Data Selection under Low Intrinsic Dimension:
from Interpolatove Decomposition to Ridge Regression

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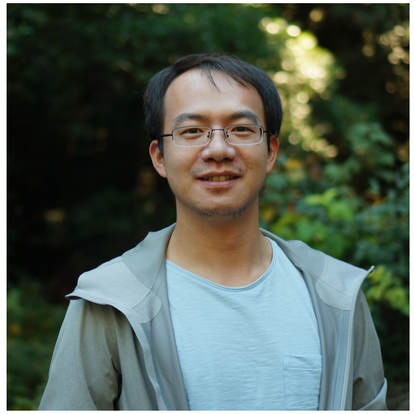
Low Intrinsic Dimension & Data Selection

- **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**

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



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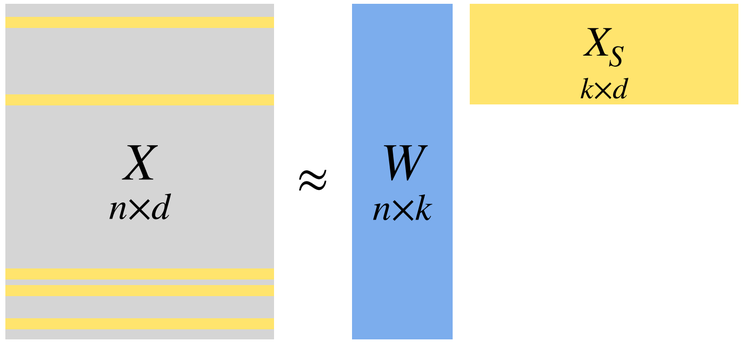
Interpolative Decomposition (ID)

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

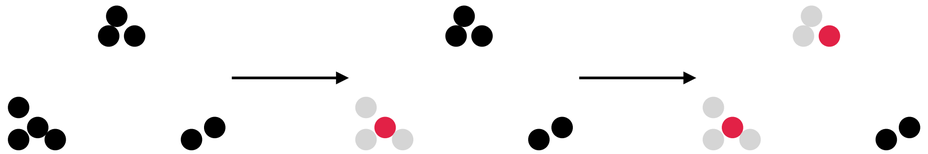


$$\mathscr{E}(S) = \|X - (XX_S^\dagger)X_S\|_F^2 \leq \tau \|X\|_F^2$$

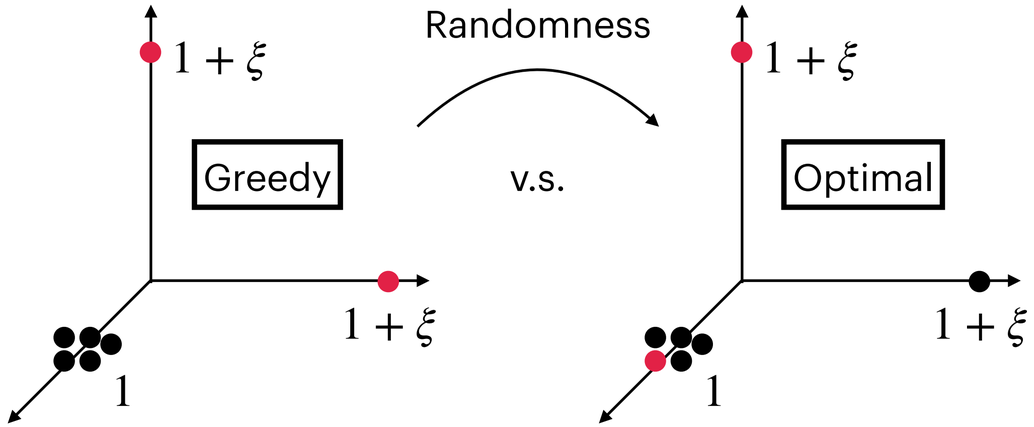
- $S = \{s_1, \cdots, s_k\} \subseteq [n]$ contains indices for a **skeleton subset** of size $|S| = k$ (usually $k \ll n$)
- $X_S = [x_{s_1}, \cdots, x_{s_k}]^\top \in \mathbb{R}^{k \times d}$ is the row skeleton submatrix corresponding to S
- $W = XX_S^\dagger \in \mathbb{R}^{n \times k}$ is an interpolation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



