Data Selection under Low Intrinsic Dimension:

from Interpolatove Decomposition to Ridge Regression

Yijun Dong

Courant Institute of Mathematical Sciences, New York University

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NYU COURANT INSTITUTE OF MATHEMATICAL SCIENCES

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Low Intrinsic Dimension & Data Selection

- **Low intrinsic dimension is ubiquitous in real world**
  - Example: A language model with 341M parameters can be finetuned in a dimension-322 subspace with less than 6K samples [Aghajanyan-Zettlemoyer-Gupta-2020]
- Learning under low intrinsic dimension **with limited data, data selection becomes crucial**

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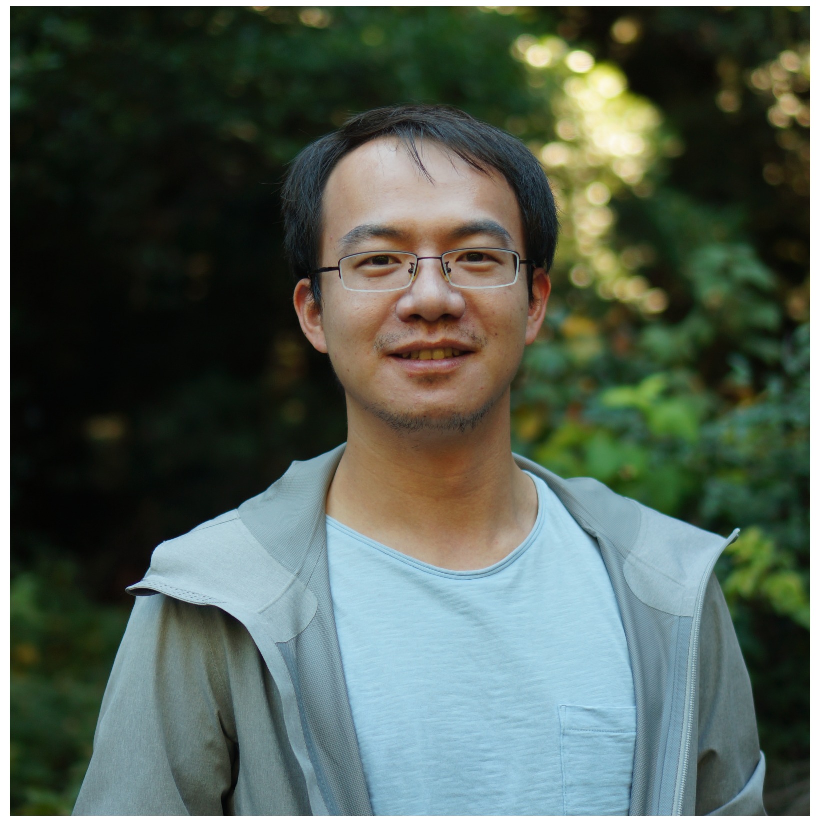
- Learning under low intrinsic dimension **with limited data, data selection becomes crucial**

How to **select informative data** for learning under **low intrinsic dimension**?

- Learning without noise: low-rank interpolative decomposition (ID)
- Learning with noise: low-rank approximation (bias) + variance reduction

Robust Blockwise Random Pivoting: Fast and Accurate Adaptive Interpolative Decomposition



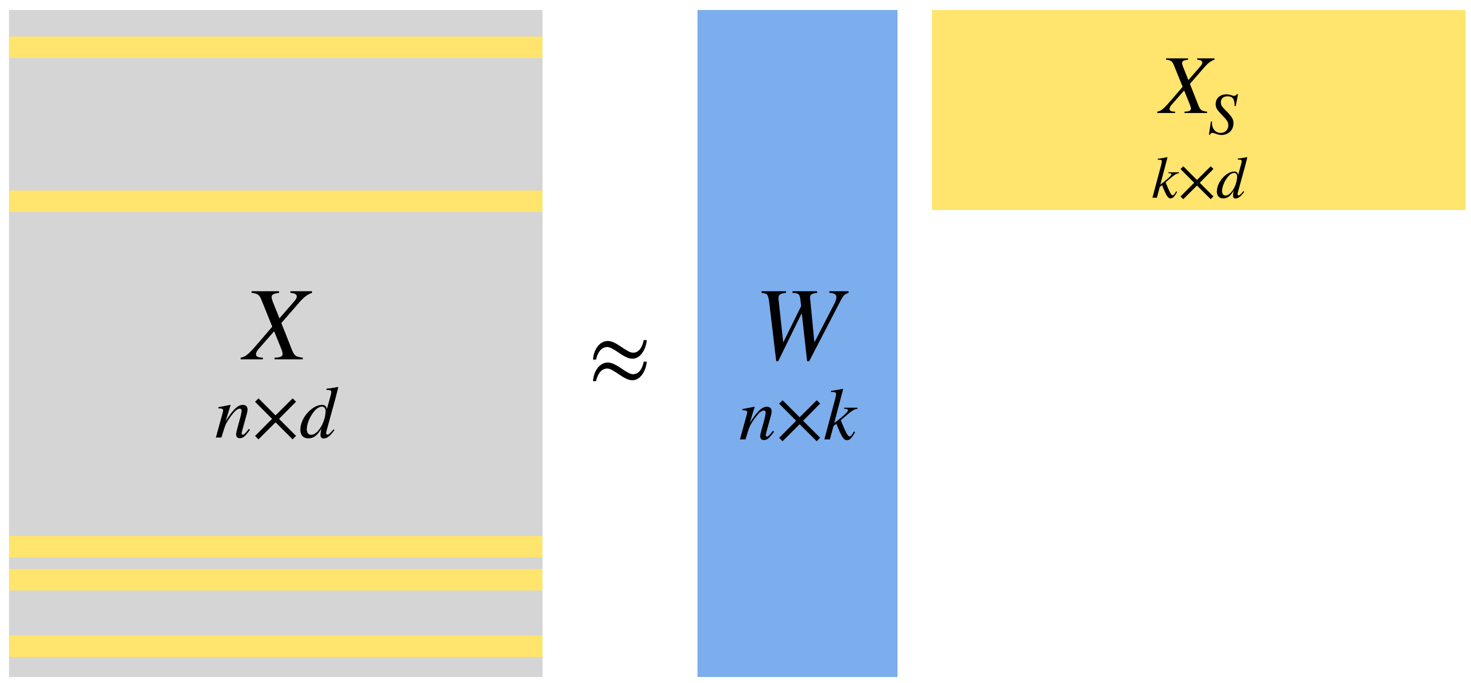
Chao Chen
NCSU

Per-Gunnar Martinsson
UT Austin

Katherine Pearce
UT Austin

Interpolative Decomposition (ID)

- Given a data matrix $X = [x_1, \cdots, x_n]^\top \in \mathbb{R}^{n \times d}$
- A target rank $1 \le r \le \mathrm{rank}(X)$
- An error tolerance $\tau > 0$
- Aim to construct an ID of X —— $X \approx (XX_S^\dagger)X_S$ such that

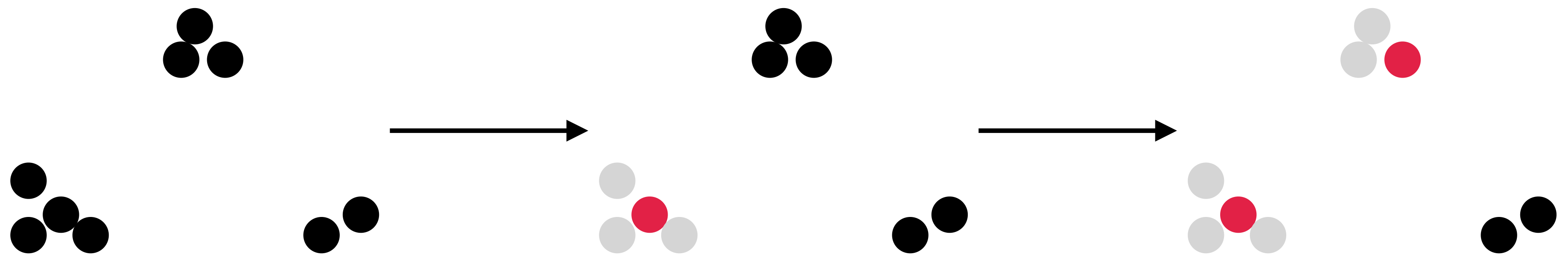


$$\mathscr{E}(S) = \|X - (XX_S^\dagger)X_S\|_F^2 \le \tau \|X\|_F^2$$

  - $S = \{s_1, \cdots, s_k\} \subseteq [n]$ contains indices for a **skeleton subset** of size $|S| = k$ (usually $k \ll n$)
  - $X_S = [x_{s_1}, \cdots, x_{s_k}]^\top \in \mathbb{R}^{k \times d}$ is the row skeleton submatrix corresponding to S
  - $W = XX_S^\dagger \in \mathbb{R}^{n \times k}$ is an interpolation matrix for the given skeleton subset S

Adaptiveness & Randomness

- **Adaptiveness**
  - Each new skeleton selection is aware of the previously selected skeleton subset
  - By selecting according to the residual
  - Common adaptive residual updates:
    - Gram-Schmidt (QR)
    - Gaussian elimination (LU)



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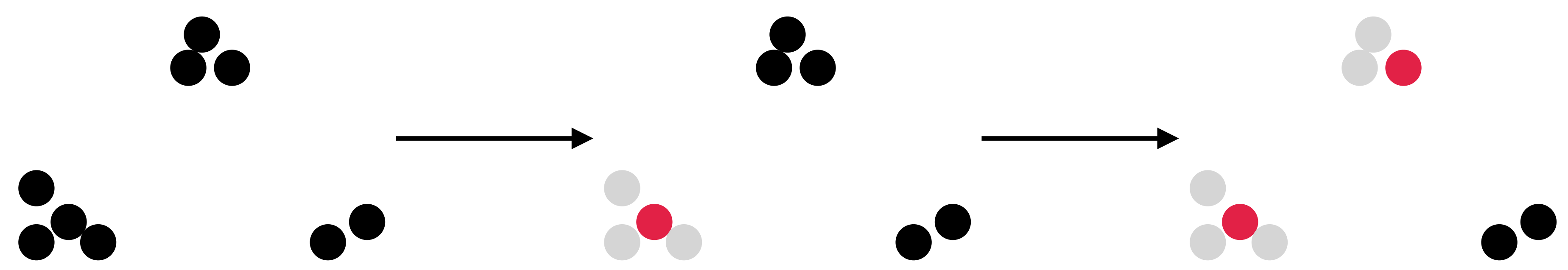
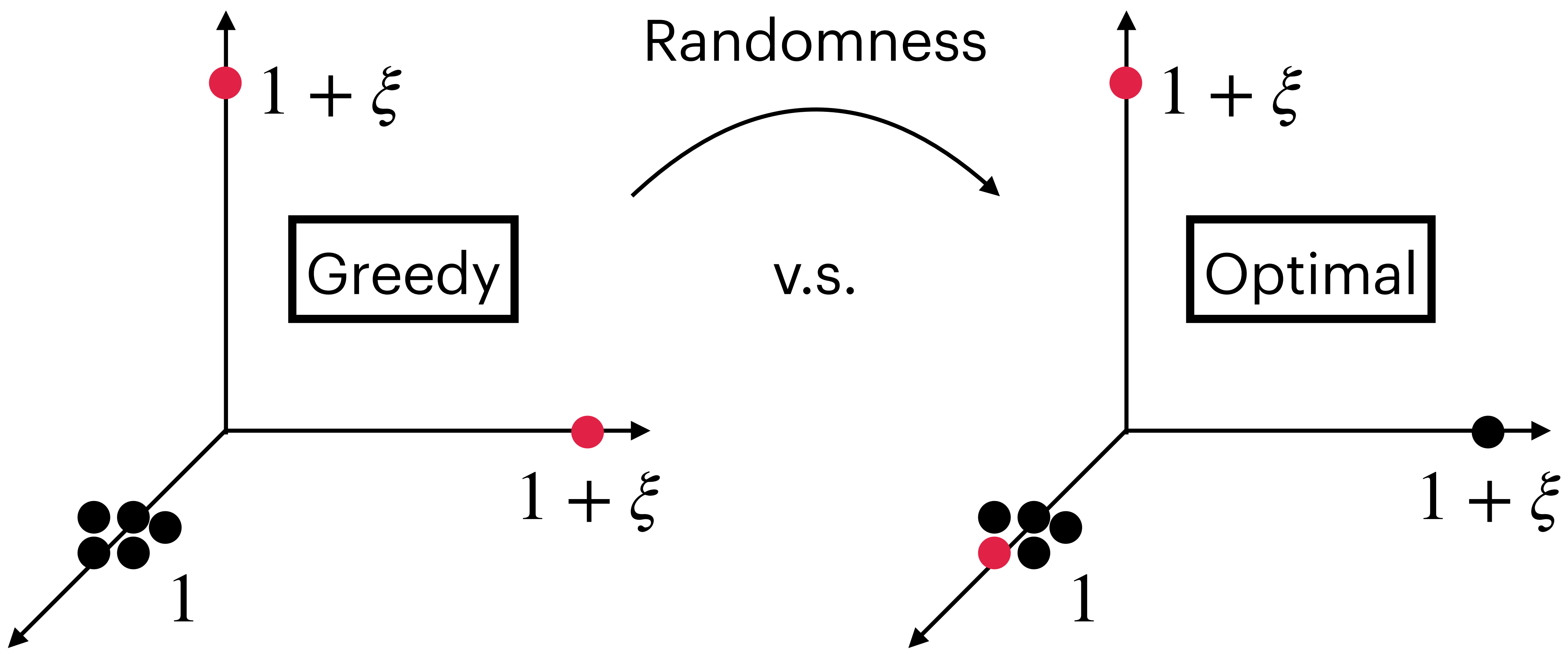


