Toward Fast and Provable Data Selection under Low Intrinsic Dimension

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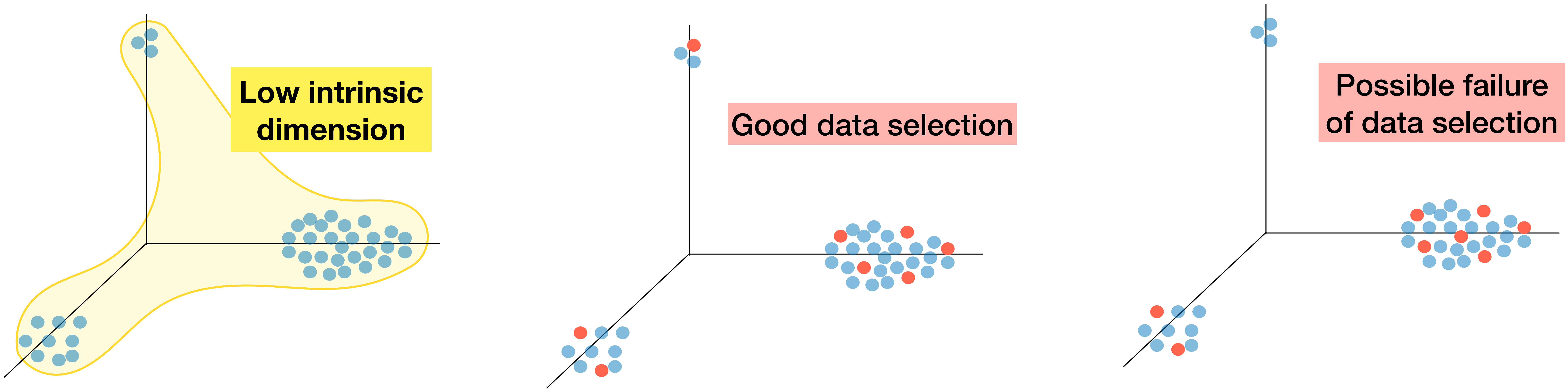
Low Intrinsic Dimension & Data Selection

- **Low intrinsic dimension is ubiquitous in real world**
  - Example: Large models can be finetuned in a lower dimension with much fewer samples than the model size [Aghajanyan-Zettlemoyer-Gupta-2020]
    - 341M parameters → dimension-322 subspace can be fine-tuned with less than 6K samples!
- Learning under low intrinsic dimension **with limited data, data selection becomes crucial**



How to **select the most informative data** for learning under **low intrinsic dimension** (e.g. finetuning)?

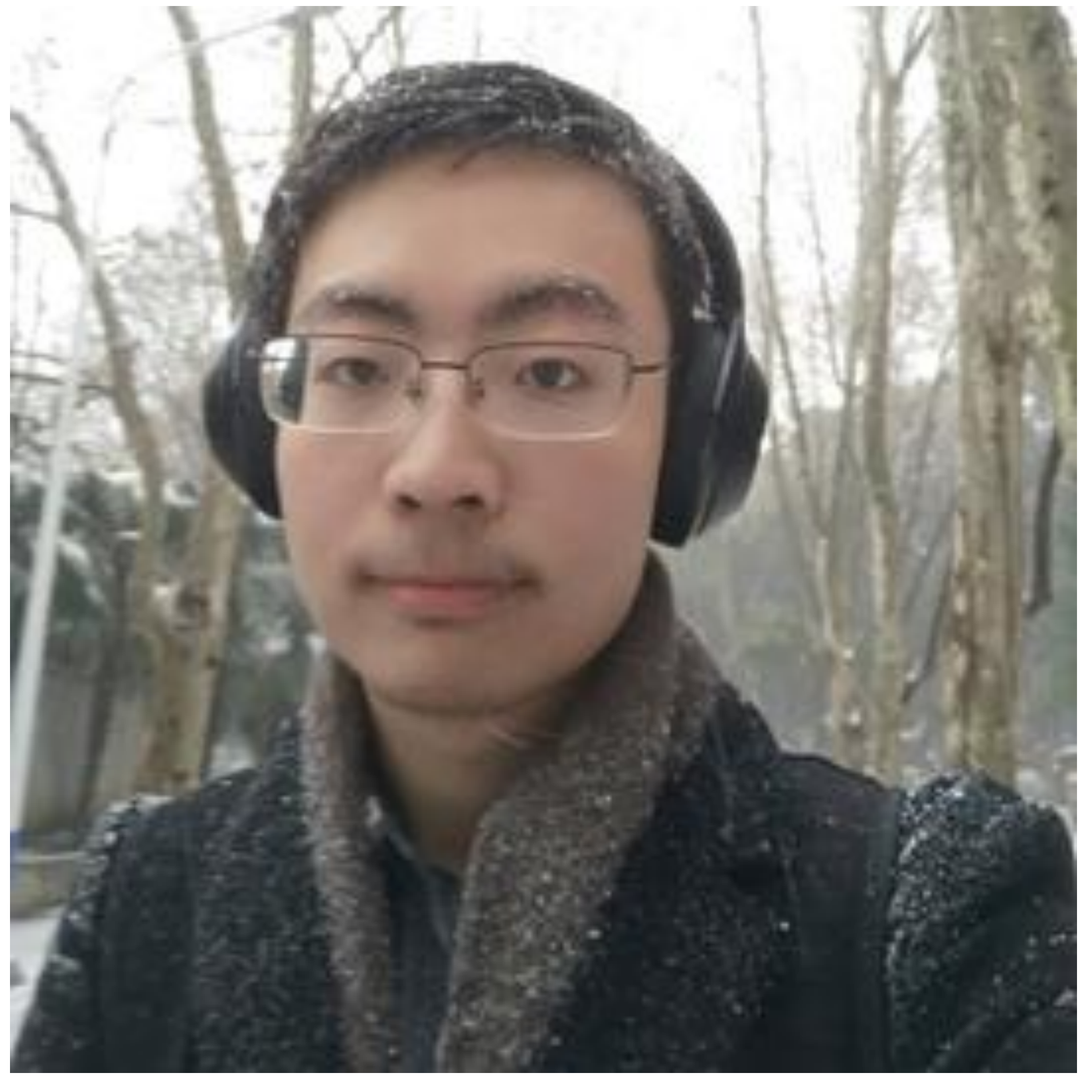
Outline

- Data selection for statistical models in kernel regime — **finetuning**
  - A theory on data selection for finetuning that
    - Extends the classical wisdom of **V-optimal experimental design** in low dimensions
    - To high-dimensional data selection under low intrinsic dimensions via **sketching**
  - A fast and effective data selection algorithm for finetuning: **Sketchy Moment Matching (SkMM)**

- Data selection for low-rank approximation — **interpolative decomposition (ID)**
  - Select minimum possible rows as a basis to form a good low-rank approximation
  - A fast and accurate adaptive ID algorithm: **Robust Blockwise Random Pivoting (RBRP)**

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

Hoang Phan
NYU



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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 $\mathbb{V}[y \mid x] \le \sigma^2$

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

Finetuning in Kernel Regime

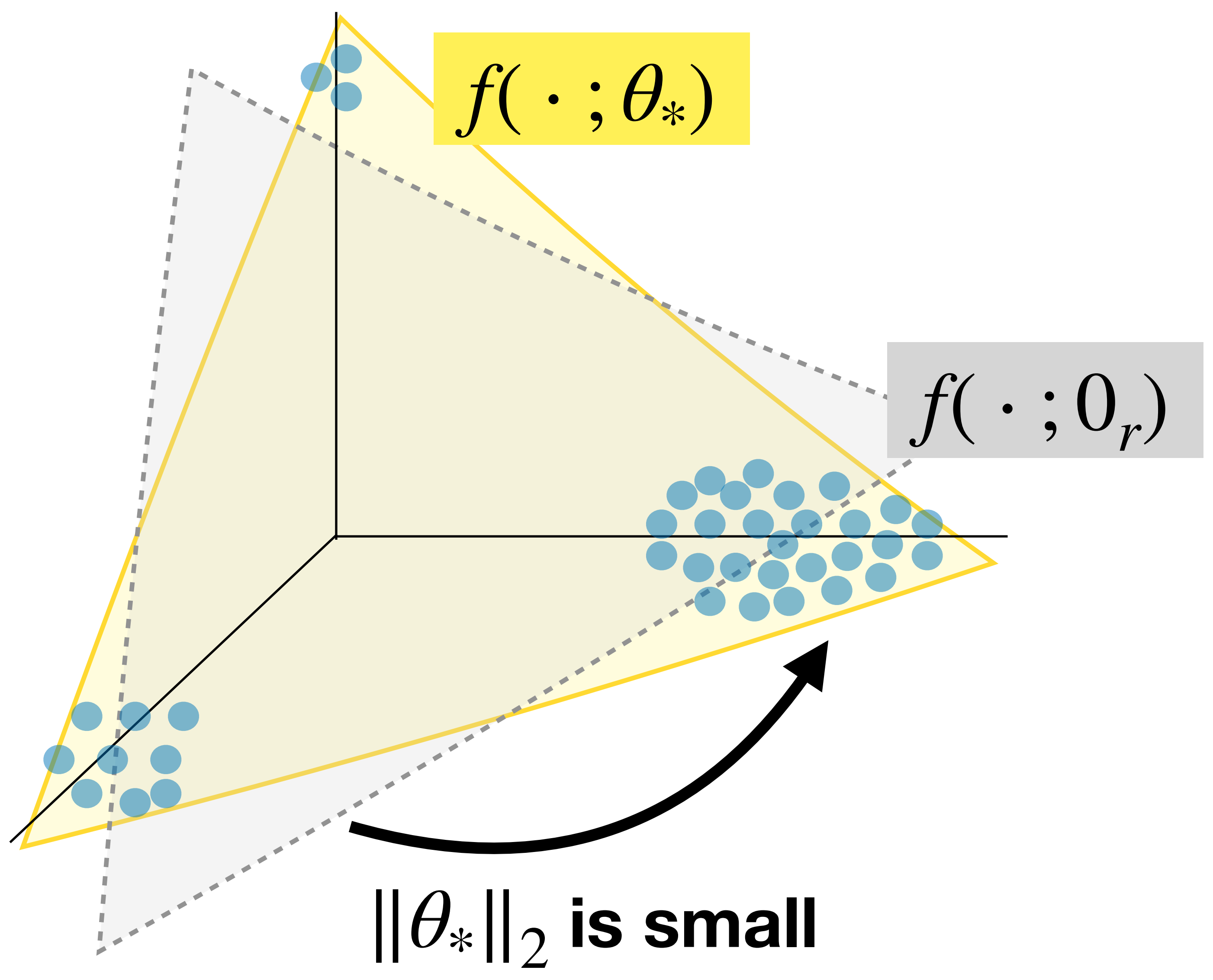
- Finetuning dynamics fall in the **kernel regime**:

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

- 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 excess risk $\mathrm{ER}(\theta_S) = \|\theta_S - \theta_*\|_\Sigma^2$ where $\Sigma = \mathbb{E}_{x\sim P}[\nabla_\theta f(x;0_r)\nabla_\theta f(x;0_r)^\top] \in \mathbb{R}^{r\times r}$



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: $\mathrm{rank}(G_S) = r \le n$ such that $\Sigma_S = G_S^\top G_S / n \succ 0$
- **V(ariance)-optimality** characterizes generalization: $\mathbb{E}[\mathrm{ER}(\theta_S)] \le \frac{\sigma^2}{n} \mathrm{tr}(\Sigma \Sigma_S^{-1})$
- If $\Sigma \preceq c_S \Sigma_S$ for some $c_S \ge \frac{n}{N}$, then $\mathbb{E}[\mathrm{ER}(\theta_S)] \le c_S \frac{\sigma^2 r}{n}$

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

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

Can the **low intrinsic dimension** of fine-tuning be leveraged when $r > n$?

With Low Intrinsic Dimension: Variance + Bias

Optimal rank-t approximation (truncated SVD)

<ins>Assumption (**Low intrinsic dimension**)</ins>: 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 $\bar{r} \ll \min\{N, r\}$

<ins>Corollary (**Exploitation + exploration**)</ins>: 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 $\mathcal{S}$: $\mathrm{tr}(\Sigma P_\mathcal{S}^\perp) \leq \dfrac{N}{n}\mathrm{tr}(\Sigma - \langle \Sigma \rangle_{\bar{r}})$. 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

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 $\Gamma_{ij} \sim \mathcal{N}(0,1/m)$

<ins>Theorem (**Gradient sketching**)</ins>: 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

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

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

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \lesssim \frac{c_S}{n}(\sigma^2 m + \mathrm{tr}(\Sigma)\|\theta_*\|_2^2)$$

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

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

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

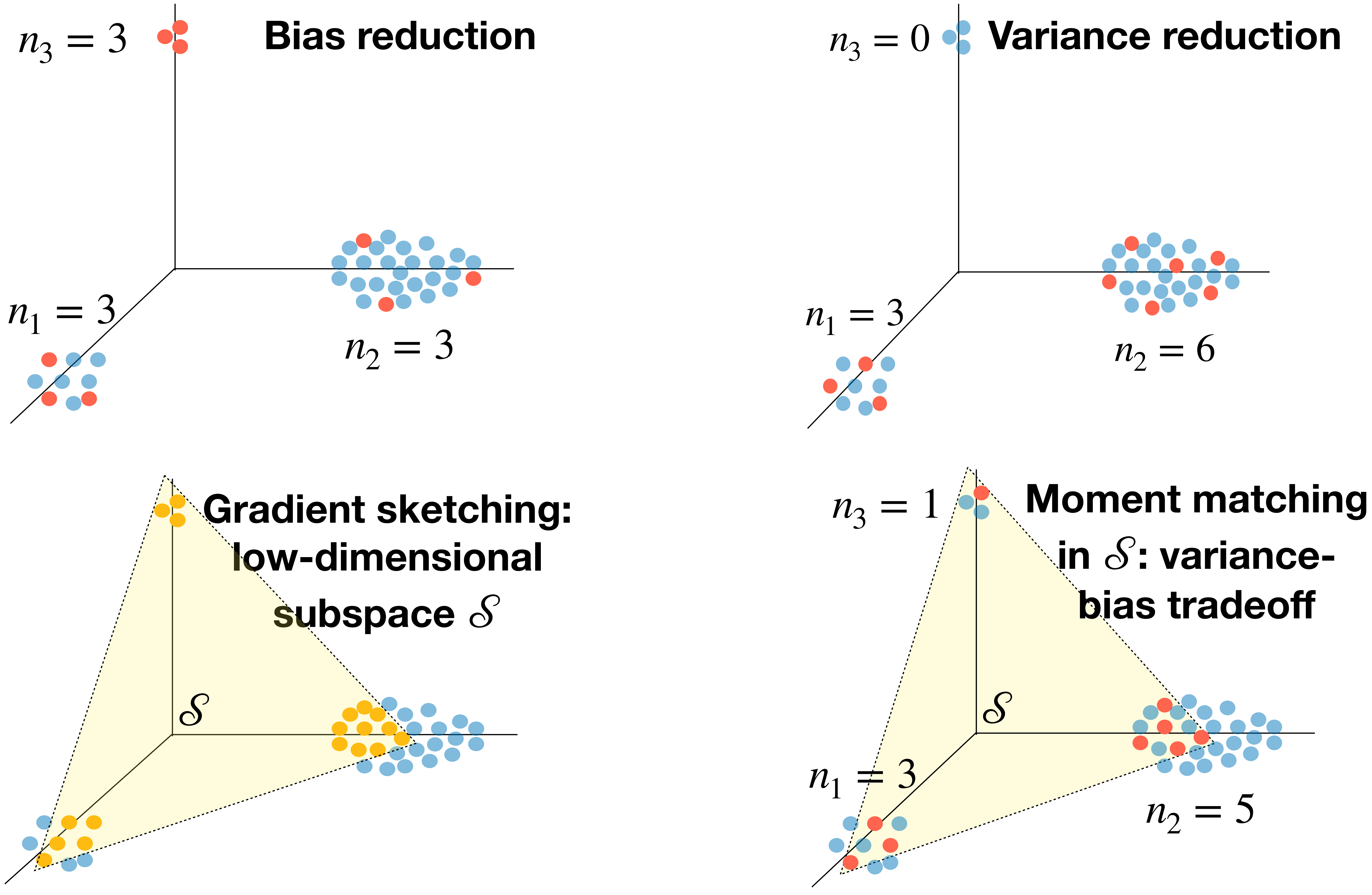
Efficiency of SkMM: (recall $m \ll \min\{N, r\}$)

- **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

SkMM simultaneously controls variance and bias



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 $\alpha > 0$

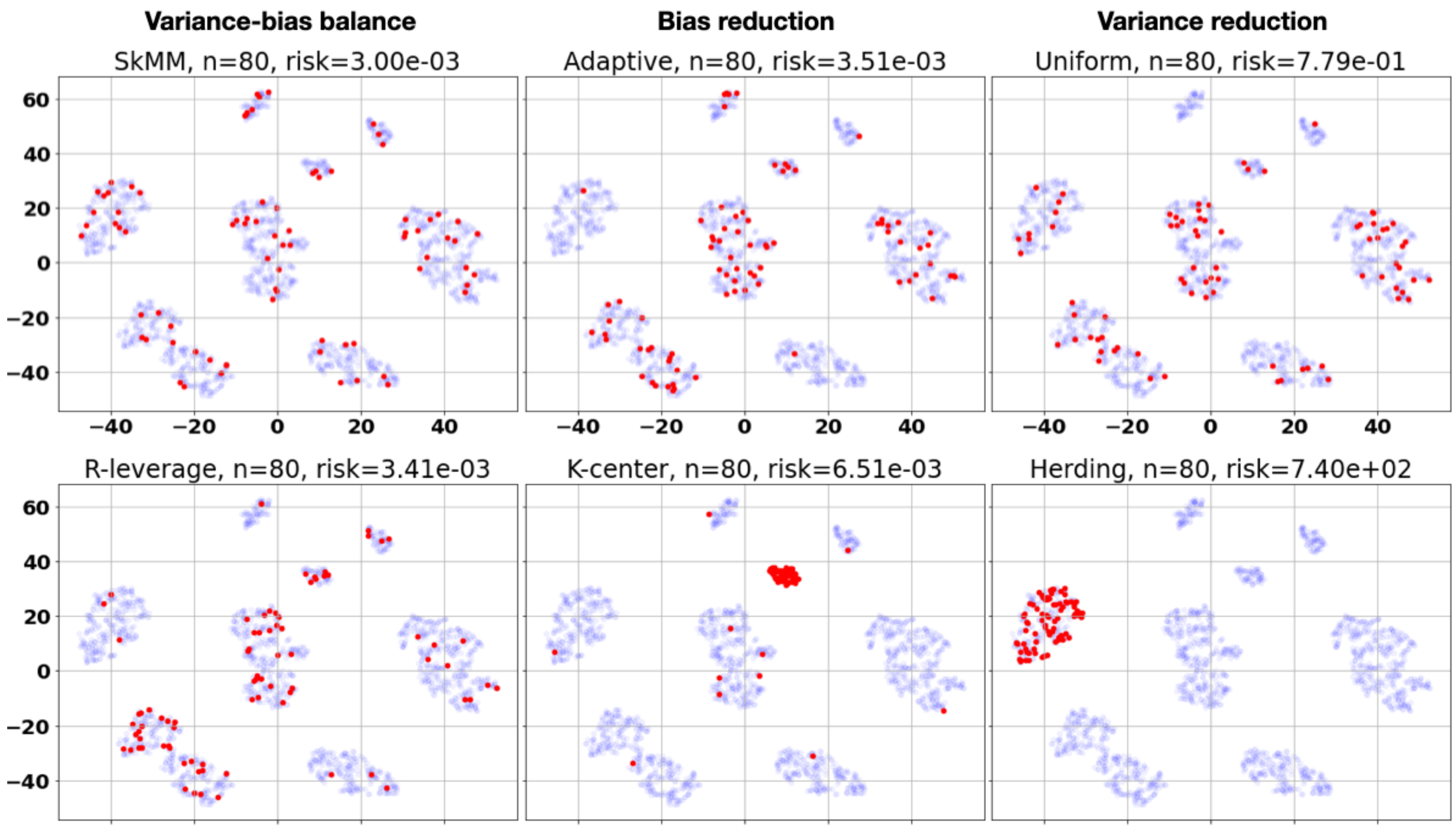
Baselines

- 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 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	$\mathbf{68.27 \pm 0.03}$	$\mathbf{71.53 \pm 0.05}$	$\mathbf{73.61 \pm 0.02}$	$\mathbf{75.12 \pm 0.01}$	$\mathbf{76.34 \pm 0.02}$
	F1	$\mathbf{65.29 \pm 0.03}$	$\mathbf{68.75 \pm 0.06}$	$\mathbf{71.14 \pm 0.03}$	$\mathbf{72.64 \pm 0.02}$	$\mathbf{74.02 \pm 0.10}$

