Asymptotics of the Sketched Pseudoinverse

December 2022

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Department of Statistics and Machine Learning

Joint work with: Hamid Javadi, Richard Baraniuk, Ryan Tibshirani

Too Much Data

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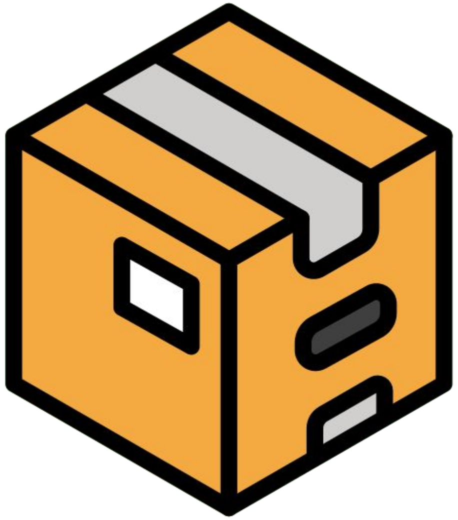

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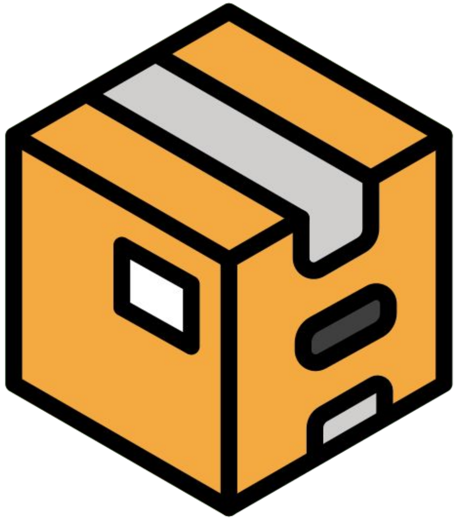

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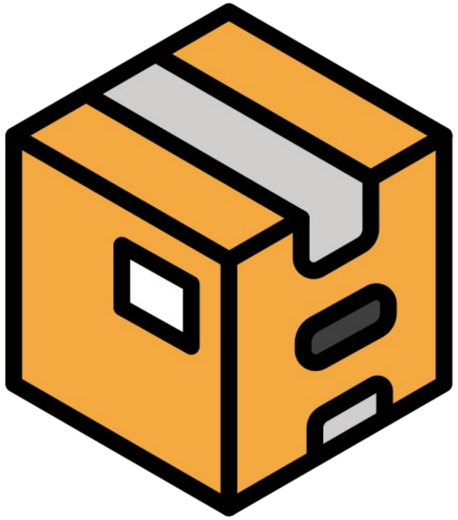

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Q: Odds of cancer in next 5 years?

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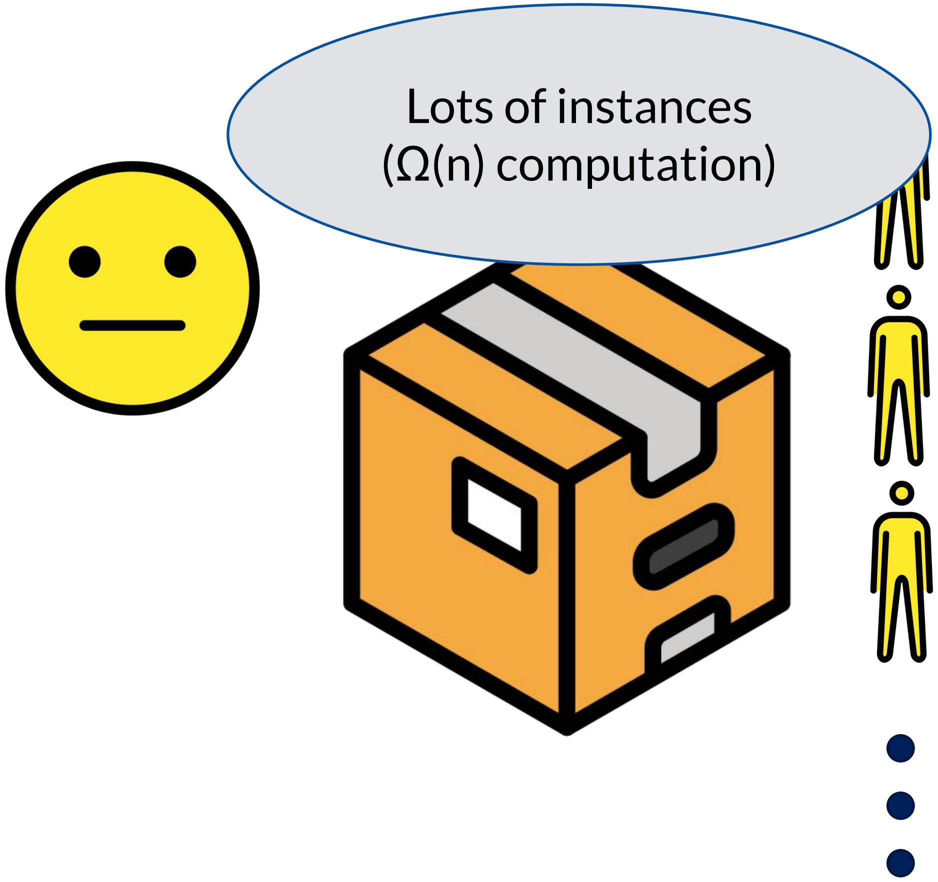