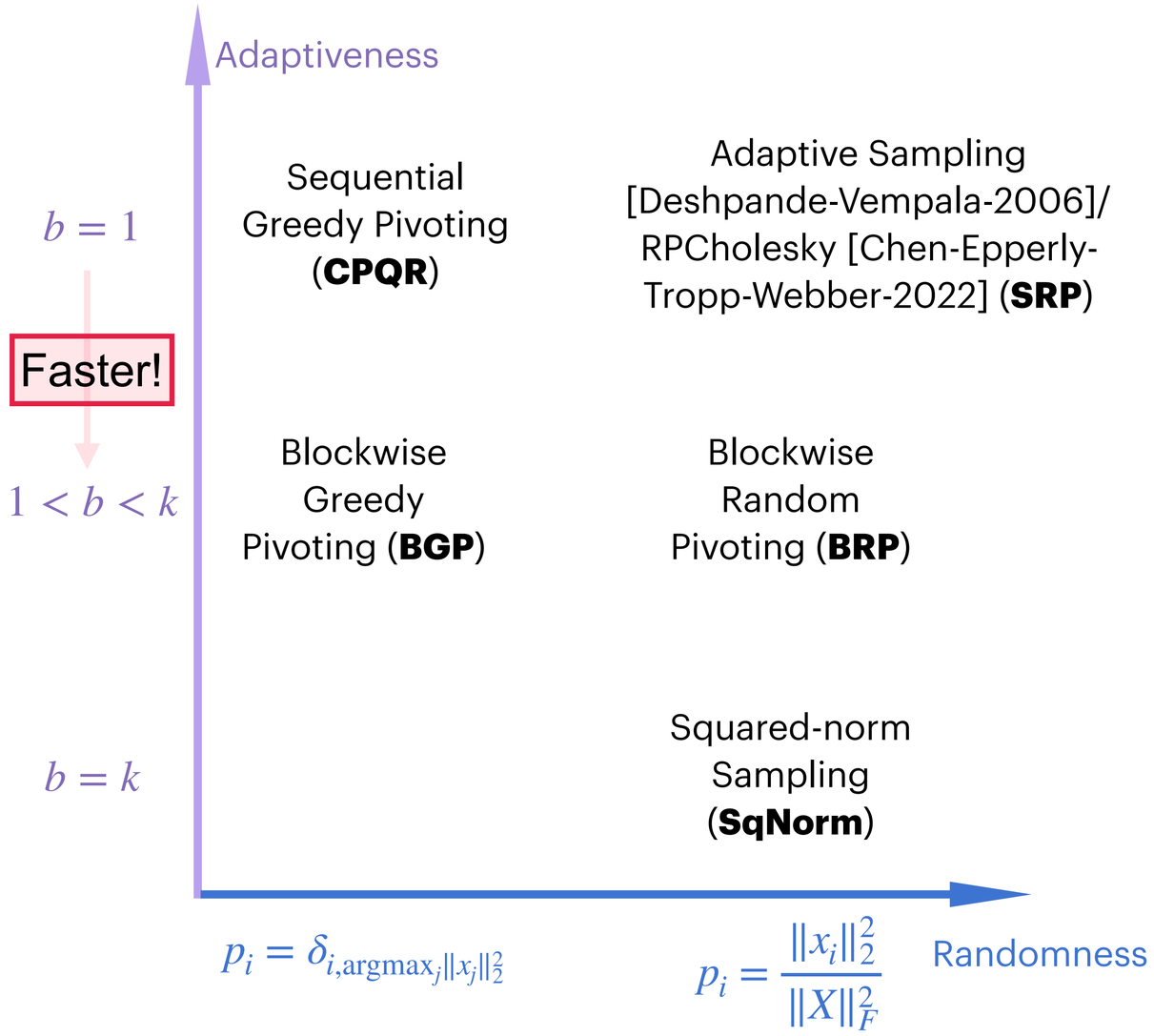
- **Randomness** (in contrast to greedy)
  - Intuition: balance exploitation with exploration
  - Effectively circumvent adversarial inputs for greedy methods
  - Achieve appealing skeleton complexities in expectation
  - Common randomness: sampling, sketching