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
Margin [19]	Acc	29.18 ± 0.12	32.73 ± 0.15	35.67 ± 0.30	38.27 ± 0.20	40.58 ± 0.06
	F1	26.15 ± 0.12	29.66 ± 0.05	32.86 ± 0.30	35.61 ± 0.17	37.77 ± 0.07
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

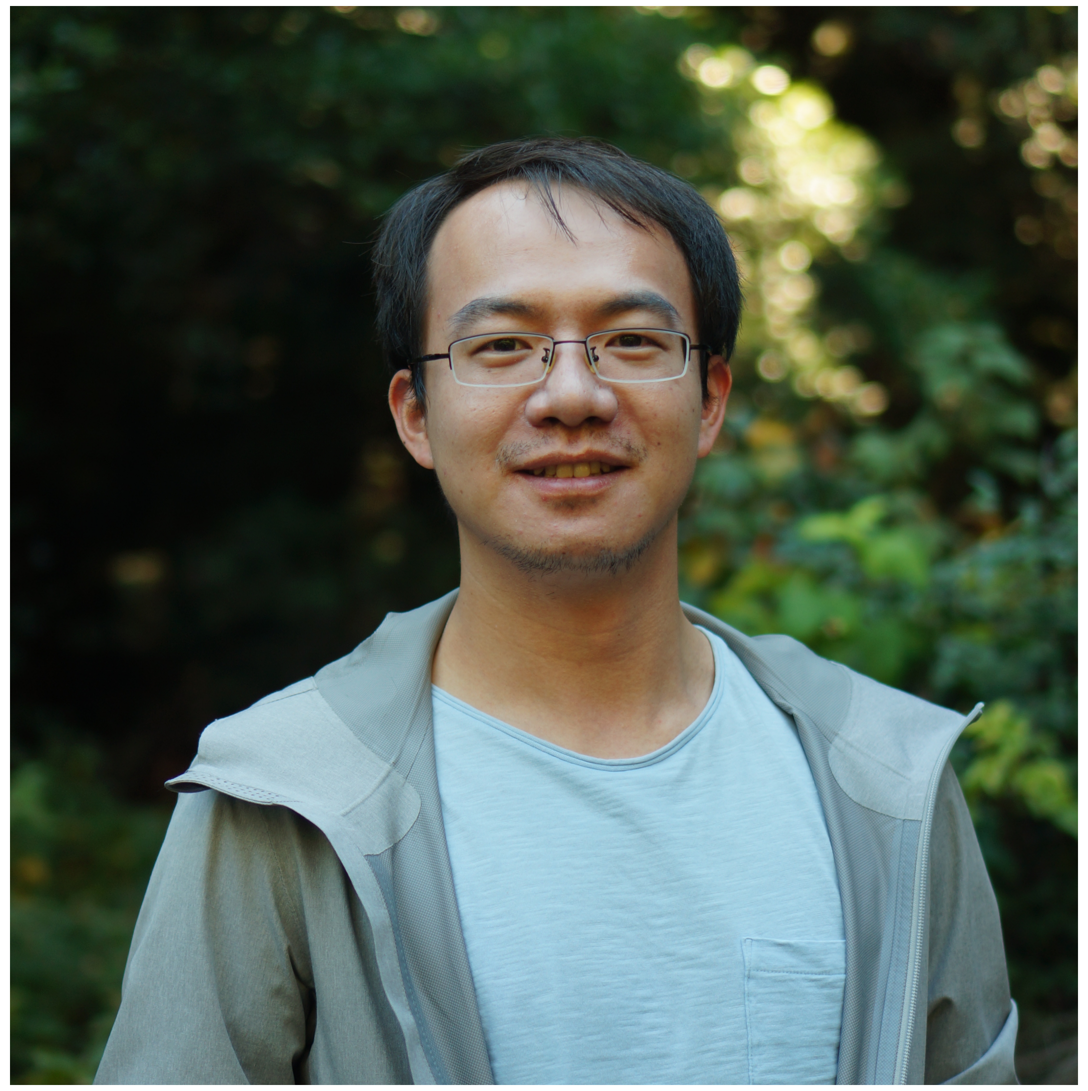
- A rigorous generalization analysis on data selection for finetuning
  - Low-dimensional data selection: variance reduction (V-optimality)
  - **High-dimensional data selection**: variance-bias tradeoff
- **Gradient sketching** provably finds a low-dimensional parameter subspace $\mathcal{S}$ with small 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**

Outline

- Data selection for statistical models in kernel regime — **finetuning**
  - A theory on data selection for finetuning that
    - Extends the classical wisdom of **V-optimal experimental design** in low dimensions
    - To high-dimensional data selection under low intrinsic dimensions via **sketching**
  - A fast and effective data selection algorithm for finetuning: **Sketchy Moment Matching (SkMM)**

- Data selection for low-rank approximation — **interpolative decomposition (ID)**
  - Select minimum possible rows as a basis to form a good low-rank approximation
  - A fast and accurate adaptive ID algorithm: **Robust Blockwise Random Pivoting (RBRP)**

Robust Blockwise Random Pivoting:
Fast and Accurate Adaptive Interpolative Decomposition



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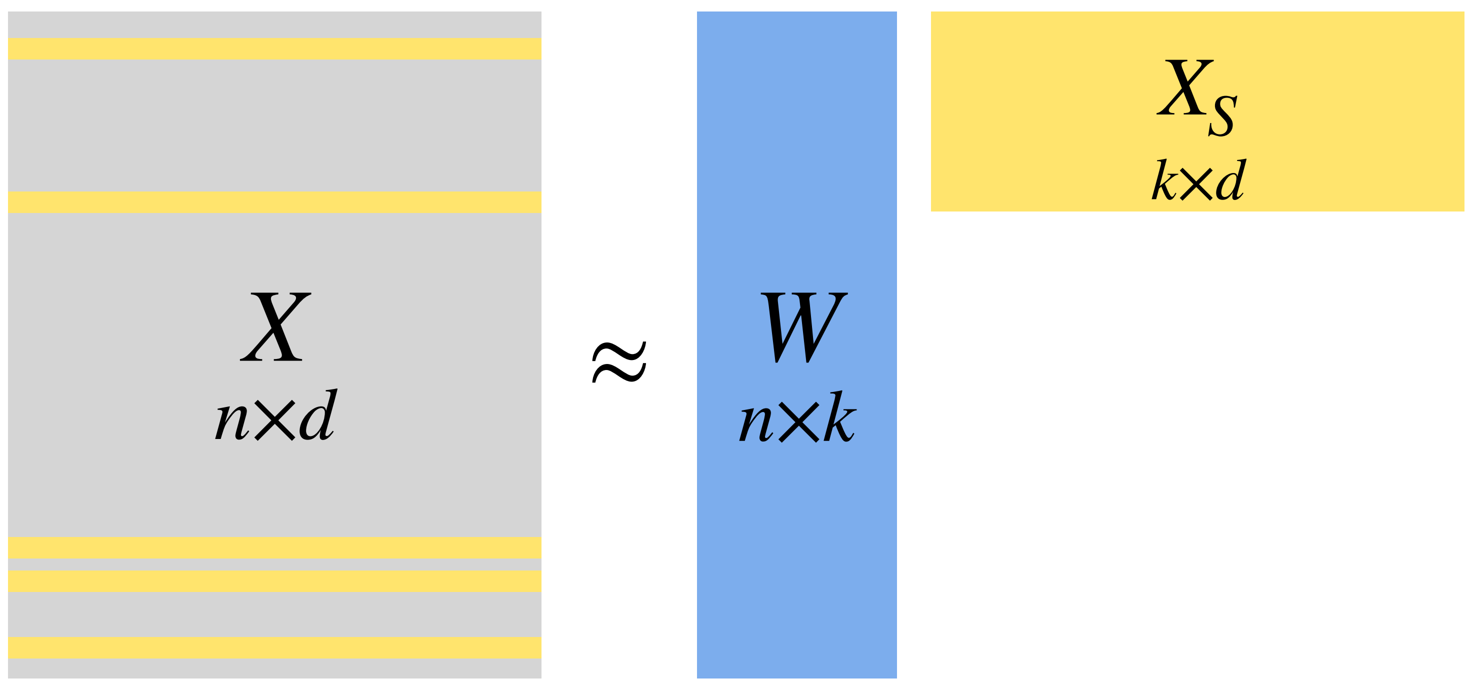
Interpolative Decomposition (ID)