- **Randomness** (in contrast to greedy)
  - Intuition: balance exploitation with exploration
  - Effectively circumvent adversarial inputs for greedy methods
  - Achieve appealing skeleton complexities in expectation
  - Common randomness: sampling, sketching



Skeleton Selection: A General Framework

A framework for (blockwise adaptive) skeleton selection

- **Inputs**: $X \in \mathbb{R}^{n \times d}$, $\tau \in (0,1)$
- $X^{(0)} \leftarrow X$, $S^{(0)} \leftarrow \varnothing$, $t \leftarrow 0$
- **while** $\mathscr{E}(S^{(t)}) > \tau \|X\|_F^2$ **do**
  - $t \leftarrow t + 1$
  - Select $|S_t| = b$ skeletons S_t based on $\left(p_i\left(X^{(t-1)}\right)\right)_{i \in [n]}$
  - $S^{(t)} \leftarrow S^{(t-1)} \cup S_t$
  - $X^{(t)} \leftarrow X^{(t-1)}\left(I_d - X_{S_t}^{\dagger} X_{S_t}\right)$
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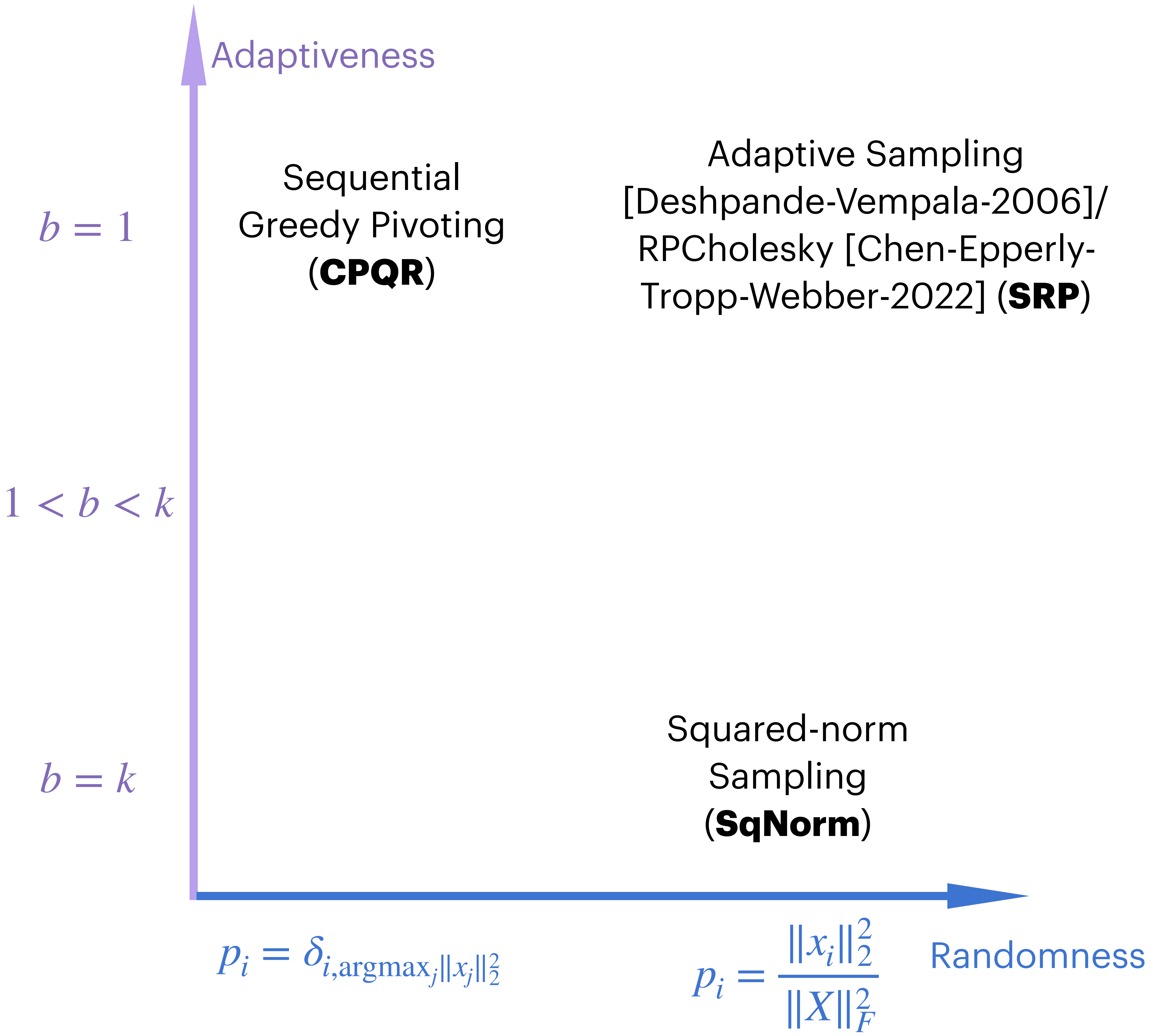

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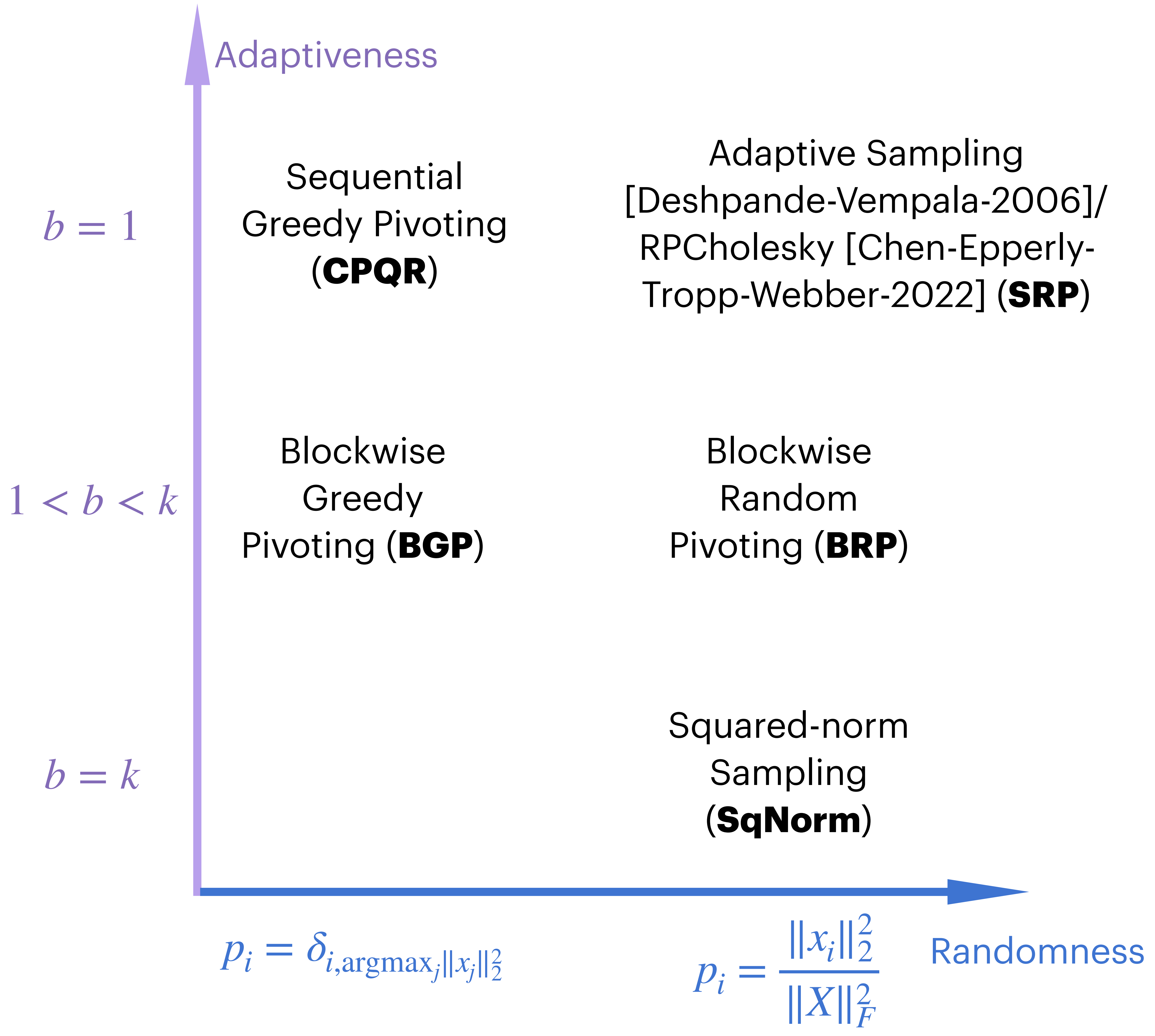

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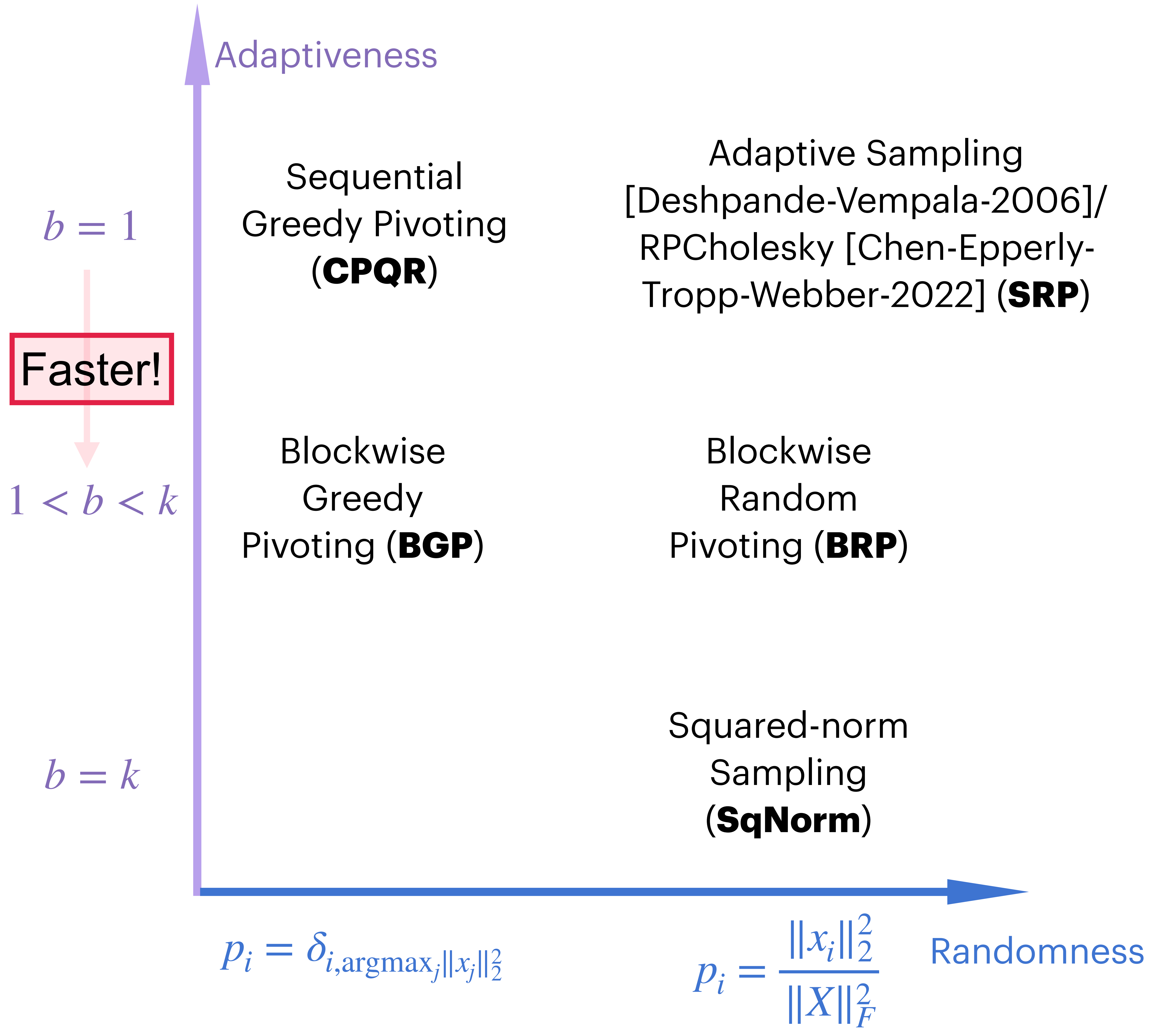