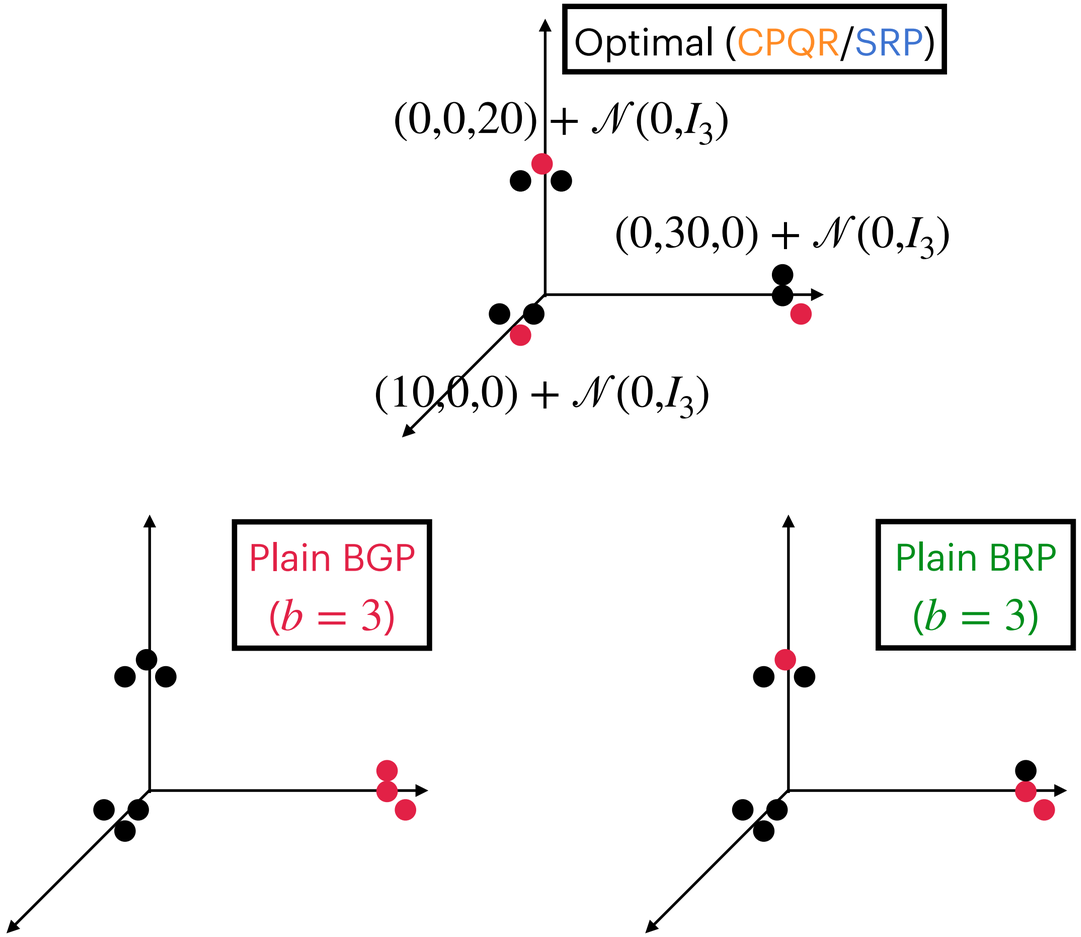
Skeleton Selection: A General Framework

A framework for (blockwise adaptive) skeleton selection

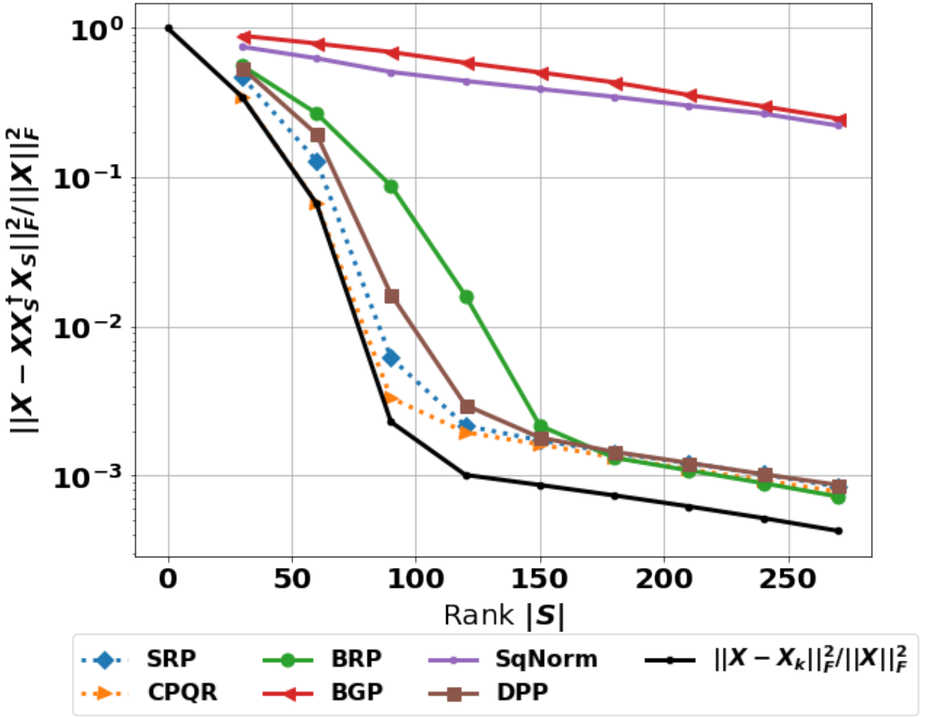
- **Inputs**: $X \in \mathbb{R}^{n \times d}$, $\tau \in (0,1)$
- $X^{(0)} \leftarrow X$, $S^{(0)} \leftarrow \emptyset$, $t \leftarrow 0$
- **while** $\mathscr{E}(S^{(t)}) > \tau \|X\|_F^2$ **do**
  - $t \leftarrow t+1$
  - Select $|S_t| = b$ skeletons S_t based on $\left(p_i\left(X^{(t-1)}\right)\right)_{i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