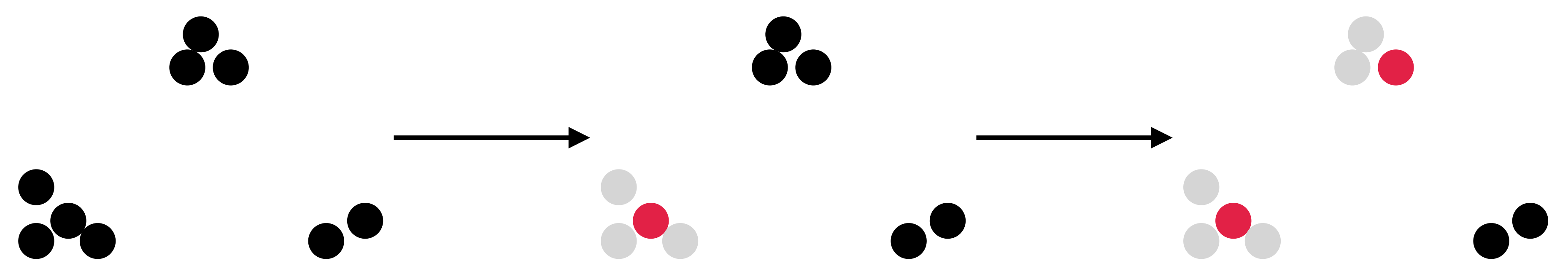
- Given a data matrix $X = [x_1, \cdots, x_n]^\top \in \mathbb{R}^{n \times d}$
- A target rank $1 \leq r \leq \operatorname{rank}(X)$
- A distortion constant $\epsilon > 0$
- Aim to construct a **(r, ϵ)-ID** of X —— $X \approx W X_S$ such that

$$\|X - W X_S\|_F^2 \leq (1 + \epsilon) \|X - X_{\langle r \rangle}\|_F^2$$

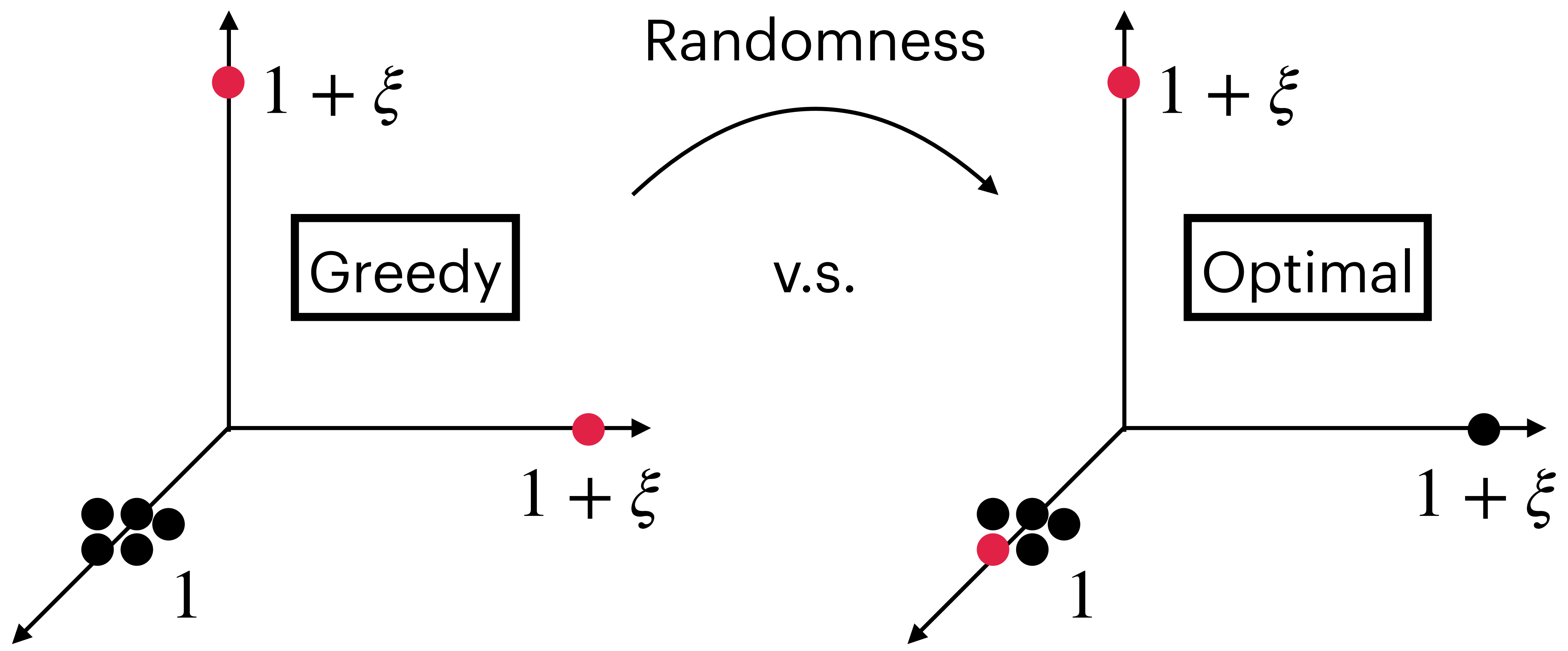
  - $S = \{s_1, \cdots, s_k\} \subseteq [n]$ contains indices for a **skeleton subset** of size $|S| = k$ (usually $k \ll n$)
  - $X_S = [x_{s_1}, \cdots, x_{s_k}]^\top \in \mathbb{R}^{k \times d}$ is the row skeleton submatrix corresponding to S
  - $W \in \mathbb{R}^{n \times k}$ is an interpolation matrix for the given skeleton subset S
  - $X_{\langle r \rangle}$ denotes the optimal rank-r approximation of X (given by the truncated SVD)

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)



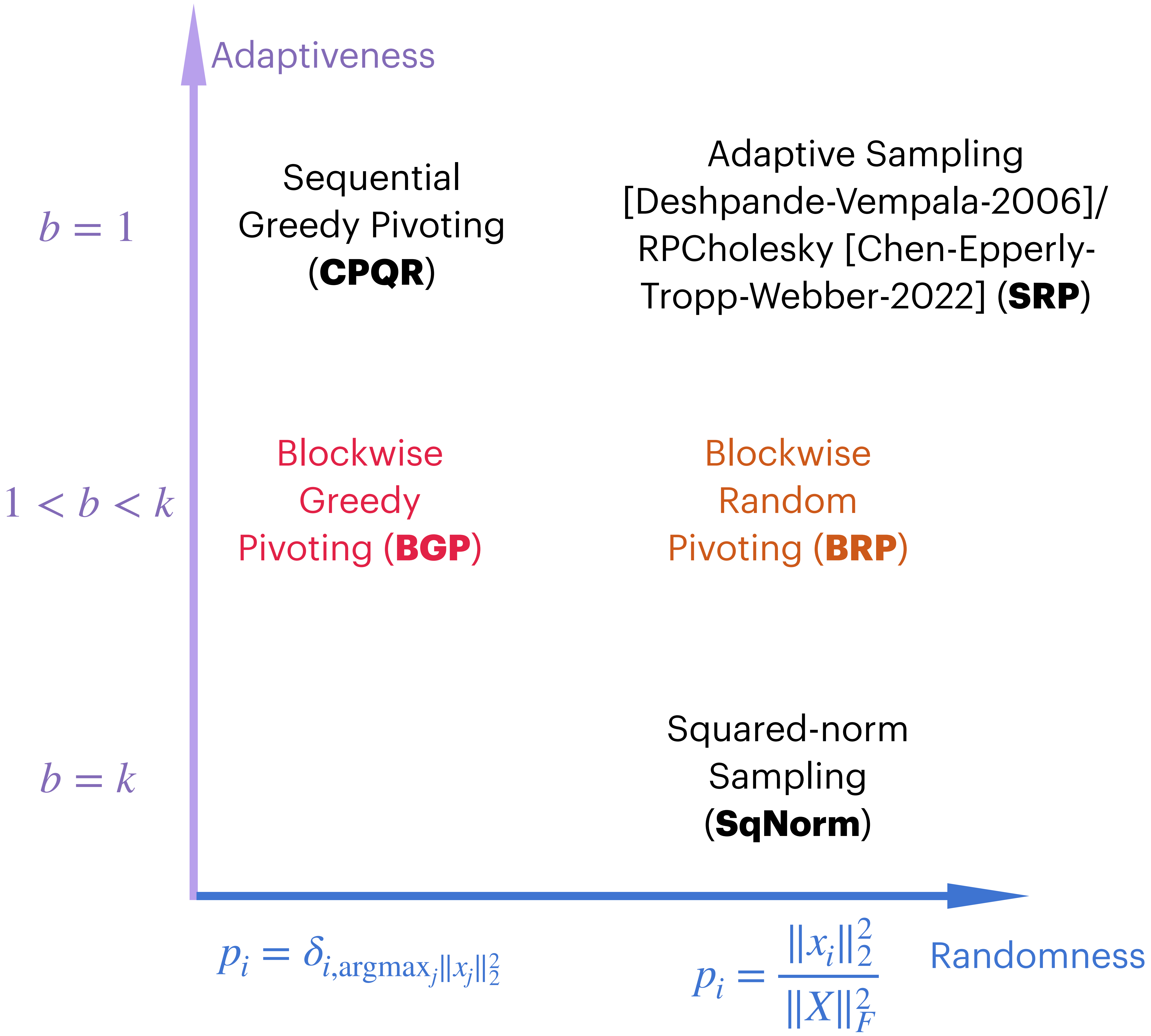
- **Randomness** (in contrast to greedy)
  - Intuition: balance exploitation with exploration
  - Effectively circumvent adversarial inputs for greedy methods
  - Achieve appealing skeleton complexities in expectation
  - Common randomness: sampling, sketching



Skeleton Selection: A General Framework

A framework for (blockwise adaptive) skeleton seletion

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



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]: $s_t \leftarrow \underset{i}{\operatorname{argmax}} \| Y_{i,:}^{(t-1)} \|_2^2$ + Gram-Schmidt
  - LU with partial pivoting (**LUPP**) [D-Martinsson-2023]: $s_t \leftarrow \underset{i}{\operatorname{argmax}} | Y_{i,t}^{(t-1)} |$ + Gaussian Elimination
- Pro: fast, accurate, robust to adversarial inputs
- Con: require prior knowledge of k

Two Stages of ID Constructions

- Stage I: Skeleton selection
  - Find a good skeleton subset S:

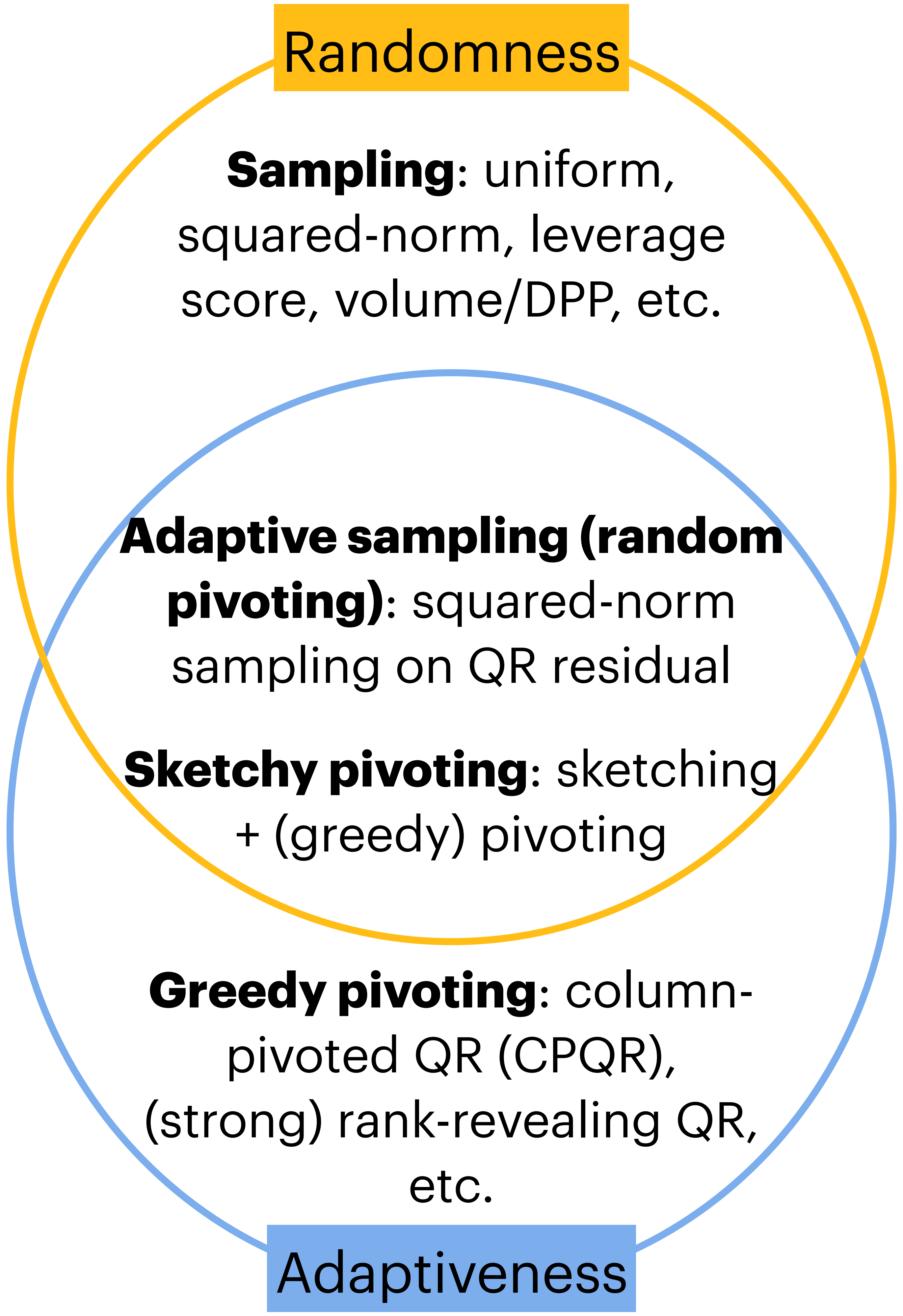
$$\min_{S\subset[n]} \min_{W\in\mathbb{R}^{n\times|S|}} \|X - WX_S\|_F^2$$

  - **Skeletonization error**: $\mathscr{E}_X(S) := \|X - XX_S^\dagger X_S\|_F^2 = \min_{W\in\mathbb{R}^{n\times|S|}} \|X - WX_S\|_F^2$
    - Naive construction of $XX_S^\dagger$ (e.g., via QR) takes $O(ndk)$ time (i.e., k additional passes through X)
- Stage II: Interpolation matrix construction
  - For some $O(ndk)$-time selection algorithms, W can be evaluated/approximated a posteriori in $O(nk^2)$ time
  - **Interpolation error**: $\mathscr{E}_X(W\,|\,S) := \|X - WX_S\|_F^2$

What are Fast & Accurate ID Algorithms?

- **Skeleton complexity**: the minimum number of skeletons $k = |S|$ that an ID algorithm needs to select in order to form a (r, ϵ)-ID (in expectation), i.e., $\mathcal{E}_X(S) \leq (1+\epsilon)\|X - X_{\langle r \rangle}\|_F^2$
- **Asymptotic complexity**: the asymptotic FLOP counts of the skeleton selection stage in an ID algorithm
- **Parallelizability**: whether the dominant cost of the skeleton selection stage in an ID algorithm can be casted as matrix-matrix (fast), instead of matrix-vector (slow), multiplications with X (i.e., applicability of Level 3 BLAS)
- **Error-revealing property**: the ability of an ID algorithm to evaluate $\mathcal{E}_X(S)$ efficiently on the fly so that the target rank k does not need to be given a priori.
  - Definition: An ID algorithm is **error-revealing** if after selecting any skeleton subset S, it can evaluate the corresponding skeletonization error $\mathcal{E}_X(S)$ efficiently in at most $O(n)$ time.
- **ID-revealing property**: if the skeleton selection stage of an ID algorithm extracts sufficient information so that
  - **Exact/inexact-ID-revealing**: $W = XX_S^\dagger$ can be evaluated exactly/approximated in $O(nk^2)$ time
  - **Non-ID-revealing** otherwise

ID Algorithms with Adaptiveness & Randomness



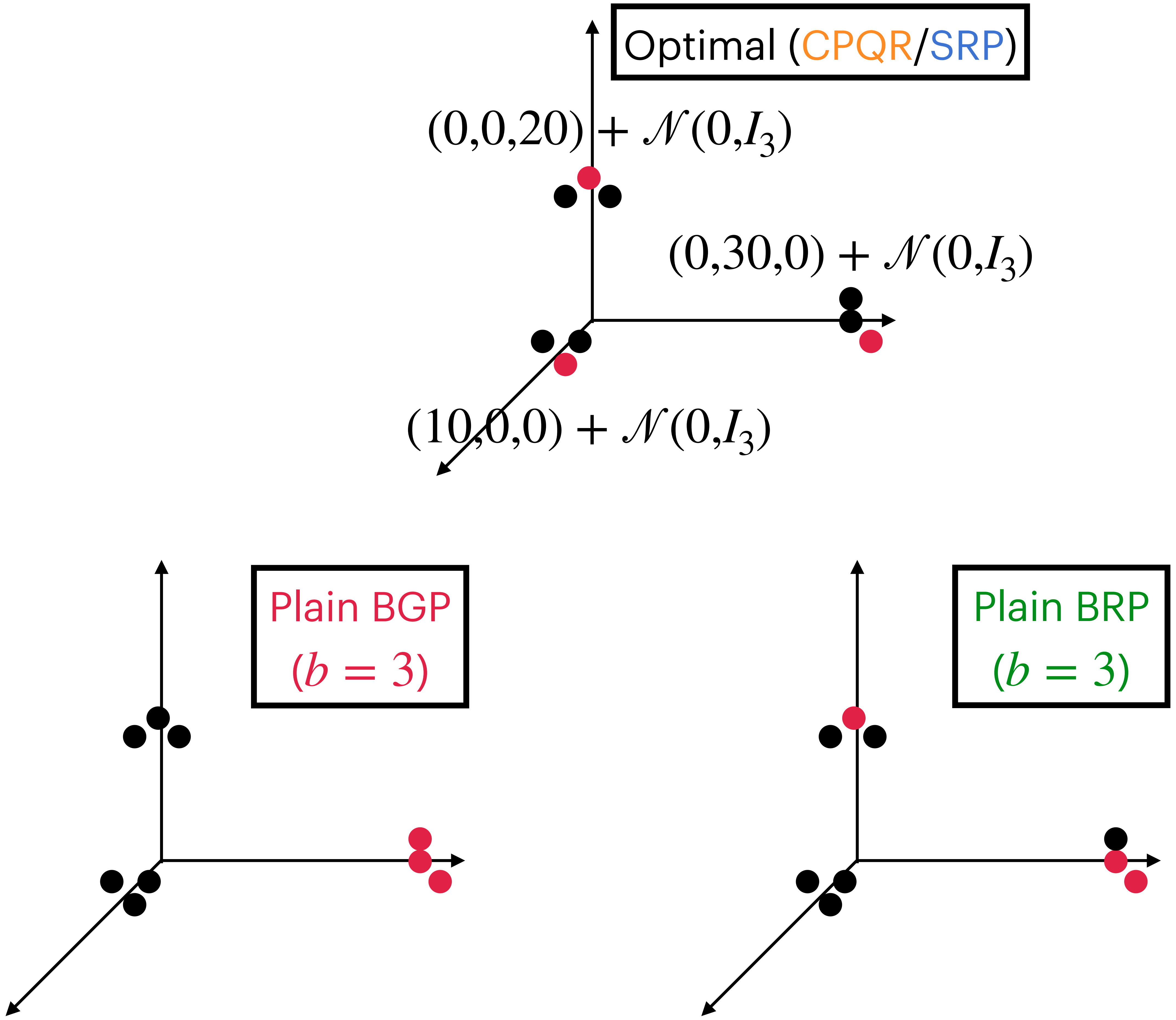
Algorithm	Skeleton Complexity	Asymp. Cost + Parallelizability	Error-reveal	ID-reveal
Greedy Pivoting	$k \geq (1+(1+\epsilon)\eta_r)n$	$O(ndk)$ sequential	✓	**Exact**
Squared-norm Sampling	$k \geq \dfrac{r-1}{\epsilon\eta_r} + \dfrac{1}{\epsilon}$	$O(nd)$ parallel	✗	Non
Random Pivoting	$k \geq k_{RP} := \dfrac{r}{\epsilon} + r\log\left(\min\left\{\dfrac{1}{\epsilon\eta_r}, \dfrac{2^{r+1}}{\epsilon}\right\}\right)$	$\boxed{O(ndk) \text{ sequential}}$	✓	**Exact**
Sketchy Pivoting	Conjecture: $k \gtrsim k_{RP}$	$O(ndk)$ parallel	✗	Inexact
RBRP	Conjecture: $k \gtrsim k_{RP}$	$\boxed{O(ndk) \text{ parallel}}$	✓	**Exact**