Skeleton Selection: Other Methods

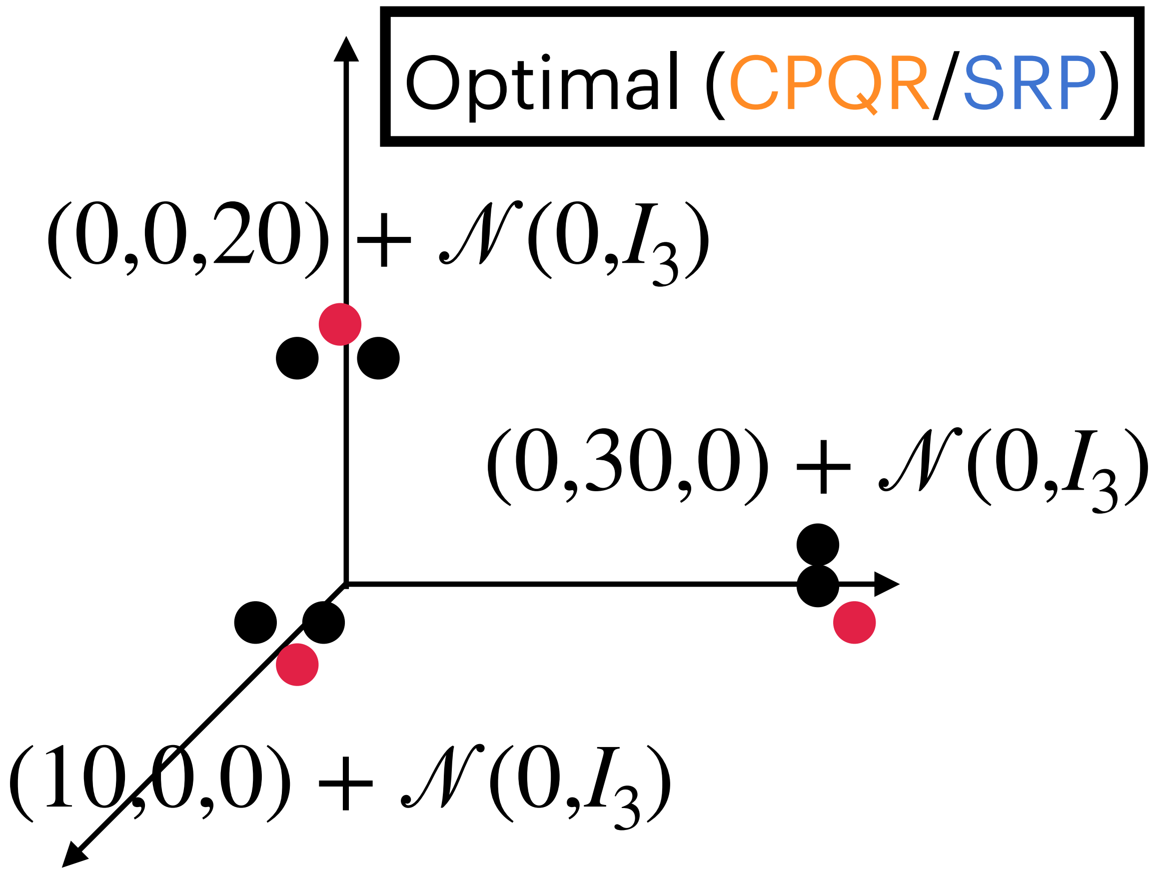
Sampling methods

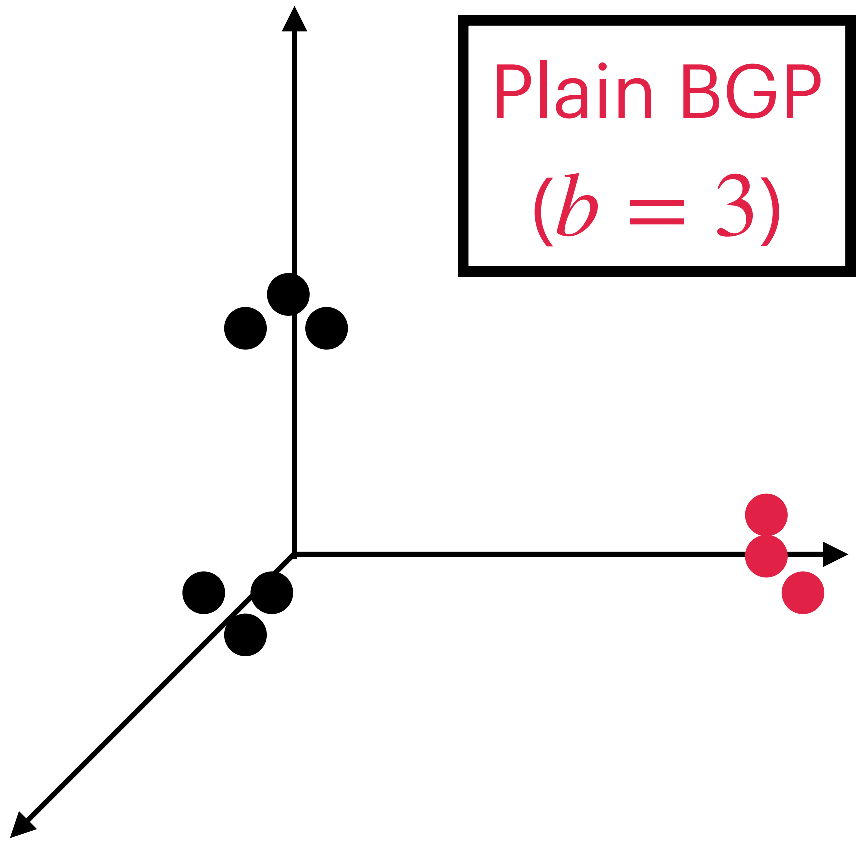
- **DPP/volume sampling** [Deshpande-Rademacher-Vempala-Wang-2006, Belabbas-Wolfe-2009, etc.]
  - Pro: nearly optimal expected skeleton complexity
  - Con: expensive to compute
- **Leverage score sampling** [Mahoney-Drineas-2009, Cohen-Musco-Musco-2017, etc.]
  - Pro: can be estimated efficiently for large-scale problems (e.g., tensor Khatri-Rao product)
  - Con: expensive to compute
- **Uniform sampling** [Cohen-Lee-Musco-Musco-Peng-Sidford-2015]
  - Pro: linear time
  - Con: require/depend on matrix incoherence

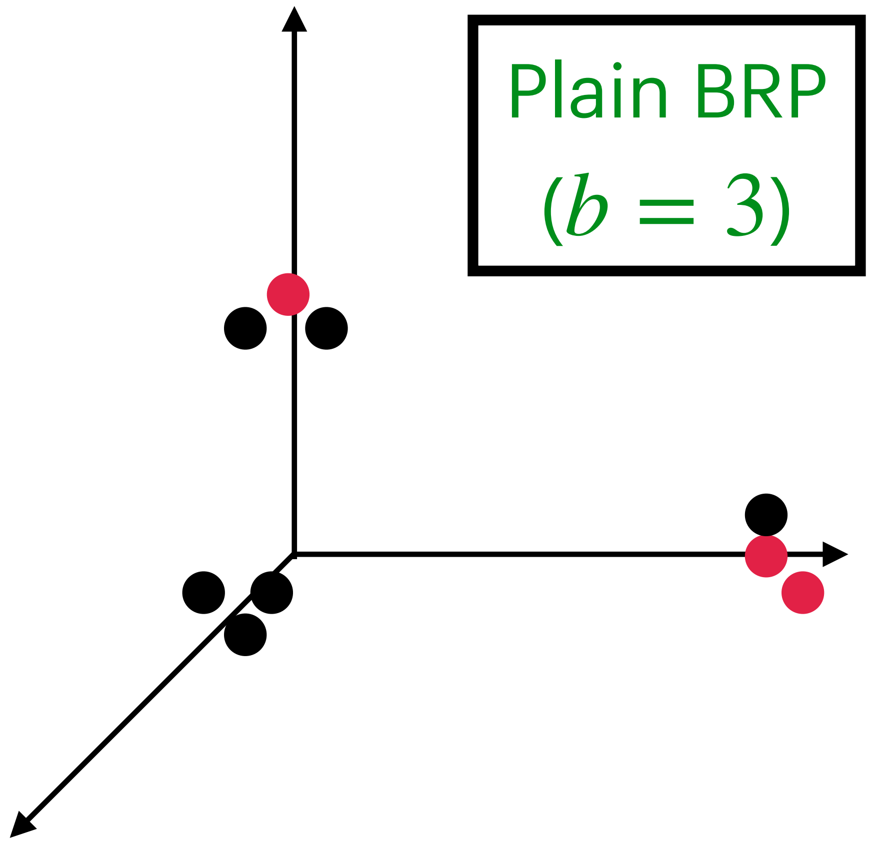
Sketchy pivoting

- **Inputs**: $X \in \mathbb{R}^{n \times d}$, $k \leq \mathrm{rank}(X)$,
- Draw JLT $\Omega \in \mathbb{R}^{d \times k}$ (e.g., $\Omega_{ij} \sim \mathcal{N}(0, 1/k)$ i.i.d.)
- Sketching $Y = X\Omega \in \mathbb{R}^{n \times k}$
- Greedy pivoting: for $t = 1, \cdots, k$
  - Row pivoted QR (**CPQR**) [Voronin-Martinsson-2017]: $s_t \leftarrow \underset{i}{\mathrm{argmax}} \, \| Y^{(t-1)}_{i,:} \|_2^2$ + Gram-Schmidt
  - LU with partial pivoting (**LUPP**) [D-Martinsson-2023]: $s_t \leftarrow \underset{i}{\mathrm{argmax}} \, | Y^{(t-1)}_{i,t} |$ + Gaussian Elimination
- Pro: fast, accurate, robust to adversarial inputs
- Con: require prior knowledge of k

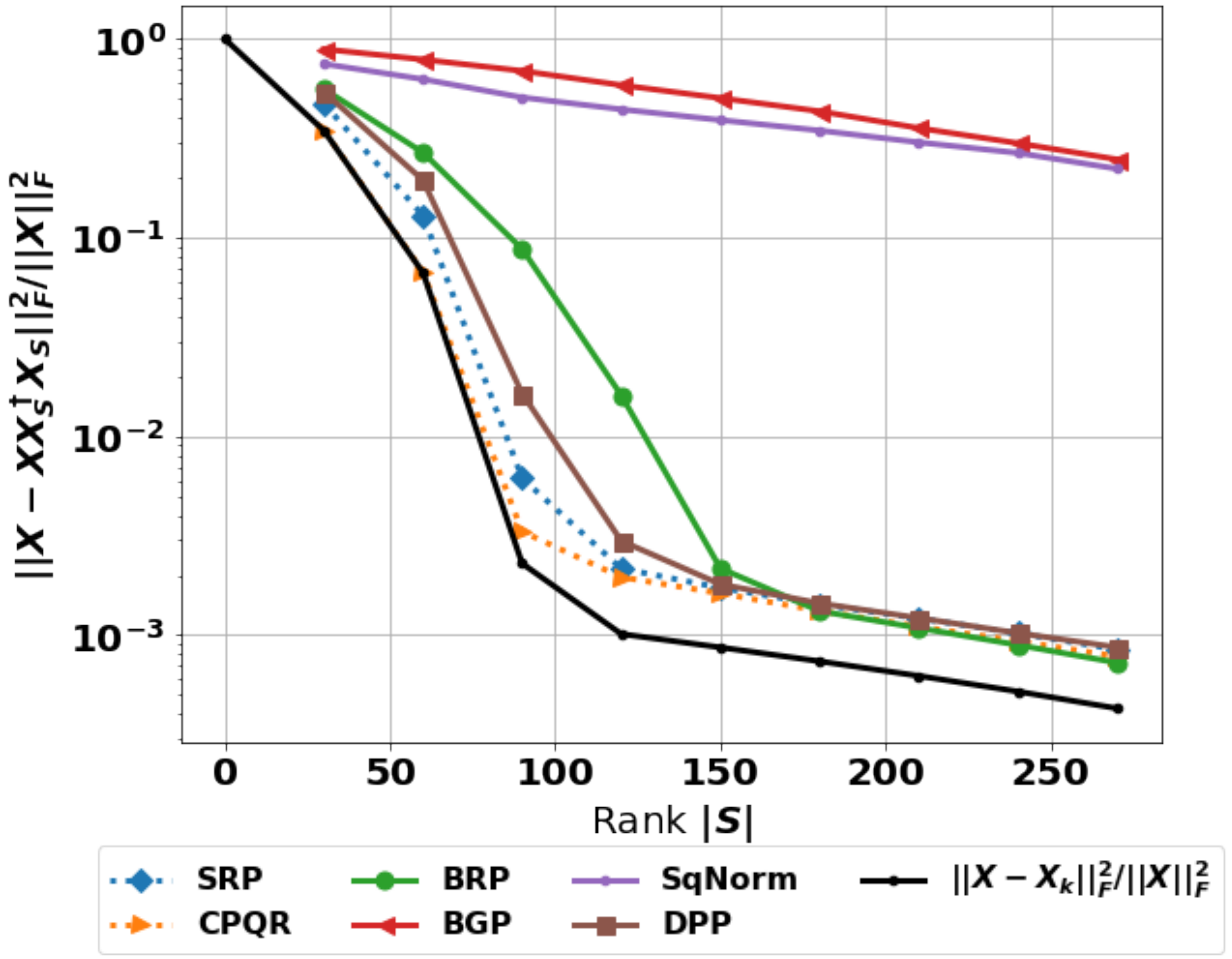
Pitfall of Plain Blockwise Greedy/Random Pivoting







