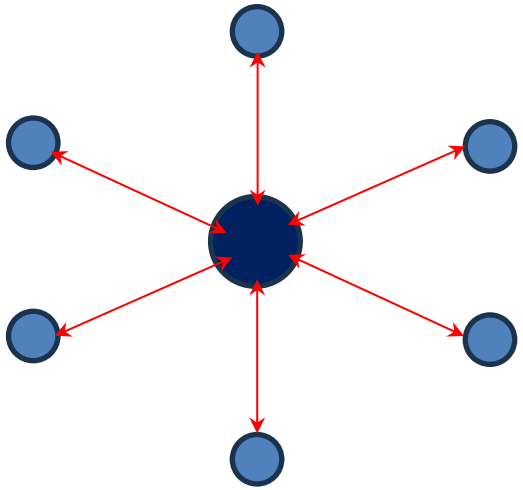




A sampling approach:

Stochastic Aggregated Double-Averaging

Consensus, Consensus!



A finite-sum problem

$$\boldsymbol{\theta}^* \in \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \left\{ f(\boldsymbol{\theta}) := \sum_{v \in \mathcal{V}} f^v(\boldsymbol{\theta}) \right\}$$

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(PSGD)

$$v_n \sim \text{Uniform}(\mathcal{V}), \text{ independent}$$
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Memory	Iteration Complexity
$O(p)$	$O(\epsilon^{-4})$

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(MISO) [Mairal '13]	$v_n \sim \text{Uniform}(\mathcal{V})$, independent $\boldsymbol{\theta}^{v_n} \leftarrow \boldsymbol{\theta}_n$, Keep other $\boldsymbol{\theta}^u$s $\nabla^v \leftarrow \nabla f^v(\boldsymbol{\theta}_n)$, Keep other ∇^us $\boldsymbol{\theta}_{n+1} \leftarrow \Pi_{\boldsymbol{\Theta}} \left(\frac{1}{\lvert\mathcal{V}\rvert} \sum_{u\in\mathcal{V}} \boldsymbol{\theta}^u - \alpha_n \frac{1}{\lvert\mathcal{V}\rvert} \sum_{u\in\mathcal{V}} \nabla^u\right)$	$O(pn)$	$O(\epsilon^{-2})$ [Karimi et al. ICML'22]

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Minimization by Incremental Surrogate Optimization

$$\boldsymbol{\theta}^* \in \arg\min_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \left\{ f(\boldsymbol{\theta}) := \sum_{v\in\mathcal{V}} f^v(\boldsymbol{\theta}) \right\}$$

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$$v_n \sim \text{Recurrent}(\mathcal{V})$$
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Iteration Complexity

$O(\epsilon^{-2})$

[Powell, Lyu ICML '24]

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- Recurrent sampling = Very general sampling scheme

  e.g., i.i.d., Markovian, Recurrent, Cyclic, etc.