* $\eta_r = \|X - X_{<r>}\|_F^2 / \|X\|_F^2$ quantifies the relative optimal rank-r approximation error of X

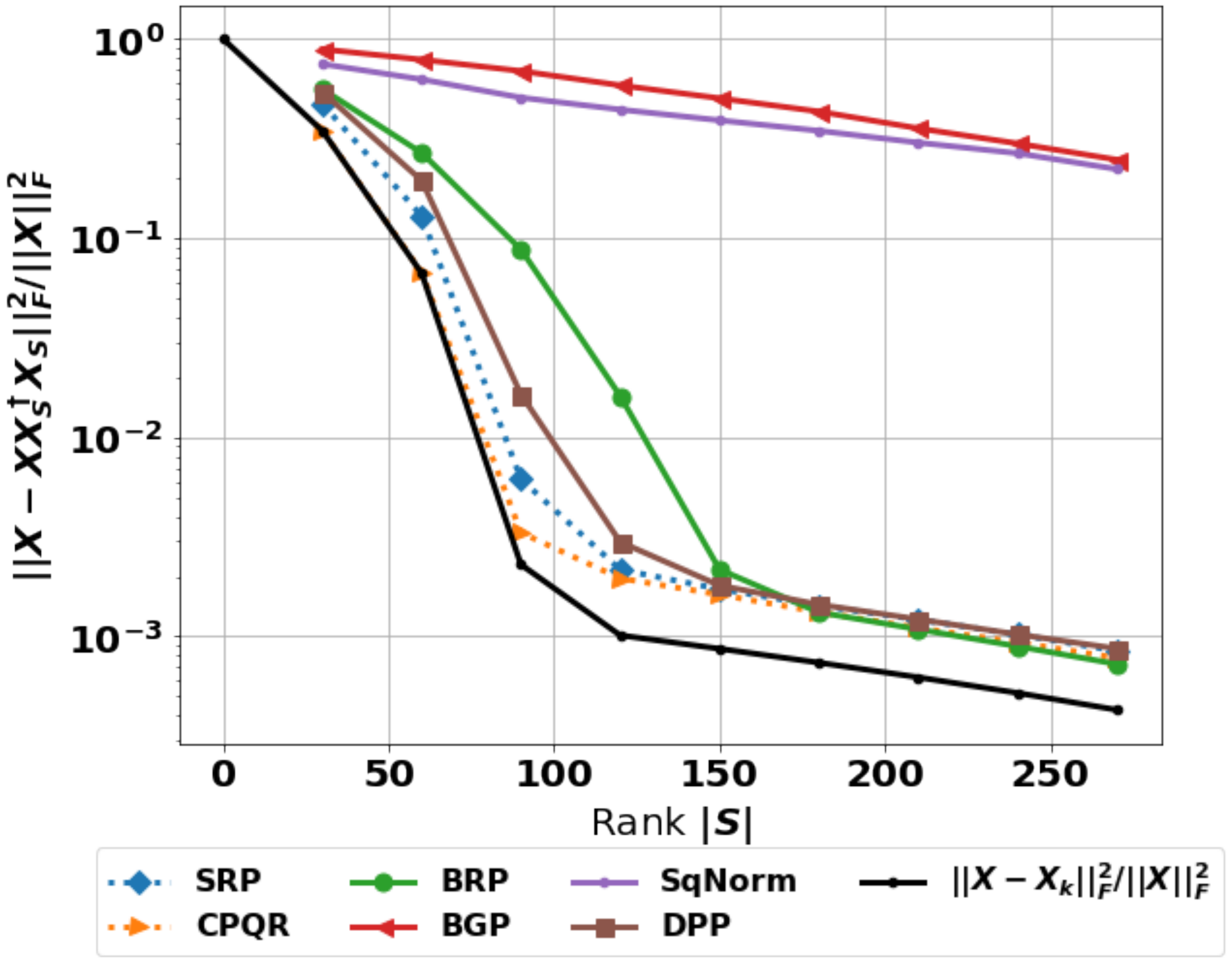
Epperly-Tropp-Webber-2024 proved this conjecture for an analogous algorithm based on rejective sampling!

Question: How to parallelize random pivoting?
Answer: Blockwise random pivoting

Pitfall of Plain Blockwise Greedy/Random Pivoting



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

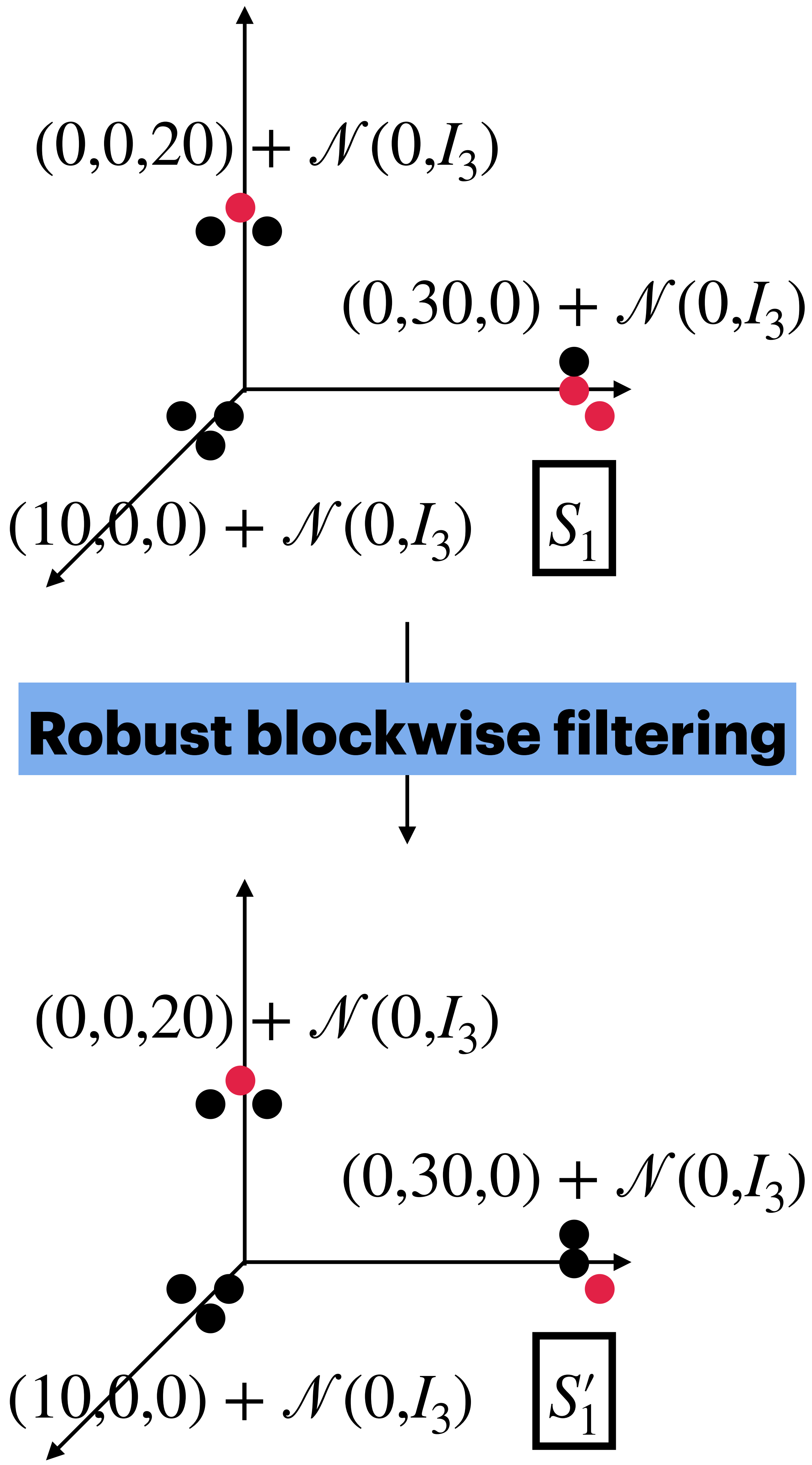


- Sequential pivoting (CPQR & SRP) is nearly optimal
- Plain blockwise pivoting (BRP/BGP, especially BGP) suffers from suboptimal skeleton complexities (up to b times)
- Squared-norm sampling (SqNorm) tends to fail