Pitfall of Plain Blockwise Greedy/Random Pivoting



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

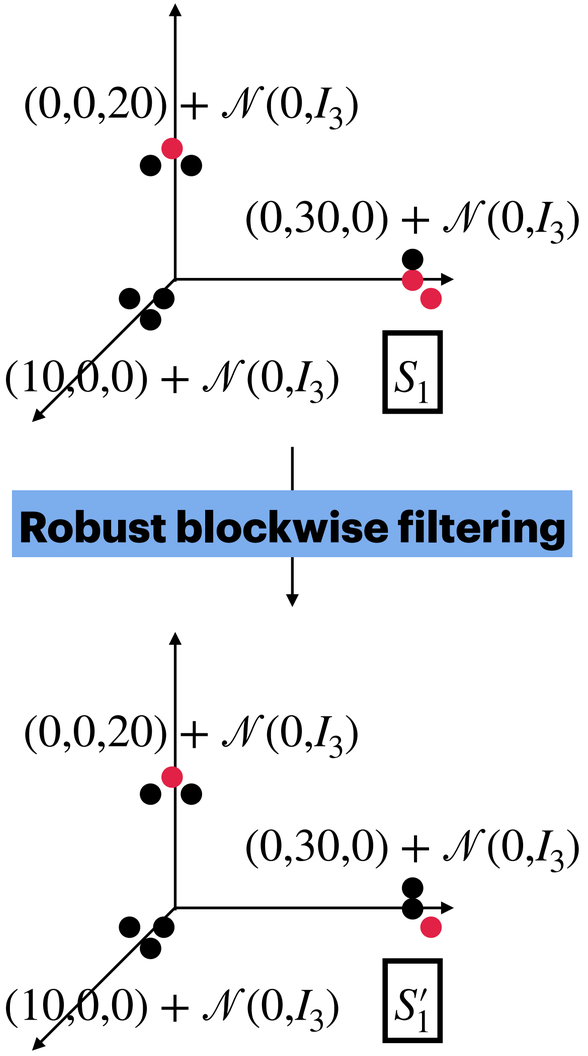


- Sequential pivoting (CPQR & SRP) is nearly optimal
- Plain blockwise pivoting (BRP/BGP, especially BGP) suffers from suboptimal skeleton complexities (up to b times)
- Squared-norm sampling (SqNorm) tends to fail

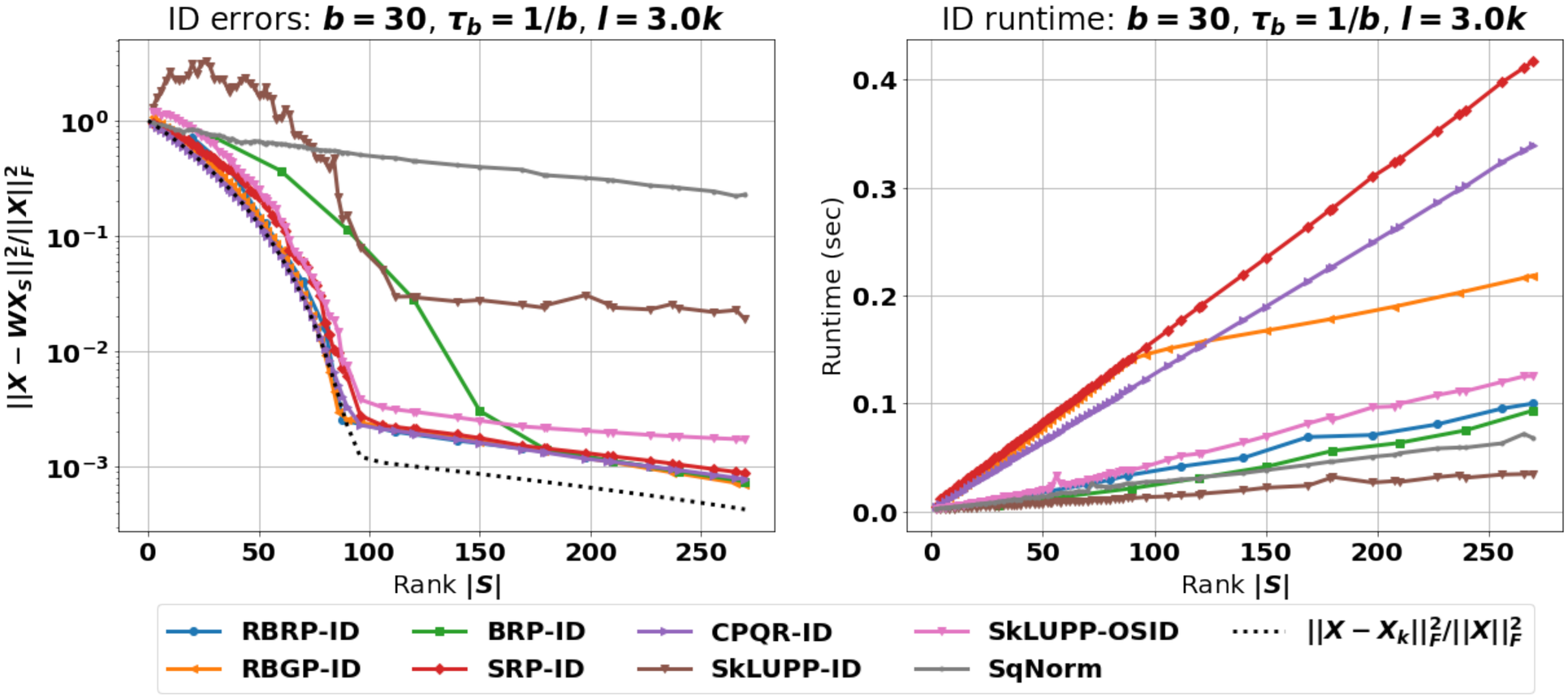
Robust Blockwise Random Pivoting

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** $\mathscr{E}(S^{(t)}) > \tau\|X\|_F^2$ $(t \leftarrow t+1)$ **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: 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