$k = 100$ clusters centered at $\{10j \cdot e_j\}_{j\in[k]}$, $n = 20k$, $d = 500$, $b = 30$



- Sequential pivoting (CPQR & SRP) is nearly optimal
- Plain blockwise pivoting (BRP/BGP, especially BGP) suffers from suboptimal skeleton complexities (up to b times)
- Squared-norm sampling (SqNorm) tends to fail

Robust Blockwise Random Pivoting

Robust Blockwise Random Pivoting (RBRP)

- **Inputs**: $X \in \mathbb{R}^{n\times d}$, $\tau \in (0,1)$
- $X^{(0)} \leftarrow X$, $S^{(0)} \leftarrow \emptyset$, $t \leftarrow 0$
- **while** $\mathcal{E}(S^{(t)}) > \tau \|X\|_F^2$ $(t \leftarrow t+1)$ **do**
  - Select $|S_t| = b$ skeletons S_t based on $\left(p_i\left(X^{(t-1)}\right)\right)_{i\in[n]}$
  - **Robust blockwise filtering (RBF)**
    - $\pi \leftarrow \mathrm{CPQR}\left(X^{(t-1)}_{S_t}\right) \in S_b$ (SRP and CPQR both work)
    - $\min_{S_t'=S_t(\pi(1:b'))} b' \ \mathrm{s.t.}\ \|X_{S_t} - X_{S_t'}\|_F^2 < \tau_b \|X_{S_t}\|_F^2$ (e.g., $\tau_b = \frac{1}{b}$)
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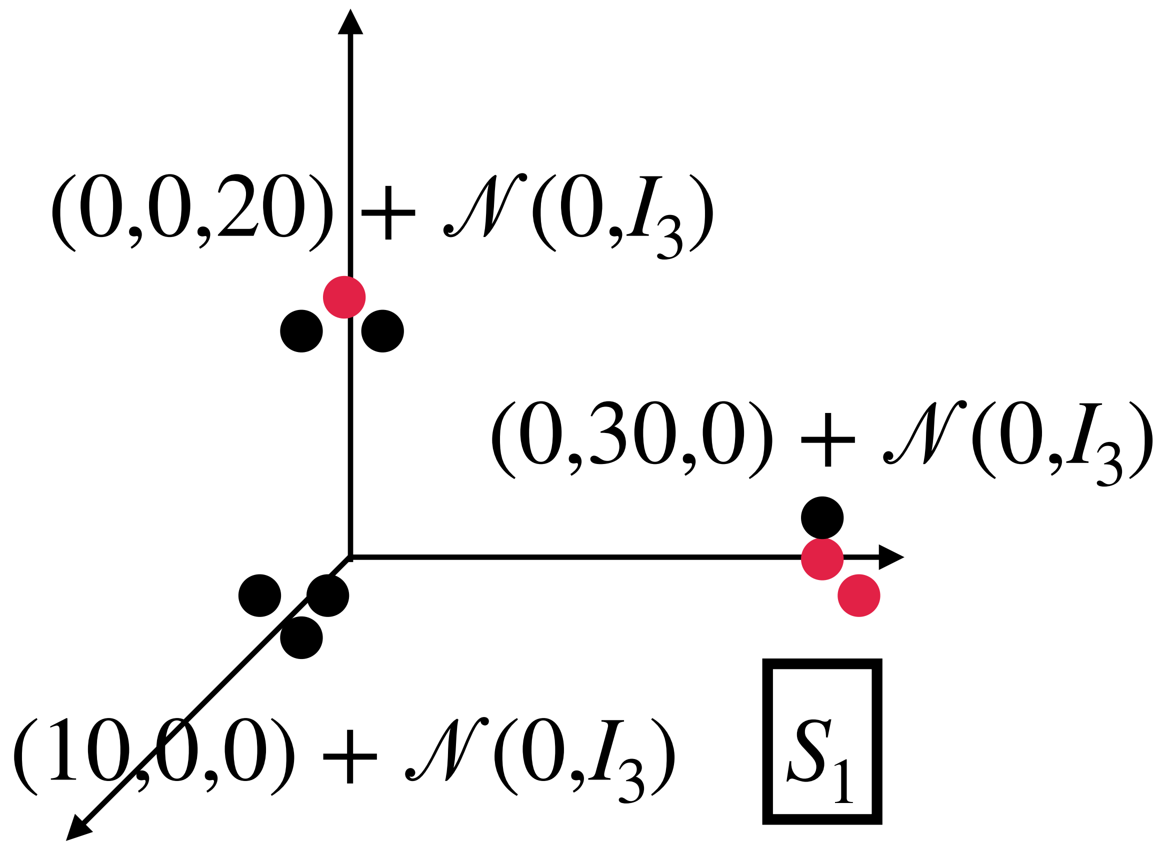

Robust Blockwise Random Pivoting

Robust **B**lockwise **R**andom **P**ivoting (**RBRP**)

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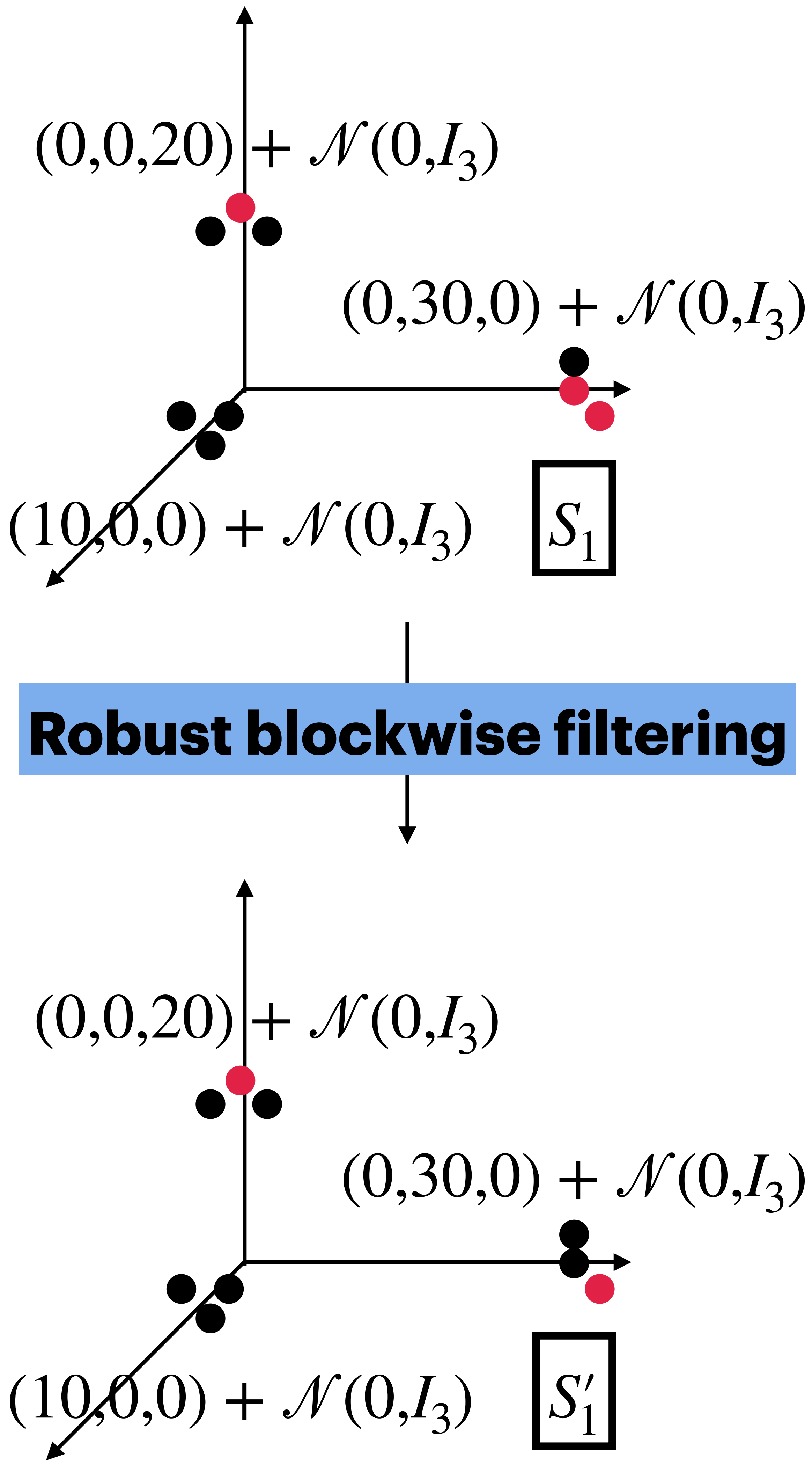
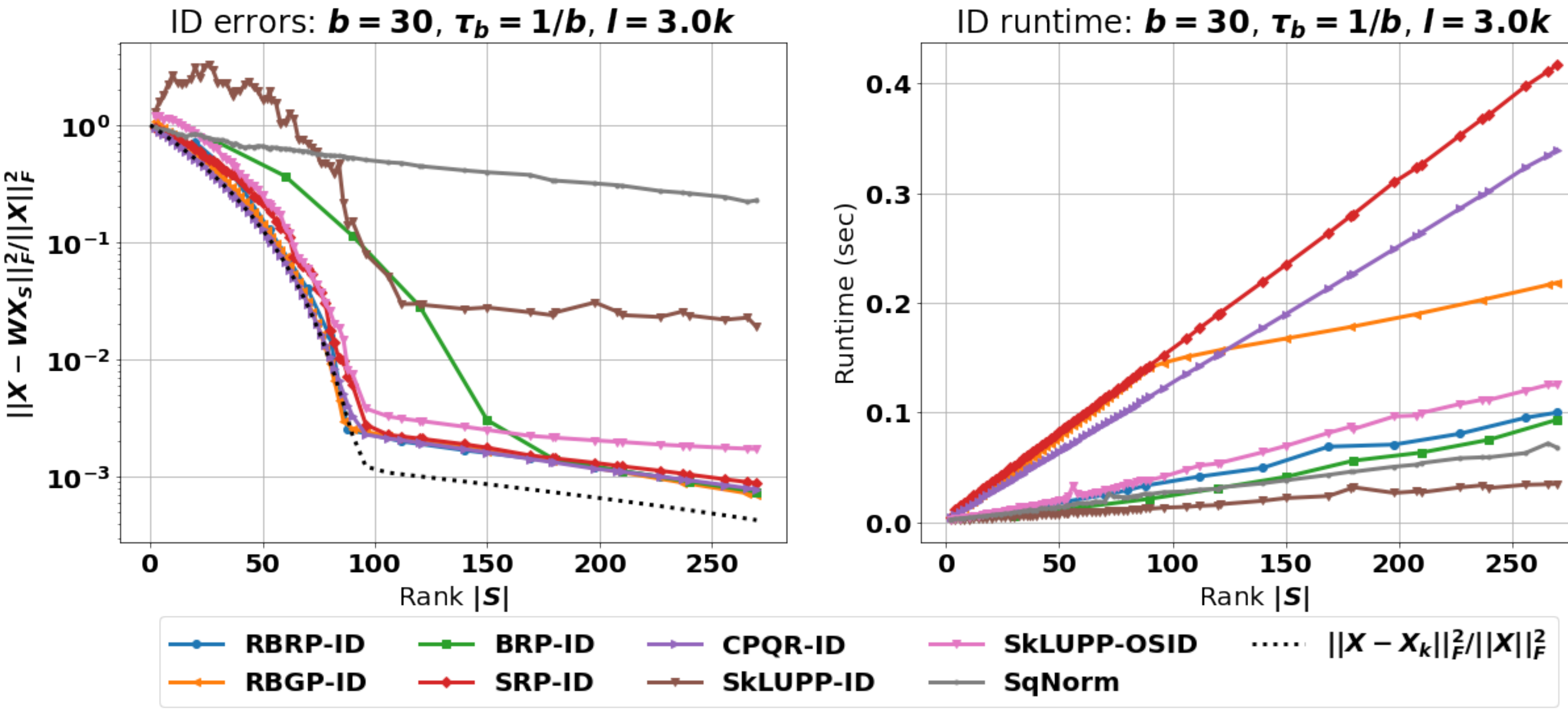


Robust Blockwise Random Pivoting: Efficiency



- GMM with $k = 100$ clusters centered at $\{10j \cdot e_j\}_{j \in [k]}$, $\Sigma = I_d$, $n = 20k$, $d = 500$, $b = 30$
- Robust blockwise filtering (RBRP and RBGP) brings nearly optimal skeleton complexities
- RBGP can be slowed down more significantly than RBRP by robust blockwise filtering

Summary and Questions

- **Blockwise pivoting** exploits the efficiency of Level-3 BLAS, bringing much **better hardware efficiency** than sequential pivoting
- For adversarial inputs, **plain blockwise pivoting can pick up redundant points**
- **Robust Blockwise Random Pivoting (RBRP)** leverages **robust blockwise filtering (RBF)**, a local greedy filtering step with negligible additional cost, as an effective remedy for such vulnerability
- Alternative to RBF, Epperly-Tropp-Webber-2024 showed that **rejective sampling** can also serve as a remedy for a closely related problem of Cholesky decomposition

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With the shared virtue of **low intrinsic dimension**, are there connections between ID and finetuning?