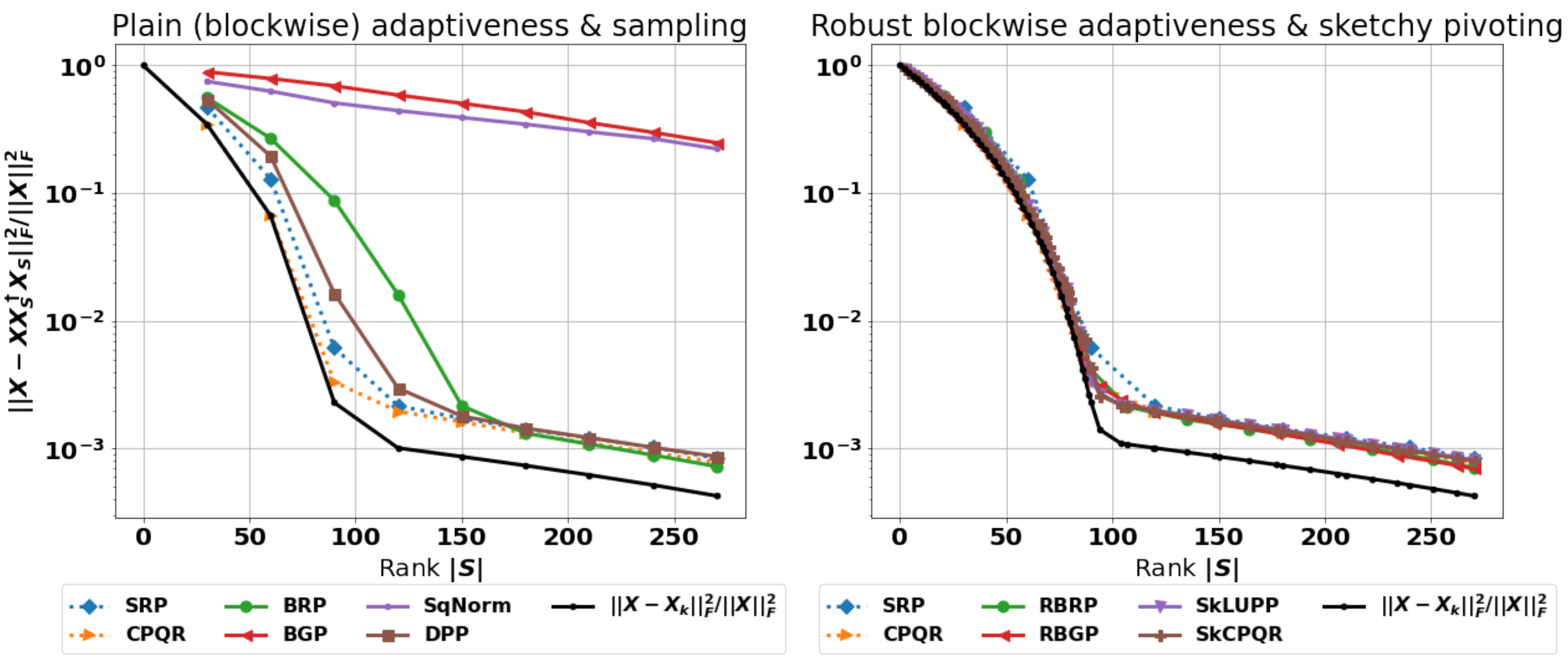
Robust Blockwise Random Pivoting

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

- **Inputs**: $X \in \mathbb{R}^{n \times d}$, $\tau = (1+\epsilon)\eta_r \in (0,1)$
- $X^{(0)} \leftarrow X$, $S^{(0)} \leftarrow \emptyset$, $t \leftarrow 0$
- **while** $\mathscr{E}(S^{(t)}) > \tau \|X\|_F^2$ $(t \leftarrow t+1)$ **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)**
    - $\pi \leftarrow \mathrm{CPQR}\left(X_{S_t}^{(t-1)}\right) \in S_b$ (SRP and CPQR both work)
    - $\min_{S_t' = S_t(\pi(1:b'))} b' \text{ s.t. } \|X_{S_t} - X_{S_t'}\|_F^2 < \tau_b \|X_{S_t}\|_F^2$ (e.g., $\tau_b = \frac{1}{b}$)
  - $S^{(t)} \leftarrow S^{(t-1)} \cup S_t'$ and $X^{(t)} \leftarrow X^{(t-1)}\left(I_d - X_{S_t'}^{\dagger} X_{S_t'}\right)$
- $S \leftarrow S^{(t)}$, $k = |S|$

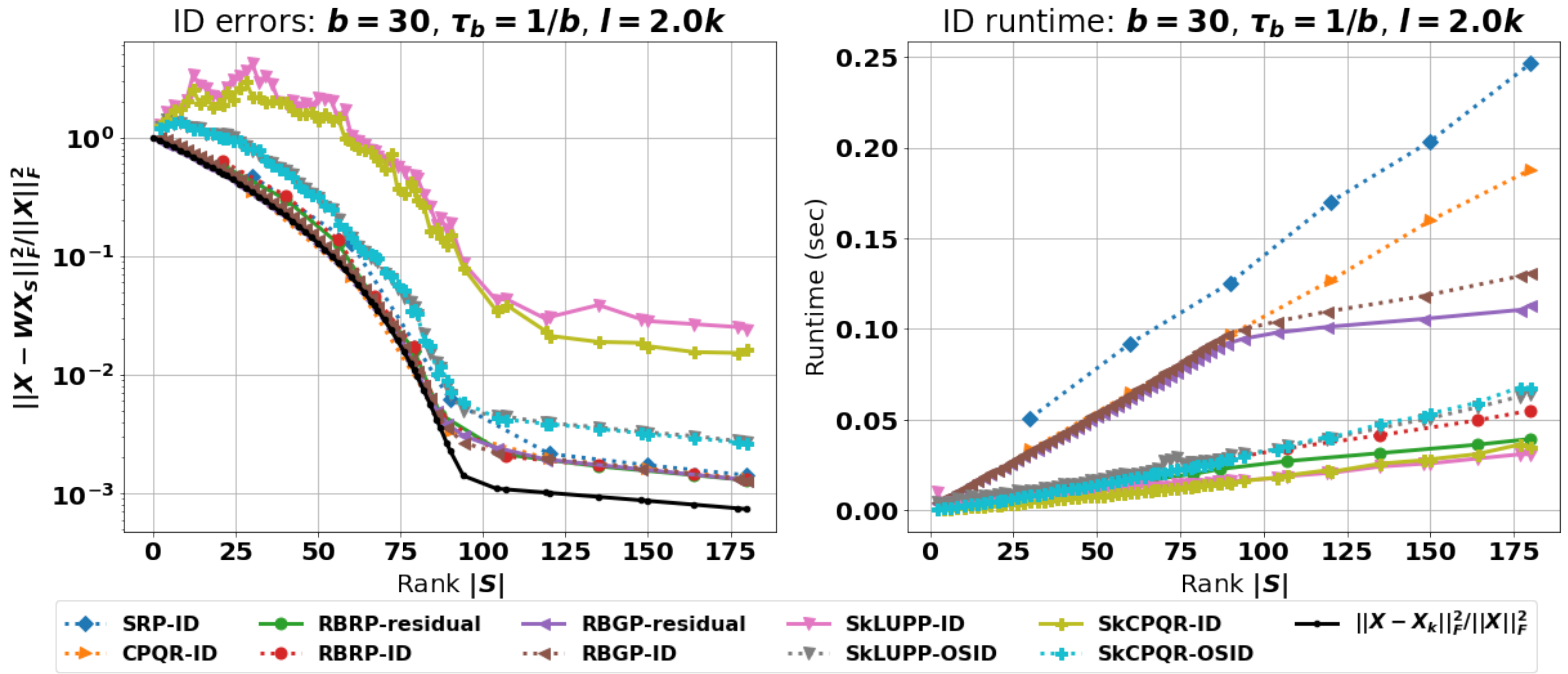


Robust Blockwise Random Pivoting: Robustness



- 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

Robust Blockwise Random Pivoting: Efficiency

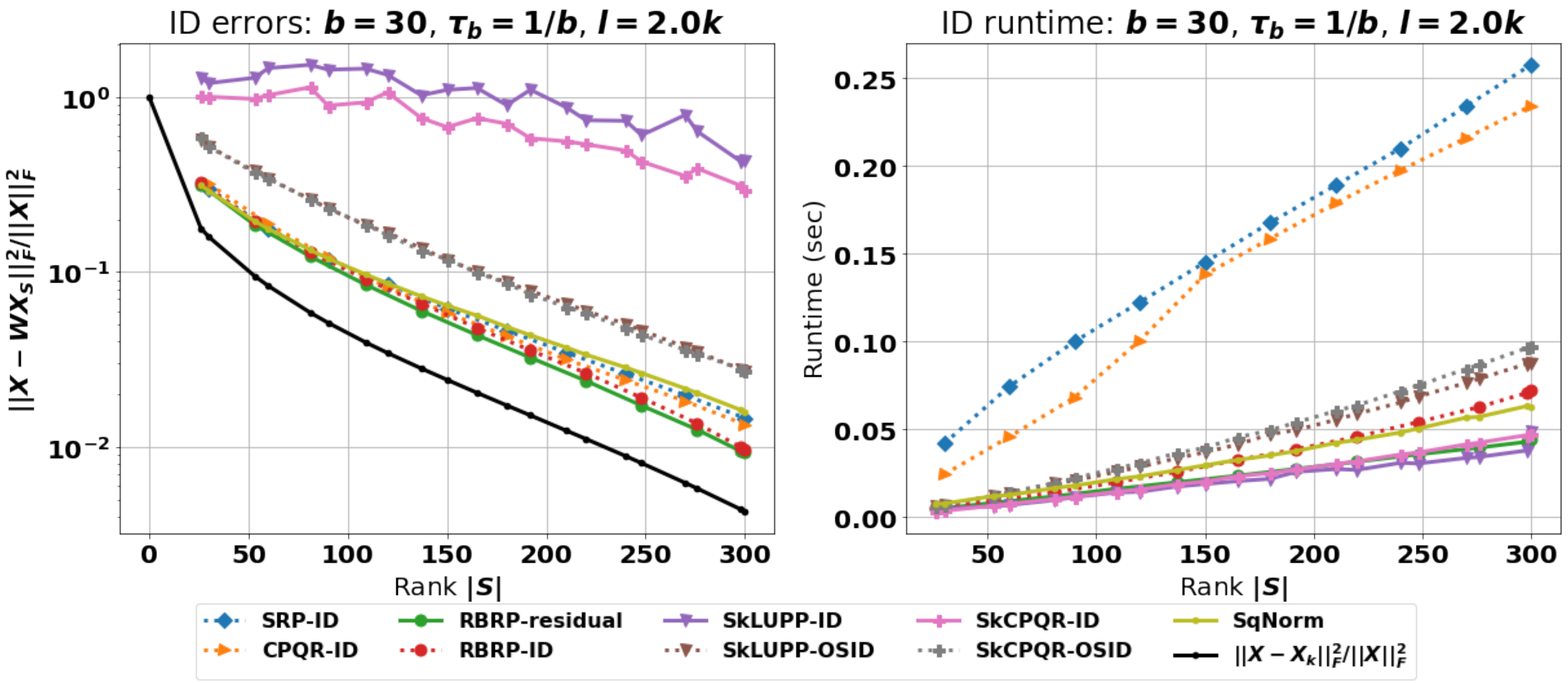


- Robust blockwise filtering (RBRP and RBGP) brings nearly optimal skeleton complexities
- RBGP tends to be slowed down much more significantly than RBRP by robust blockwise filtering
- For ID: RBRP-ID is almost as fast as sketchy pivoting (SkLUPP-ID/SkCPQR-ID), while enjoying much better interpolation error $\mathscr{E}_X(W|S) = \mathscr{E}_X(S)$ thanks to its exact-ID-revealing property.