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**:

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

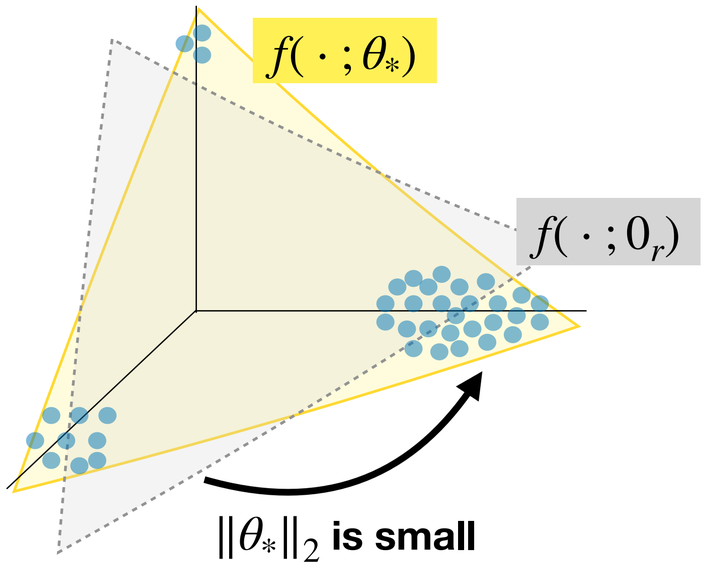
- With a **suitable pre-trained initialization** (i.e. $f(\cdot,0_r)$ is close to $f(\,\cdot\,,\theta_*)$), $\|\theta_*\|_2$ is small

- 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 $\Sigma_S = G_S^\top G_S/n \succeq 0$



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:

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

Low-rank approximation error of ID!

Theorem (**Variance-bias tradeoff**): 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

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

- 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

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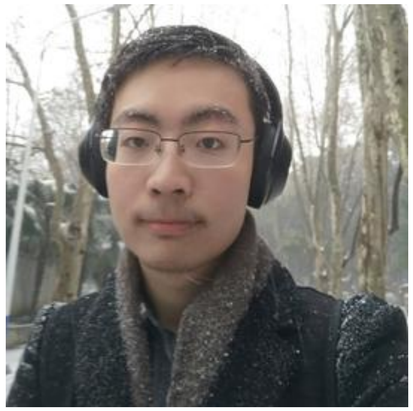

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In Low Dimension: Variance Reduction

- 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: $\mathbb{E}[\mathrm{ER}(\theta_S)] \le \frac{\sigma^2}{n}\mathrm{tr}(\Sigma\Sigma_S^{-1})$

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

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

Optimal rank-t approximation (truncated SVD)

Assumption (**Low intrinsic dimension**): For $\Sigma = G^\top G/N$, let $\bar{r} = \min\{t \in [r] \mid \mathrm{tr}(\Sigma - \langle\Sigma\rangle_t) \le \mathrm{tr}(\Sigma)/N\}$ 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)?

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

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 $m = \max\{\sqrt{\mathrm{tr}(\Sigma)/\gamma_S}, 11\bar{r}\}$,

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

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 $i \in [N]$ and $s_i = 0$ otherwis
- Sample a size-n coreset $S \subset$ that solves the optimization p

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

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

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

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

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): $O(\mathrm{nnz}(G)\log m)$
- **ing** takes $O(m^3)$ for spectral The optimization takes $O(Nm)$