Beyond low-rank approximation, are “redundant” points necessarily bad?

Data Selection for Finetuning

- Large full dataset $X = [x_1, \cdots, x_N]^\top \subset \mathcal{X}^N$, $y = [y_1, \cdots, y_N] \in \mathbb{R}^N$ drawn i.i.d. from unknown distribution P
- Finetuning function class $\mathcal{F} = \{f(\,\cdot\,; \theta) : \mathcal{X} \to \mathbb{R} \mid \theta \in \Theta\}$ with parameters $\Theta \subset \mathbb{R}^r$
- Pre-trained initialization $0_r \in \mathbb{R}^r$ (without loss of generality)
- Ground truth $\theta_* \in \Theta$ such that $\mathbb{E}[y \mid x] = f(x; \theta_*)$ and $\mathbb{V}[y \mid x] \leq \sigma^2$

Select a small coreset $(X_S, y_S) \subset \mathcal{X}^n \times \mathbb{R}^n$ of size n indexed by $S \subset [N]$ such that:

$$(1) \quad \theta_S = \arg\min_{\theta \in \Theta} \frac{1}{n} \|f(X_S; \theta) - y_S\|_2^2 + \alpha \|\theta\|_2^2$$

- Low-dimensional data selection: $r \leq n$, (1) = linear regression ($\alpha = 0$)
- **High-dimensional data selection**: $r > n$, (1) = ridge regression ($\alpha > 0$)

Finetuning falls in the Kernel Regime

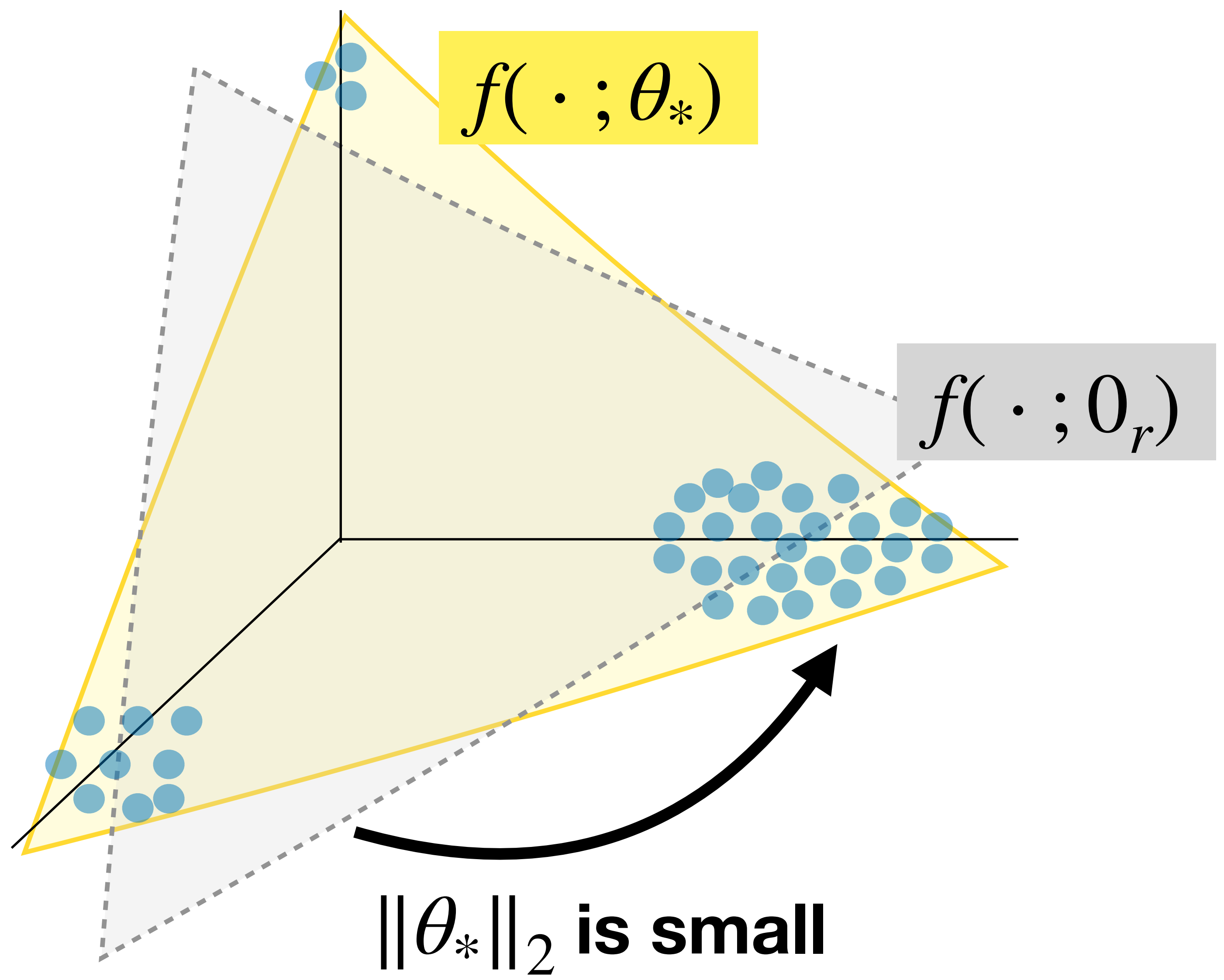
- Finetuning dynamics fall in the **kernel regime**:

$$f(x;\theta) \approx f(x;0_r) + \nabla_\theta f(x;0_r)^\top \theta$$

- With a **suitable pre-trained initialization** (i.e. $f(\cdot,0_r)$ is close to $f(\,\cdot\,,\theta_*)$), $\|\theta_*\|_2$ is small
- Let $G = \nabla_\theta f(X;0_r) \in \mathbb{R}^{N\times r}$ and $G_S = \nabla_\theta f(X_S;0_r) \in \mathbb{R}^{n\times r}$, (1) is well approximated by:

$$(2) \quad \theta_S = \arg\min_{\theta\in\Theta} \frac{1}{n}\|G_S\theta - (y_S - f(X_S;0_r))\|_2^2 + \alpha\|\theta\|_2^2$$

- Aim to control the excess risk $\mathrm{ER}(\theta_S) = \|\theta_S - \theta_*\|_\Sigma^2$ where $\Sigma = \mathbb{E}_{x\sim P}[\nabla_\theta f(x;0_r)\nabla_\theta f(x;0_r)^\top] \in \mathbb{R}^{r\times r}$
- Let $\Sigma_S = G_S^\top G_S/n \succeq 0$



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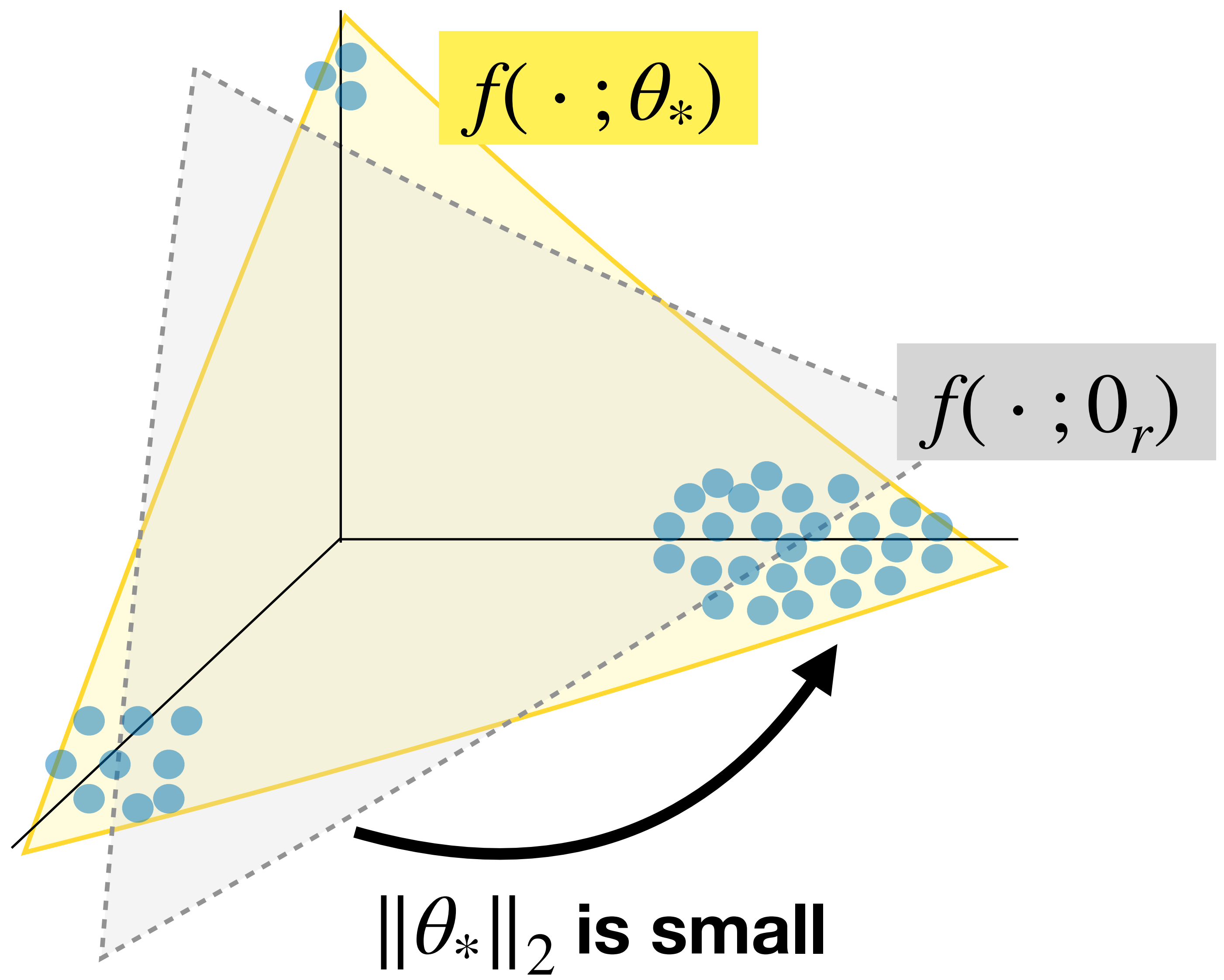

r = number of finetunable parameters

($n < r$ in overparametrized regime)

Qs: Are there connections between ID and finetuning?

- In the **noiseless setting** $\sigma = 0$, the generalization error is controlled by the bias:

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \le \mathrm{tr}(\Sigma - \Sigma G_S^{\dagger} G_S) \|\theta_*\|_2^2$$

Low-rank approximation error of ID!

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Low-rank approximation error of ID!