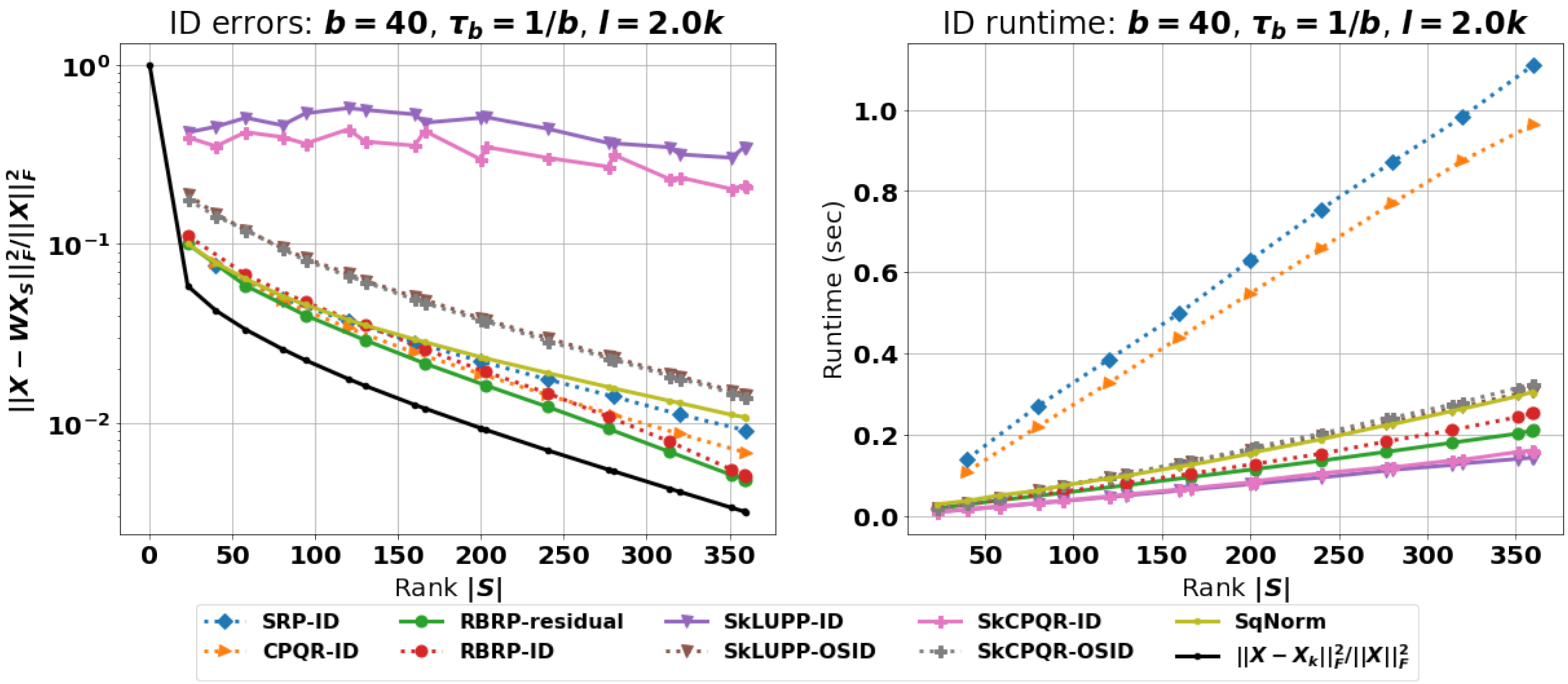
Exact- v.s. Inexact-ID-revealing Algorithms

- **Exact-ID-revealing algorithms**
  - Sequential/blockwise random/greedy pivoting algorithms (SRP, CPQR, BRP, BGP, RBRP, RBGP)
  - The skeleton selection process generates sufficient information for solving the least square problem $\min_{W \in \mathbb{R}^{n \times k}} \|X - WX_S\|_F^2$ in $O(nk^2)$ time
- **Inexact-ID-revealing algorithms**
  - Sketchy pivoting algorithms (SkLUPP, SkCPQR)
  - The skeleton selection process generates sufficient information for solving the **sketched** least square problem $\min_{W \in \mathbb{R}^{n \times k}} \|X\Omega - WX_S\Omega\|_F^2$ in $O(nk^2)$ time
  - Oversampled sketchy ID (**OSID**): for $|S| = k$
    - Sketching with oversampling $Y = X\Omega \in \mathbb{R}^{n \times l}$ such that $l = O(k)$
    - $W = YY_S^\dagger$ can be computed in $O(nlk) = O(nk^2)$ time
  - Suboptimal interpolation error: $\mathcal{E}_X(W | S) - \mathcal{E}_X(S) = O(k/l)$

More Numerical Comparisons: MNIST



More Numerical Comparisons: CIFAR-10



Takeaways

- A fast & accurate ID algorithm that finds $\|X - WX_S\|_F^2 \leq (1+\epsilon)\|X - X_{\langle r \rangle}\|_F^2$
  - With **nearly optimal skeleton complexity** in practice
  - Computationally efficient in terms of both **asymptotic complexity** and **parallelizability**
  - **Error-revealing** without requiring prior knowledge of the target skeleton subset size
  - **Exact-ID-revealing** where the optimal interpolation matrix can be computed efficiently
- **Combining adaptiveness and randomness** is a key for designing robust skeleton selection algorithms with competitive skeleton complexity
- A critical challenge is to **relax the sequential natural of adaptive selection**
- We introduced **Robust Blockwise Random Pivoting (RBRP)**, a parallelizable blockwise adaptive selection scheme that achieves comparable skeleton complexity as its sequential counterpart

Thank You! Happy to take any questions

SkMM: https://arxiv.org/pdf/2407.06120

RBRP: https://arxiv.org/abs/2309.16002

Qs: Are there connections between ID and finetuning?

<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

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

<u>Bias reduction $\asymp$ learning in noiseless settings $\asymp$ minimizing skeletonization error of ID</u>

- In the noiseless setting $\sigma = 0$, the expected excess risk is controlled by the variance only:

$$\mathbb{E}[\mathrm{ER}(\theta_S)] \le \min_{\mathcal{S}\subset\mathrm{Range}(\Sigma_S)} 2\mathrm{tr}(\Sigma P_{\mathcal{S}}^{\perp})\|\theta_*\|_2^2$$

  - $\mathrm{tr}(\Sigma P_{\mathcal{S}}^{\perp}) = \|G P_{\mathcal{S}}^{\perp}\|_F^2 / N$ can be viewed as a low-rank approximation error
  - Taking $\mathcal{S} = \mathrm{Row}(G_S)$, $\mathrm{tr}(\Sigma P_{\mathcal{S}}^{\perp})$ is effectively the skeletonization error of the ID associated with S

Qs: What's wrong with adaptive sampling for finetuning?

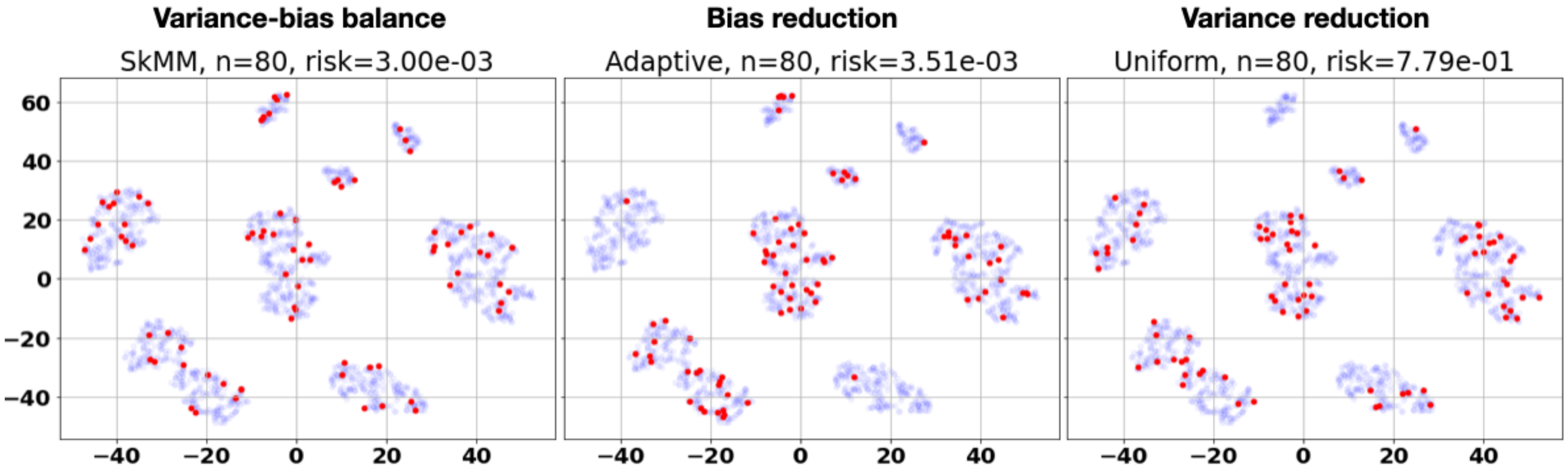


Table 1: Empirical risk $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_S)$ on the GMM dataset at various n, under the same hyperparameter tuning where ridge regression over the full dataset $\mathcal{D}$ with $N = 2000$ samples achieves $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_{[N]}) =$ **2.95e-3**.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