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

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

SkMM 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 $\alpha > 0$

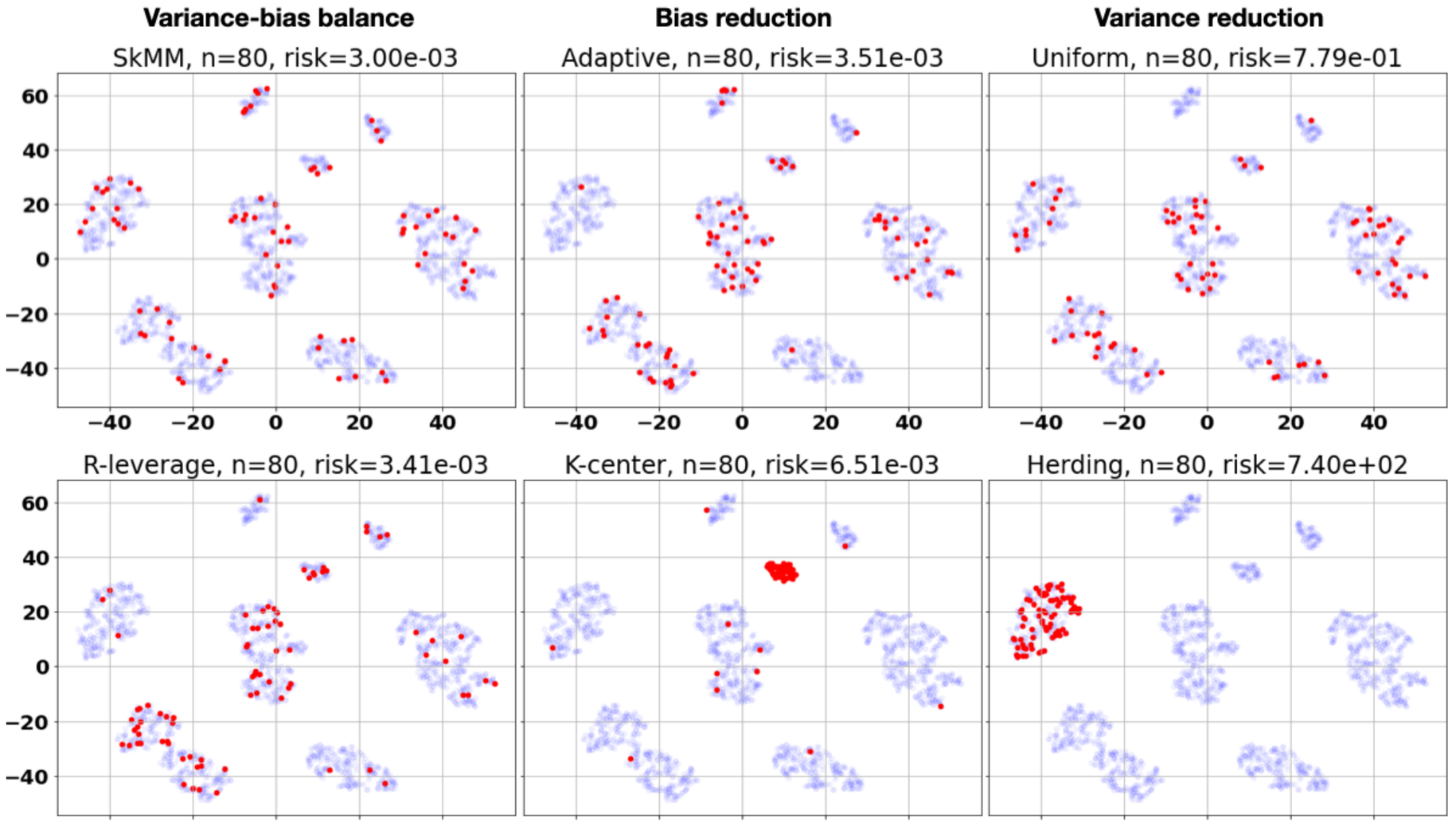
Baselines

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

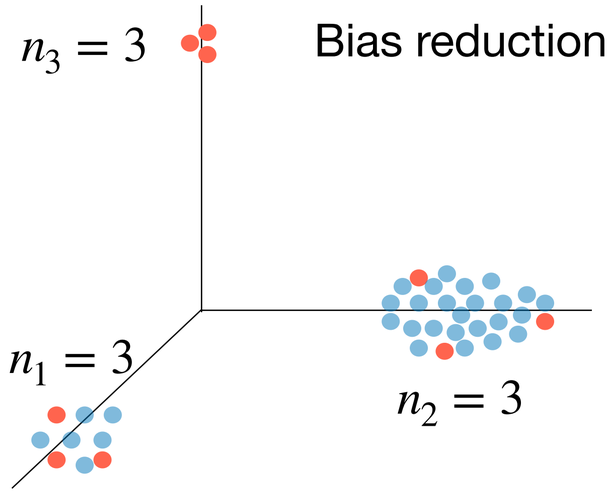
Table 1: Empirical risk $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_S)$ on the GMM dataset at various n, under the same hyperparameter tuning where ridge regression over the full dataset $\mathcal{D}$ with $N = 2000$ samples achieves $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_{[N]}) =$ **2.95e-3**.