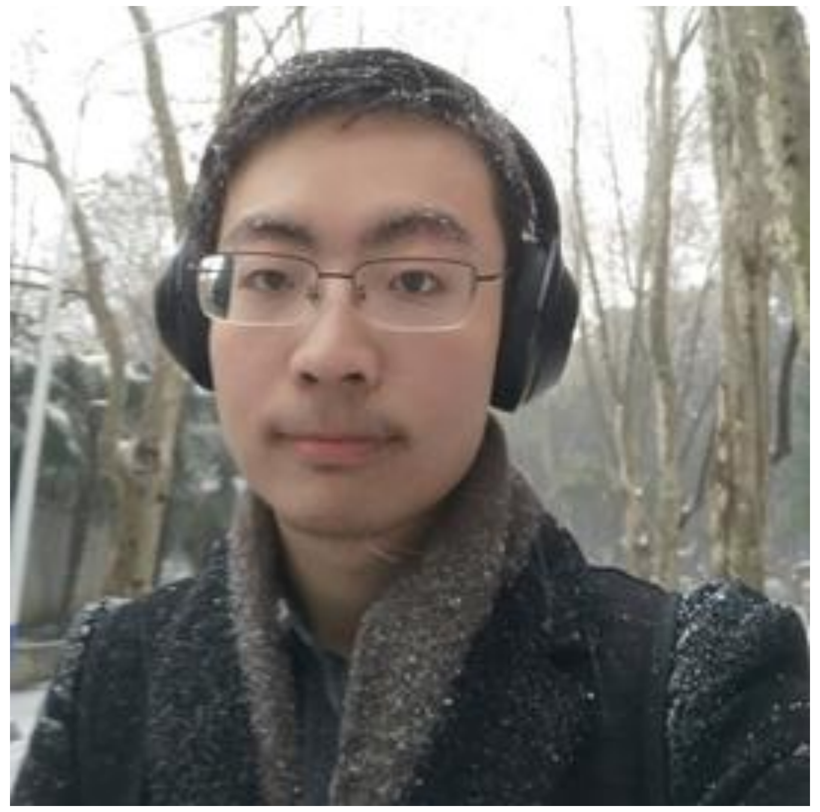
<u>Theorem (**Variance-bias tradeoff**)</u>: Given a coreset S of size n, let $P_{\mathcal{S}} \in \mathbb{R}^{r\times r}$ be the orthogonal projector onto any subspace $\mathcal{S} \subset \mathrm{Range}(\Sigma_S)$, and $P_{\mathcal{S}}^\perp = I_r - P_{\mathcal{S}}$. There exists $\alpha > 0$ such that (2) satisfies

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \le \min_{\mathcal{S}\subset\mathrm{Range}(\Sigma_S)} \underbrace{\frac{2\sigma^2}{n}\mathrm{tr}(\Sigma(P_{\mathcal{S}}\Sigma_S P_{\mathcal{S}})^\dagger)}_{\text{variance}} + \underbrace{2\mathrm{tr}(\Sigma P_{\mathcal{S}}^\perp)\|\theta_*\|_2^2}_{\text{bias}}$$

- For a noiseless finetuning problem, accurate ID brings good data selection
- In high-dimensional data selection, **bias** is controlled by the **low-rank approximation error**
- Will see: learning with noise $\sigma > 0$, “redundant” points are critical for **variance reduction**!

Sketchy Moment Matching: Toward Fast and Provable Data Selection for Finetuning

Hoang Phan
NYU



Xiang Pan
NYU

Qi Lei
NYU

In Low Dimension: Variance Reduction

- Consider **fixed design** for simplicity: $\Sigma = \mathbb{E}_{x \sim P}[\nabla_\theta f(x; 0_r) \nabla_\theta f(x; 0_r)^\top] = G^\top G / N$
- **Low-dimensional** data selection: $\mathrm{rank}(G_S) = r \leq n$ such that $\Sigma_S = G_S^\top G_S / n \succ 0$
- **V(ariance)-optimality** characterizes generalization: $\mathbb{E}[\mathrm{ER}(\theta_S)] \leq \frac{\sigma^2}{n} \mathrm{tr}(\Sigma \Sigma_S^{-1})$

Uniform sampling achieves nearly optimal sample complexity in low dimension: Assuming $\|\nabla_\theta f(\cdot\,; 0_r)\|_2 \leq B$ and $\Sigma \succeq \gamma I_r$. With probability $\geq 1 - \delta$, X_S sampled uniformly from X satisfies

$$\Sigma \preceq c_S \Sigma_S \text{ for any } c_S > 1 \text{ when } n \gtrsim \frac{B^4}{\gamma^2 (1 - c_S^{-1})^2} (r + \log(1/\delta))$$

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Optimal rank-t approximation (truncated SVD)

Assumption (**Low intrinsic dimension**): For $\Sigma = G^\top G / N$, let $\bar{r} = \min\{t \in [r] \mid \mathrm{tr}(\Sigma - \langle \Sigma \rangle_t) \leq \mathrm{tr}(\Sigma)/N\}$ be the intrinsic dimension of the learning problem. Assume $\bar{r} \ll \min\{N, r\}$

Can the **low intrinsic dimension** of fine-tuning be leveraged when $r > n$ (Σ_S is low-rank)?

With Low Intrinsic Dimension: Variance + Bias

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Corollary (**Exploitation + exploration**): Given $S \subset [N]$, for $\mathcal{S} \subseteq \mathrm{Range}(\Sigma_S)$ with $\mathrm{rank}(P_\mathcal{S}) \asymp \overline{r}$, if

- **Variance** is controlled by **exploiting** information in $\mathcal{S}$: $P_\mathcal{S}(c_S \Sigma_S - \Sigma) P_\mathcal{S} \succeq 0$ for some $c_S \geq n/N$; and
- **Bias** is controlled by **exploring** $\mathrm{Range}(\Sigma)$ for an informative $\mathcal{S}$: $\mathrm{tr}(\Sigma P_\mathcal{S}^\perp) \leq \dfrac{N}{n} \mathrm{tr}(\Sigma - \langle \Sigma \rangle_{\overline{r}})$. Then,

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \leq \text{variance} + \text{bias} \lesssim \frac{1}{n}(c_S \sigma^2 \overline{r} + \mathrm{tr}(\Sigma) \|\theta_*\|_2^2)$$

With Low Intrinsic Dimension: Variance + Bias

Optimal rank-t approximation (truncated SVD)

Assumption (**Low intrinsic dimension**): For $\Sigma = G^\top G/N$, let $\bar{r} = \min\{t \in [r] \mid \mathrm{tr}(\Sigma - \langle\Sigma\rangle_t) \leq \mathrm{tr}(\Sigma)/N\}$ be the intrinsic dimension of the learning problem. Assume $\bar{r} \ll \min\{N, r\}$

Corollary (**Exploitation + exploration**): Given $S \subset [N]$, for $\mathcal{S} \subseteq \mathrm{Range}(\Sigma_S)$ with $\mathrm{rank}(P_\mathcal{S}) \asymp \bar{r}$, if

- **Variance** is controlled by **exploiting** information in $\mathcal{S}$: $P_\mathcal{S}(c_S\Sigma_S - \Sigma)P_\mathcal{S} \succeq 0$ for some $c_S \geq n/N$; and
- **Bias** is controlled by **exploring** $\mathrm{Range}(\Sigma)$ for an informative $\mathcal{S}$: $\mathrm{tr}(\Sigma P_\mathcal{S}^\perp) \leq \frac{N}{n}\mathrm{tr}(\Sigma - \langle\Sigma\rangle_{\bar{r}})$. Then,

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \leq \text{variance} + \text{bias} \lesssim \frac{1}{n}(c_S\sigma^2\bar{r} + \mathrm{tr}(\Sigma)\|\theta_*\|_2^2)$$

- **Sample efficiency**: With suitable selection of $S \subset [N]$, the sample complexity of finetuning is **linear in the intrinsic dimension** $\bar{r}$, independent of the (potentially high) parameter dimension r

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How to explore the intrinsic low-dimensional structure **efficiently** for data selection?

Explore Low Intrinsic Dimension: Gradient Sketching

- **Gradient sketching**: Randomly projecting the high-dimensional gradients $G = \nabla_\theta f(X; 0_r) \in \mathbb{R}^{N \times r}$ with $r > n$ to a lower-dimension $m = O(\bar{r}) \ll r$ via a Johnson-Lindenstrauss transform (JLT) $\Gamma \in \mathbb{R}^{r \times m}$
  - Common JLT: a Gaussian random matrix with i.i.d entries $\Gamma_{ij} \sim \mathcal{N}(0, 1/m)$

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Theorem (**Gradient sketching**): For Gaussian embedding $\Gamma \in \mathbb{R}^{r\times m}$ with $m \geq 11\bar{r}$, let $\widetilde{\Sigma} = \Gamma^\top \Sigma \Gamma$ and $\widetilde{\Sigma}_S = \Gamma^\top \Sigma_S \Gamma$. If the coreset $S \subset [N]$ satisfies $\mathrm{rank}(\Sigma_S) = n > m$ and the $\lceil 1.1\bar{r} \rceil$-th largest eigenvalue $s_{\lceil 1.1\bar{r}\rceil}(\Sigma_S) \geq \gamma_S > 0$, then with probability at least 0.9 over Γ, there exists $\alpha > 0$ such that

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \lesssim \underbrace{\frac{\sigma^2}{n}\mathrm{tr}(\widetilde{\Sigma}(\widetilde{\Sigma}_S)^\dagger)}_{\text{variance}} + \underbrace{\frac{\sigma^2}{n}\frac{1}{m\gamma_S}\|\widetilde{\Sigma}(\widetilde{\Sigma}_S)^\dagger\|_2 \mathrm{tr}(\Sigma)}_{\text{sketching error}} + \underbrace{\frac{1}{n}\|\widetilde{\Sigma}(\widetilde{\Sigma}_S)^\dagger\|_2 \mathrm{tr}(\Sigma)\|\theta_*\|_2^2}_{\text{bias}}$$

- If S further satisfies $\widetilde{\Sigma} \preceq c_S \widetilde{\Sigma}_S$ for some $c_S \geq n/N$, with $m = \max\{\sqrt{\mathrm{tr}(\Sigma)/\gamma_S}, 11\bar{r}\}$,

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Control Variance: Sketchy Moment Matching (SkMM)

Gradient sketching

- Draw a (fast) JLT (e.g. Gaussian random matrix) $\Gamma \in \mathbb{R}^{r \times m}$
- Sketch the gradients $\widetilde{G} = \nabla_\theta f(X; 0_r)\Gamma \in \mathbb{R}^{N \times m}$

Moment matching

- Spectral decomposition $\widetilde{\Sigma} = \widetilde{G}^\top \widetilde{G}/N = V \Lambda V^\top$ with $V = [v_1, \cdots, v_m]$, $\Lambda = \mathrm{diag}(\lambda_1, \cdots, \lambda_m)$
- Initialize $s = [s_1, \cdots, s_N]$ with $s_i = 1/n$ for n uniformly sampled $i \in [N]$ and $s_i = 0$ otherwise
- Sample a size-n coreset $S \subset [N]$ according to the distribution s that solves the optimization problem

$$\min_{s \in [0,1/n]^N} \min_{\gamma = [\gamma_1, \cdots, \gamma_m] \in \mathbb{R}^m} \sum_{j=1}^{m} \left(v_j^\top \widetilde{G}^\top \mathrm{diag}(s) \widetilde{G} v_j - \gamma_j \lambda_j\right)^2$$

$$\text{s.t.} \quad \|s\|_1 = 1, \quad \gamma_j \geq 1/c_S \ \forall\, j \in [m]$$

Efficiency of SkMM: (recall $m \ll \min\{N, r\}$)

- **Gradient sketching** is parallelizable with input-sparsity time: for $\mathrm{nnz}(G)$ = #nonzeros in G
  - Gaussian embedding: $O(\mathrm{nnz}(G)m)$
  - Fast JLT (sparse sign): $O(\mathrm{nnz}(G)\log m)$
- **Moment matching** takes $O(m^3)$ for spectral decomposition. The optimization takes $O(Nm)$ per iteration

Relaxation of $\widetilde{\Sigma} \preceq c_S \widetilde{\Sigma}_S$:

- $\widetilde{\Sigma} \preceq c_S \widetilde{\Sigma}_S \iff V^\top (\widetilde{(G)}_S^\top \widetilde{(G)}_S / n) V \succeq \Lambda / c_S$
- Assume Σ, Σ_S commute such that imposing m diagonal constraints is sufficient

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$$\text{s.t.} \quad \|s\|_1 = 1, \quad \gamma_j \geq 1/c_S \ \forall\, j \in [m]$$

Select $S \subset [N]$ of size $|S| = n$ that reduces the sketched V-optimality:

$$\mathrm{tr}(\widetilde{\Sigma}(\widetilde{\Sigma}_S)^\dagger)$$

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SkMM on Synthetic Data: Regression

Synthetic high-dimensional linear probing

- Gaussian mixture model (GMM) $G \in \mathbb{R}^{N \times r}$
- $N = 2000$, $r = 2400 > N$
- $\bar{r} = 8$ well separated clusters of random sizes
- Grid search for the nearly optimal $\alpha > 0$