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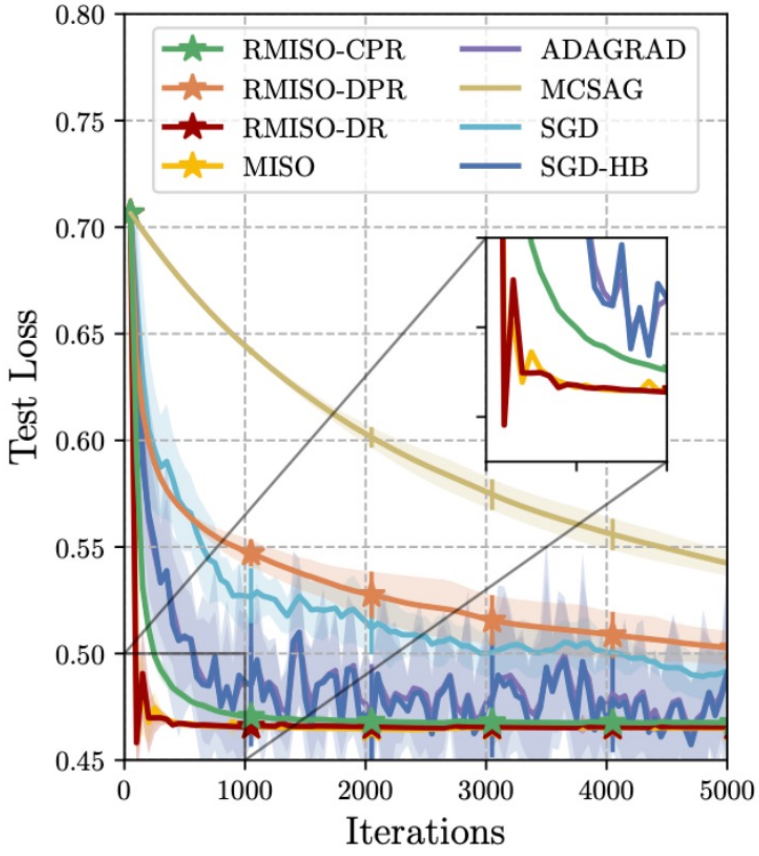
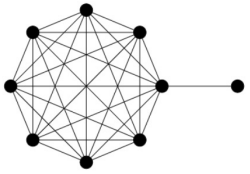
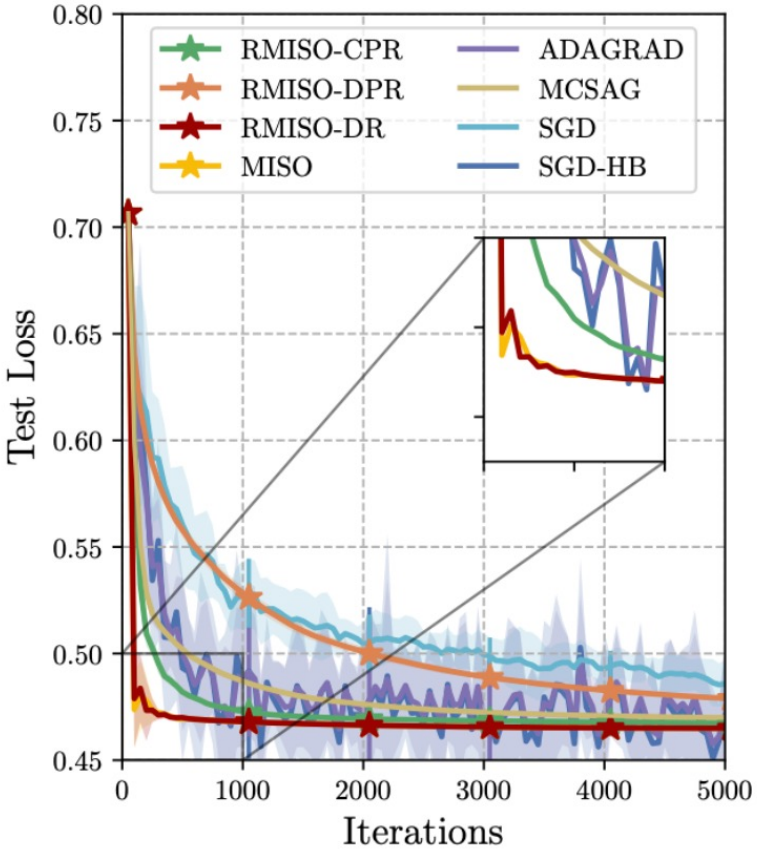
  e.g., i.i.d., Markovian, Recurrent, Cyclic, etc.

- The implied constant in $O(\epsilon^{-2})$ is significantly improved

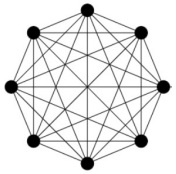


(a) Lonely graph





(b) Complete graph



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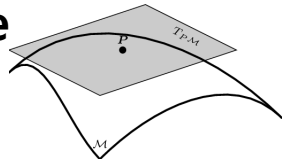

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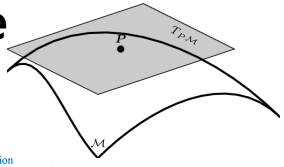
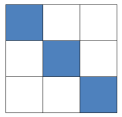
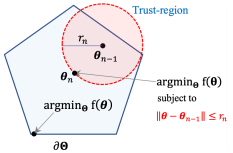
    - Block optimization and Trust-Region







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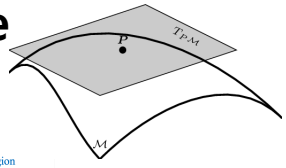

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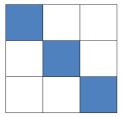

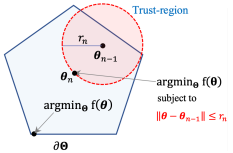

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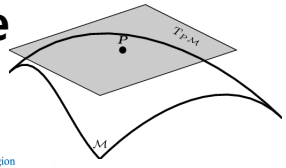

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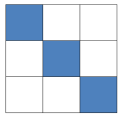

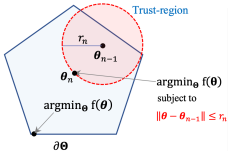

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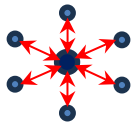
  - **Finite-sum problem with arbitrary sampling**
    - Aggregation with parameter and gradient averaging



Thank you very much!

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