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

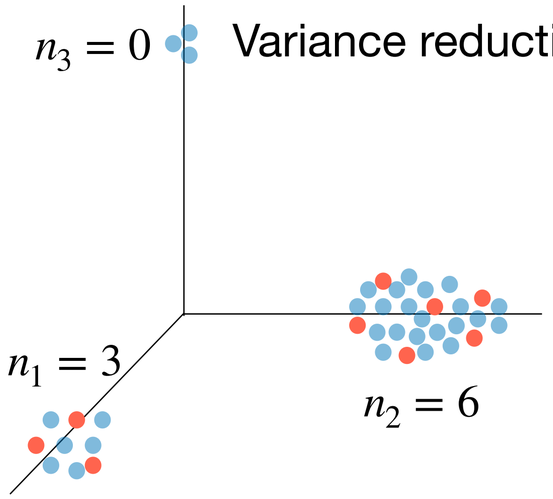
SkMM on Synthetic Data: Regression



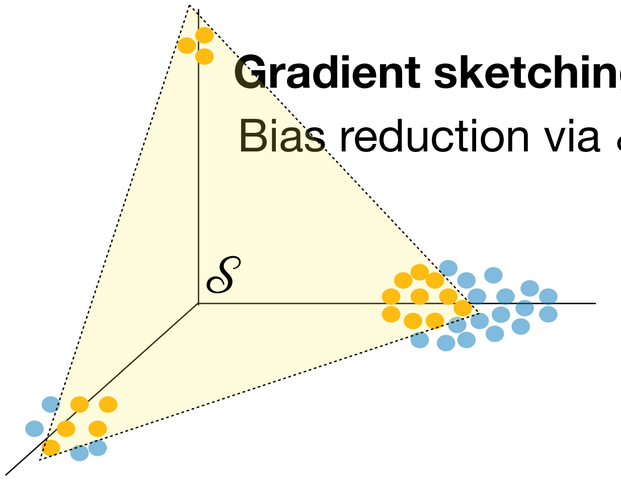
SkMM simultaneously controls variance and bias



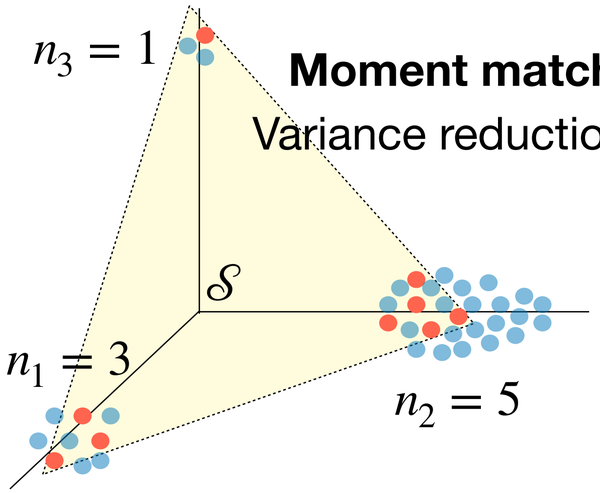
Bias reduction



Variance reduction



Gradient sketching:
Bias reduction via $\mathcal{S}$



Moment matching:
Variance reduction in $\mathcal{S}$

Thank You! Happy to take any questions

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*.