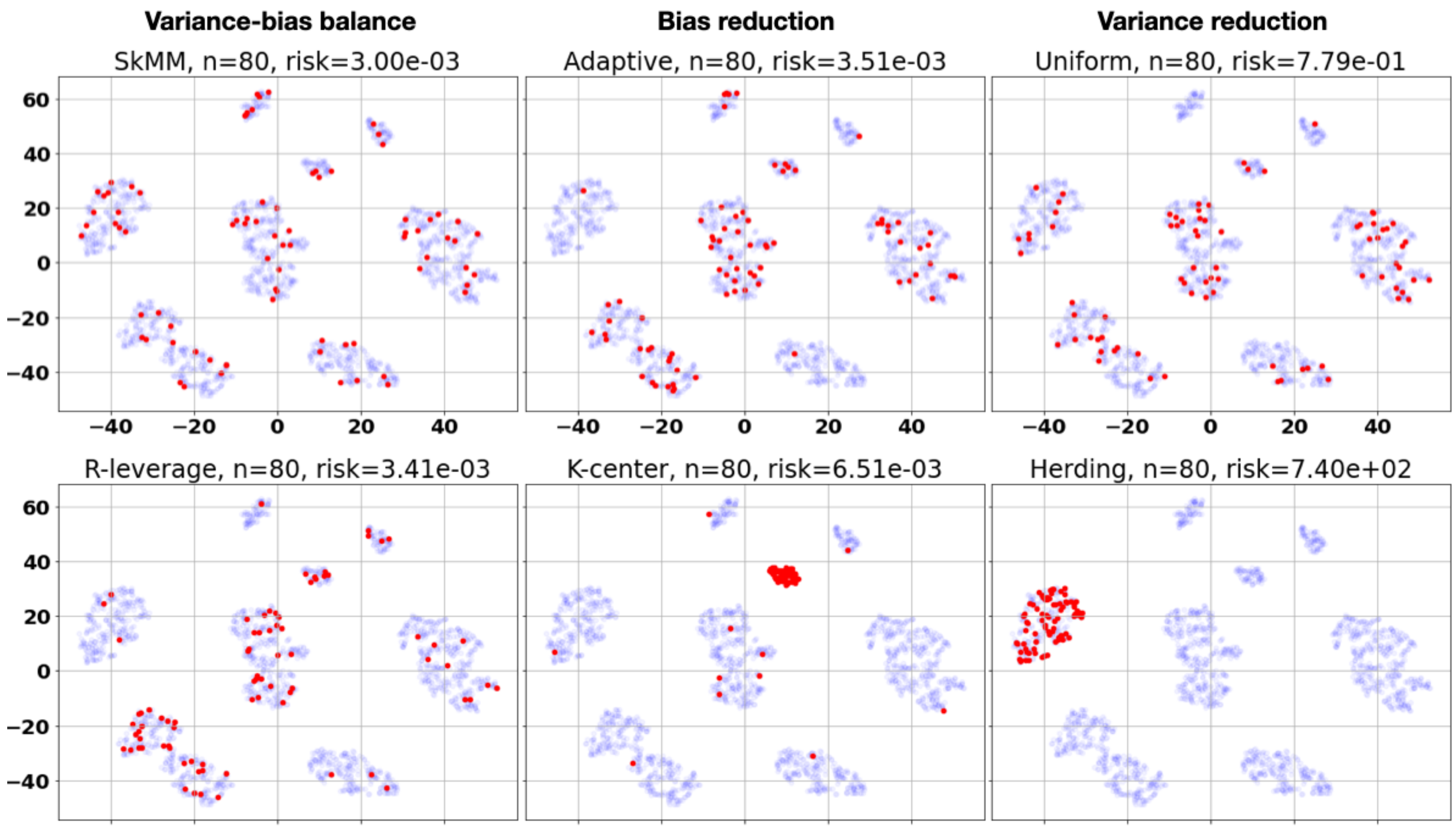
Baselines

- Herding
- Uniform sampling
- K-center greedy
- Adaptive sampling/random pivoting
- T(runcated)/R(idge) leverage score sampling

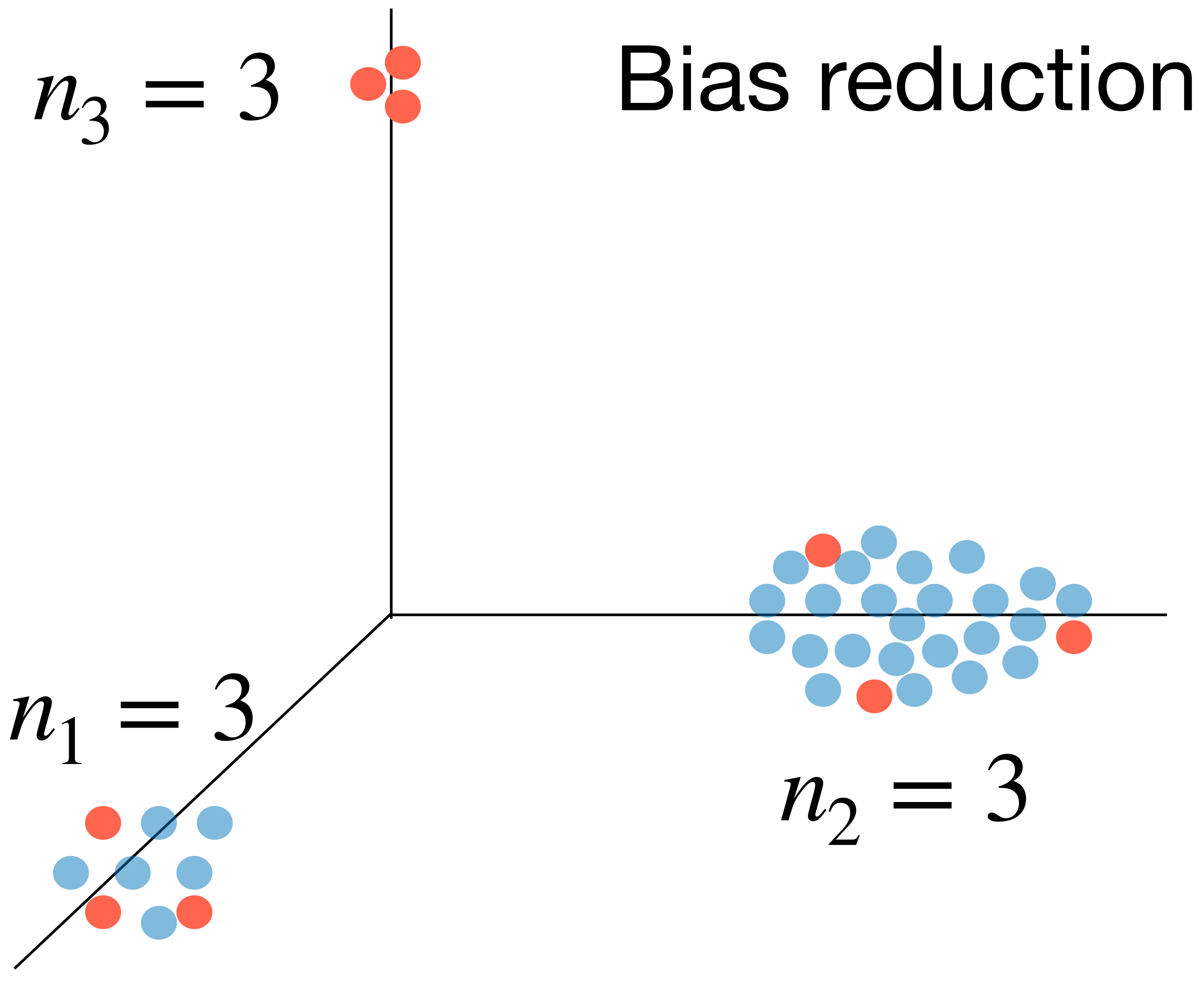
Table 1: Empirical risk $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_S)$ on the GMM dataset at various n, under the same hyperparameter tuning where ridge regression over the full dataset $\mathcal{D}$ with $N = 2000$ samples achieves $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_{[N]}) =$ **2.95e-3**. For methods involving sampling, results are reported over 8 random seeds.

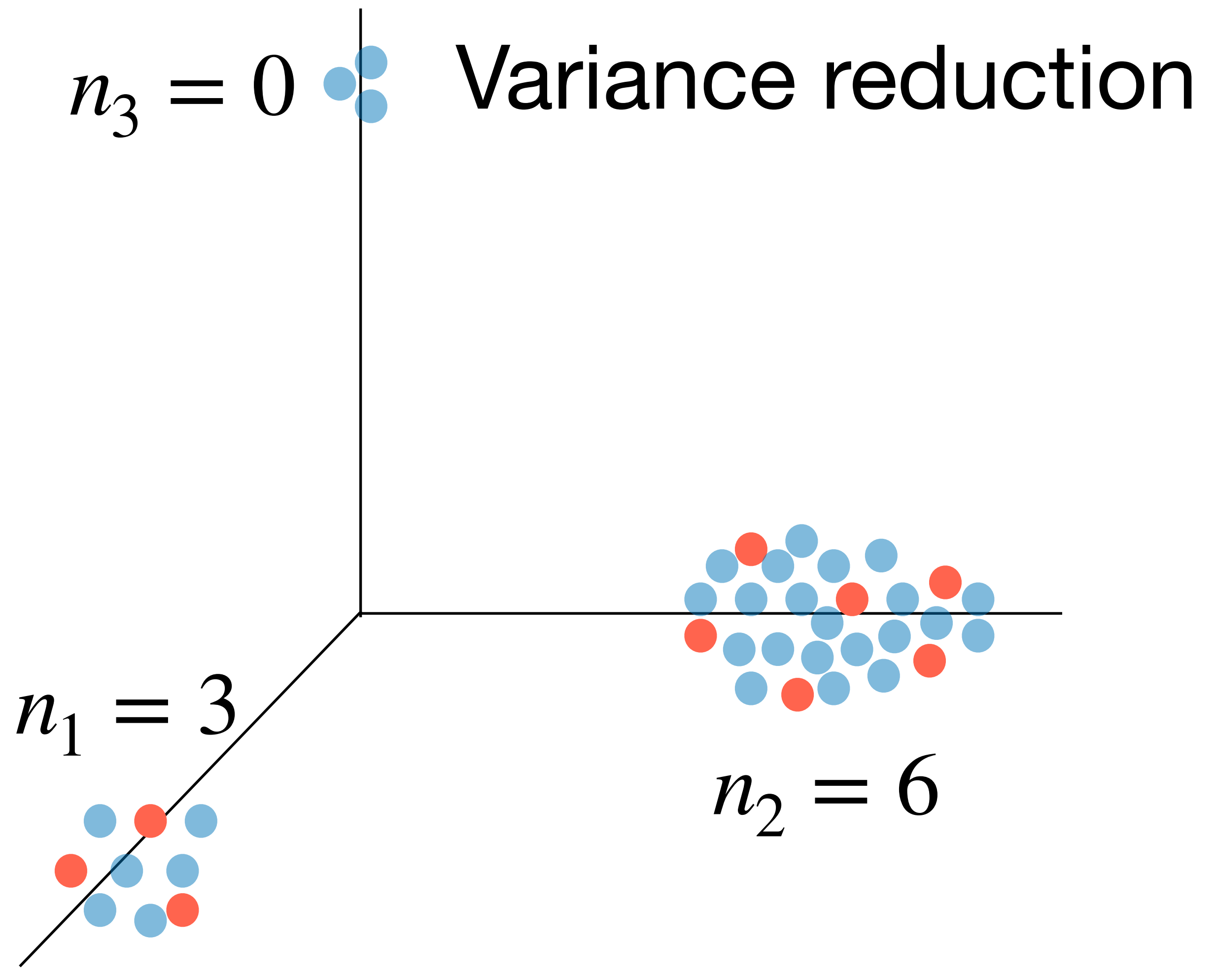
n	48	64	80	120	400	800	1600
Herding	7.40e+2	7.40e+2	7.40e+2	7.40e+2	7.38e+2	1.17e+2	**2.95e-3**
Uniform	(1.14 ± 2.71)e-1	(1.01 ± 2.75)e-1	(3.44 ± 0.29)e-3	(3.13 ± 0.14)e-3	(2.99 ± 0.03)e-3	**(2.96 ± 0.01)e-3**	**(2.95 ± 0.00)e-3**
K-center	(1.23 ± 0.40)e-2	(9.53 ± 0.60)e-2	(1.12 ± 0.45)e-2	(2.73 ± 1.81)e-2	(5.93 ± 4.80)e-2	(1.18 ± 0.64)e-1	(1.13 ± 0.70)e+0
Adaptive	(3.81 ± 0.65)e-3	(3.79 ± 1.37)e-3	(4.83 ± 1.90)e-3	(4.03 ± 1.35)e-3	(3.40 ± 0.67)e-3	(7.34 ± 3.97)e-3	(3.19 ± 0.16)e-3
T-leverage	(0.99 ± 1.65)e-2	(3.63 ± 0.49)e-3	(3.30 ± 0.30)e-3	(3.24 ± 0.14)e-3	**(2.98 ± 0.01)e-3**	**(2.96 ± 0.01)e-3**	**(2.95 ± 0.00)e-3**
R-leverage	(4.08 ± 1.58)e-3	(3.48 ± 0.43)e-3	(3.25 ± 0.31)e-3	(3.09 ± 0.06)e-3	(3.00 ± 0.02)e-3	(2.97 ± 0.01)e-3	**(2.95 ± 0.00)e-3**
SkMM	**(3.54 ± 0.51)e-3**	**(3.31 ± 0.15)e-3**	**(3.12 ± 0.07)e-3**	**(3.07 ± 0.08)e-3**	**(2.98 ± 0.02)e-3**	**(2.96 ± 0.01)e-3**	**(2.95 ± 0.00)e-3**

SkMM on Synthetic Data: Regression



SkMM simultaneously controls variance and bias





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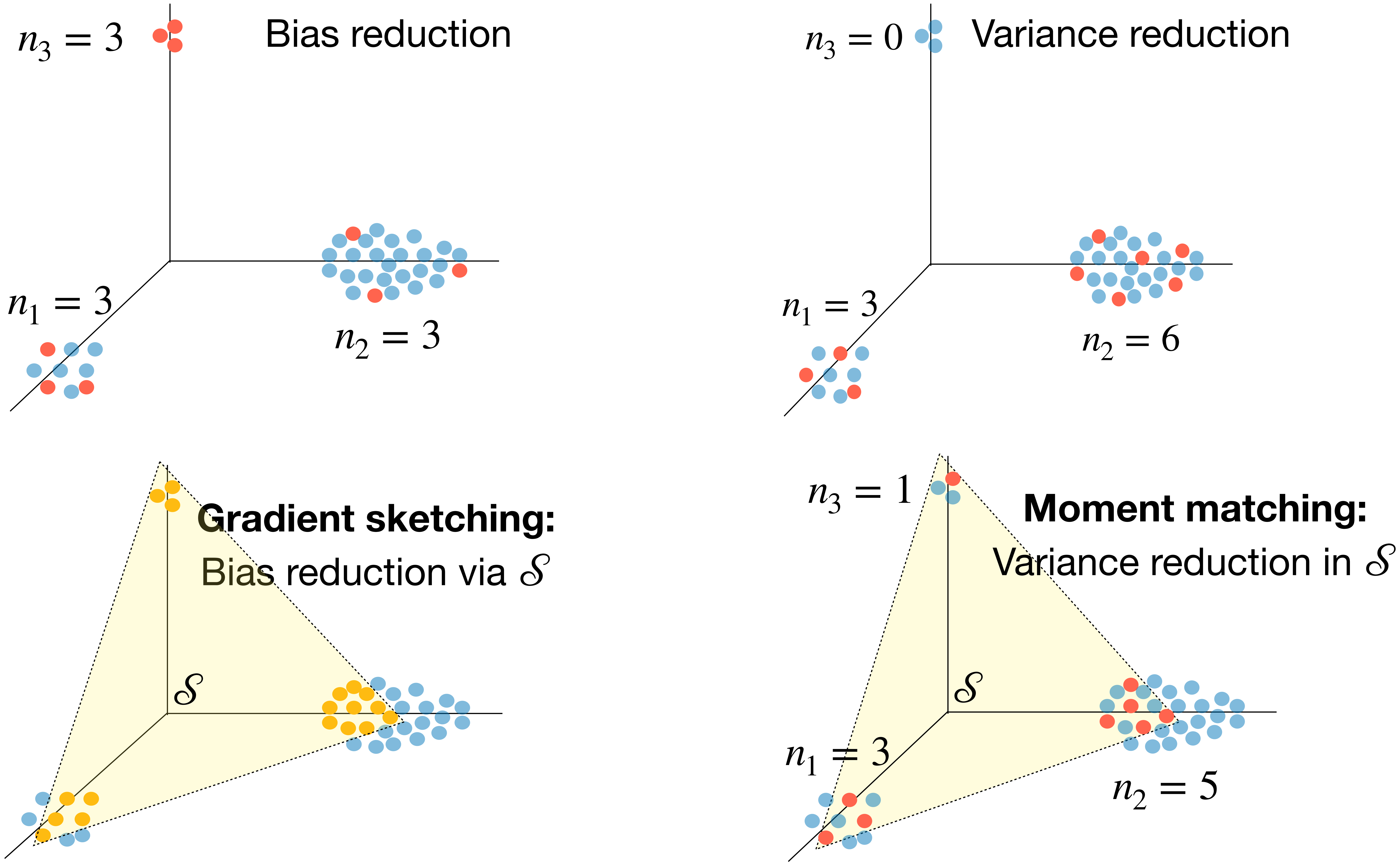

SkMM for Classification: Linear Probing (LP)

Table 2: Accuracy and F1 score (%) of LP over CLIP on StanfordCars

	n	2000	2500	3000	3500	4000
Uniform Sampling	Acc	67.63 ± 0.17	70.59 ± 0.19	72.49 ± 0.19	74.16 ± 0.22	75.40 ± 0.16
	F1	64.54 ± 0.18	67.79 ± 0.23	70.00 ± 0.20	71.77 ± 0.23	73.14 ± 0.12
Herding [90]	Acc	67.22 ± 0.16	71.02 ± 0.13	73.17 ± 0.22	74.64 ± 0.18	75.71 ± 0.29
	F1	64.07 ± 0.23	68.28 ± 0.15	70.64 ± 0.28	72.22 ± 0.26	73.26 ± 0.39
Contextual Diversity [1]	Acc	67.64 ± 0.13	70.82 ± 0.23	72.66 ± 0.12	74.46 ± 0.17	75.77 ± 0.12
	F1	64.51 ± 0.17	68.18 ± 0.25	70.05 ± 0.11	72.13 ± 0.15	73.35 ± 0.07
Glister [43]	Acc	67.60 ± 0.24	70.85 ± 0.27	73.07 ± 0.26	74.63 ± 0.21	76.00 ± 0.20
	F1	64.50 ± 0.34	68.07 ± 0.38	70.47 ± 0.35	72.18 ± 0.25	73.69 ± 0.24
GraNd [63]	Acc	67.27 ± 0.07	70.38 ± 0.07	72.56 ± 0.05	74.67 ± 0.06	75.77 ± 0.12
	F1	64.04 ± 0.09	67.48 ± 0.09	69.81 ± 0.08	72.13 ± 0.05	73.44 ± 0.13
Forgetting [79]	Acc	67.59 ± 0.10	70.99 ± 0.05	72.54 ± 0.07	74.81 ± 0.05	75.74 ± 0.01
	F1	64.85 ± 0.13	68.53 ± 0.07	70.30 ± 0.05	72.59 ± 0.04	73.74 ± 0.02
DeepFool [59]	Acc	67.77 ± 0.29	70.73 ± 0.22	73.24 ± 0.22	74.57 ± 0.23	75.71 ± 0.15
	F1	64.16 ± 0.68	68.49 ± 0.53	70.93 ± 0.32	72.44 ± 0.27	73.79 ± 0.15
Entropy [19]	Acc	67.95 ± 0.11	71.00 ± 0.10	73.28 ± 0.10	75.02 ± 0.08	75.82 ± 0.06
	F1	64.55 ± 0.10	67.95 ± 0.12	70.68 ± 0.12	72.46 ± 0.12	73.29 ± 0.04
Margin [19]	Acc	67.53 ± 0.14	71.19 ± 0.09	73.09 ± 0.14	74.66 ± 0.11	75.57 ± 0.13
	F1	64.16 ± 0.15	68.33 ± 0.14	70.37 ± 0.17	72.03 ± 0.11	73.14 ± 0.20
Least Confidence [19]	Acc	67.68 ± 0.11	70.99 ± 0.14	73.04 ± 0.05	74.65 ± 0.09	75.58 ± 0.08
	F1	64.09 ± 0.20	68.03 ± 0.20	70.30 ± 0.07	72.02 ± 0.10	73.15 ± 0.12
SkMM-LP	Acc	**68.27 ± 0.03**	**71.53 ± 0.05**	**73.61 ± 0.02**	**75.12 ± 0.01**	**76.34 ± 0.02**
	F1	**65.29 ± 0.03**	**68.75 ± 0.06**	**71.14 ± 0.03**	**72.64 ± 0.02**	**74.02 ± 0.10**

StanfordCar dataset

- 196 imbalanced classes
- $N = 16{,}185$ images

Linear probing (LP)

- CLIP-pre-trained ViT
- $r = 100{,}548$

Last-two-layer finetuning (FT)

- ImageNet-pre-trained ResNet18
- $r = 2{,}459{,}844$

SkMM for Classification: Last-two-layer Finetuning (FT)

Table 3: Accuracy and F1 score (%) of FT over (the last two layers of) ResNet18 on StanfordCars

	n	2000	2500	3000	3500	4000
Uniform Sampling	Acc	29.19 ± 0.37	32.83 ± 0.19	35.69 ± 0.35	38.31 ± 0.16	40.35 ± 0.26
	F1	26.14 ± 0.39	29.91 ± 0.16	32.80 ± 0.37	35.38 ± 0.19	37.51 ± 0.23
Herding [90]	Acc	29.19 ± 0.21	32.42 ± 0.16	35.83 ± 0.24	38.30 ± 0.19	40.51 ± 0.19
	F1	25.90 ± 0.24	29.48 ± 0.23	32.89 ± 0.27	35.50 ± 0.22	37.56 ± 0.21
Contextual Diversity [1]	Acc	28.50 ± 0.34	32.66 ± 0.27	35.67 ± 0.32	38.31 ± 0.15	40.53 ± 0.18
	F1	25.65 ± 0.40	29.79 ± 0.29	32.86 ± 0.31	35.55 ± 0.14	37.81 ± 0.23
Glister [43]	Acc	29.16 ± 0.26	32.91 ± 0.19	36.03 ± 0.20	38.16 ± 0.12	40.47 ± 0.16
	F1	26.33 ± 0.19	30.05 ± 0.28	$\mathbf{33.26 \pm 0.18}$	35.41 ± 0.14	37.63 ± 0.17
GraNd [63]	Acc	28.59 ± 0.17	32.67 ± 0.20	35.83 ± 0.16	38.58 ± 0.15	40.70 ± 0.11
	F1	25.66 ± 0.15	29.70 ± 0.22	32.76 ± 0.16	35.72 ± 0.15	37.83 ± 0.11
Forgetting [79]	Acc	28.61 ± 0.31	32.48 ± 0.28	35.18 ± 0.24	37.78 ± 0.22	40.24 ± 0.13
	F1	25.64 ± 0.25	29.58 ± 0.30	32.38 ± 0.20	35.16 ± 0.18	37.41 ± 0.14
DeepFool [59]	Acc	24.97 ± 0.20	29.02 ± 0.17	32.60 ± 0.18	35.59 ± 0.24	38.20 ± 0.22
	F1	22.11 ± 0.11	26.08 ± 0.29	29.83 ± 0.27	32.92 ± 0.33	35.47 ± 0.22
Entropy [19]	Acc	28.87 ± 0.13	32.84 ± 0.20	35.64 ± 0.20	37.96 ± 0.11	40.29 ± 0.27
	F1	25.95 ± 0.17	30.03 ± 0.17	32.85 ± 0.23	35.19 ± 0.12	37.33 ± 0.34
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Least Confidence [19]	Acc	29.05 ± 0.07	32.88 ± 0.13	35.66 ± 0.18	38.25 ± 0.20	39.91 ± 0.09
	F1	26.18 ± 0.04	30.03 ± 0.14	32.79 ± 0.15	35.42 ± 0.16	37.14 ± 0.12
SkMM-FT	Acc	$\mathbf{29.44 \pm 0.09}$	$\mathbf{33.48 \pm 0.04}$	$\mathbf{36.11 \pm 0.12}$	$\mathbf{39.18 \pm 0.03}$	$\mathbf{41.77 \pm 0.07}$
	F1	$\mathbf{26.71 \pm 0.10}$	$\mathbf{30.75 \pm 0.05}$	33.24 ± 0.05	$\mathbf{36.38 \pm 0.05}$	$\mathbf{39.07 \pm 0.10}$

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Takeaways

- A rigorous generalization analysis on data selection for finetuning
  - Low-dimensional data selection: variance reduction (V-optimality)
  - **High-dimensional data selection**: variance-bias tradeoff
- **Gradient sketching** provably finds a low-dimensional parameter subspace $\mathcal{S}$ with small bias
  - Reducing variance over $\mathcal{S}$ preserves the fast-rate generalization $O(\dim(\mathcal{S})/n)$
- **SkMM** — a scalable two-stage data selection method for finetuning that simultaneously
  - **Explores** the high-dimensional parameter space via **gradient sketching** and
  - **Exploits** the information in the low-dimensional subspace via **moment matching**

Thank You!

Dong, Y., Phan, H., Pan, X., & Lei, Q. Sketchy Moment Matching: Toward Fast and Provable Data Selection for Finetuning. In *The Thirty-eighth Annual Conference on Neural Information Processing Systems*.

Dong, Y., Chen, C., Martinsson, P. G., & Pearce, K. (2023). Robust blockwise random pivoting: Fast and accurate adaptive interpolative decomposition. *arXiv preprint arXiv:2309.16002*.