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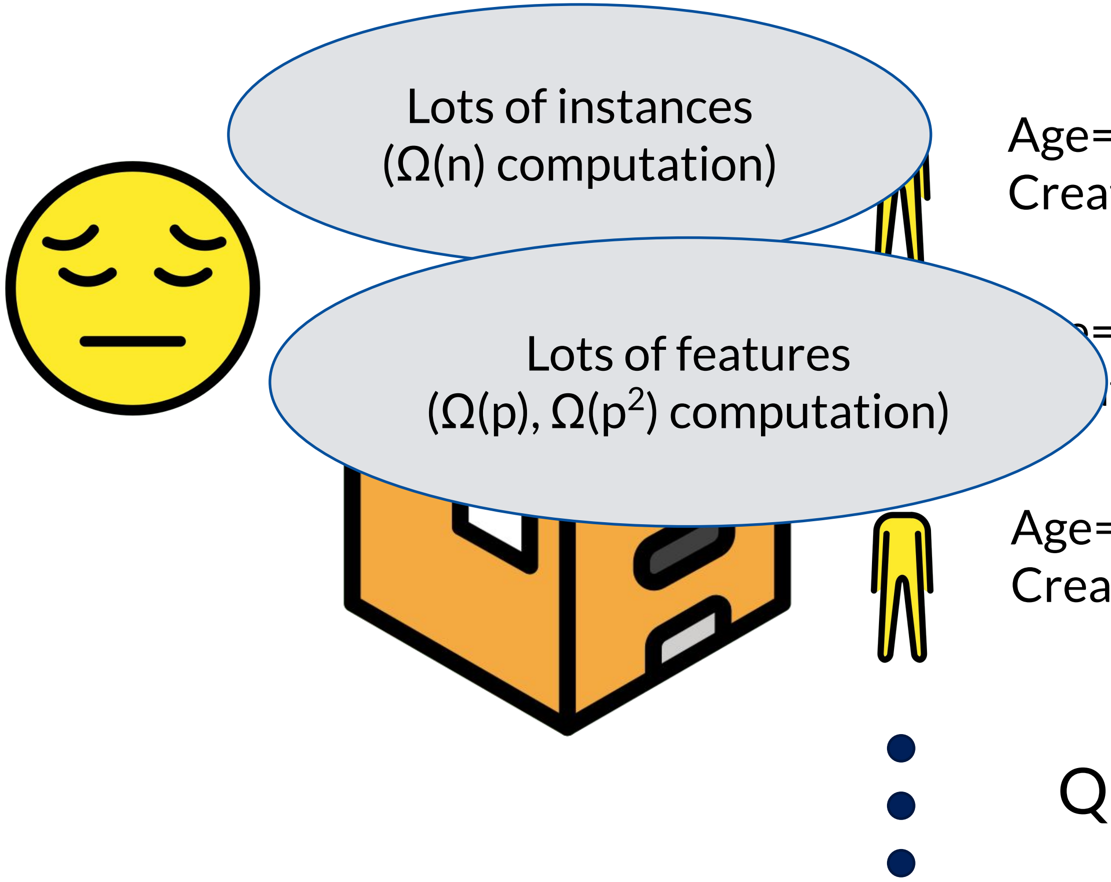

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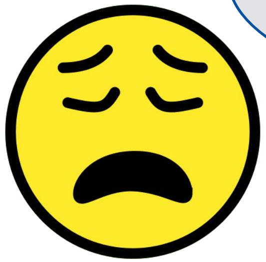

Lots of instances
($\Omega(n)$ computation)

Lots of features
($\Omega(p)$, $\Omega(p^2)$ computation)

Curse of dimensionality
(Too many solutions)

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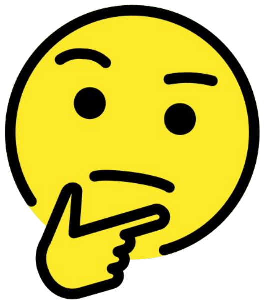
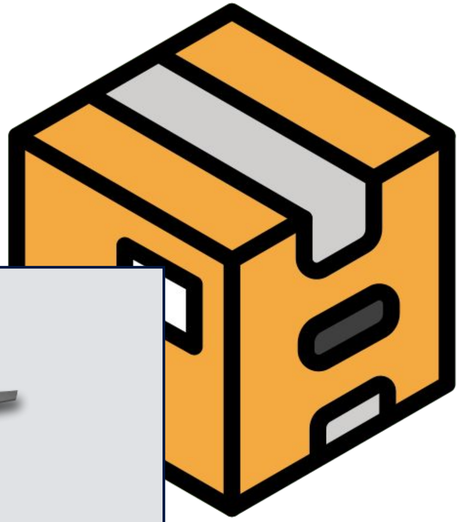
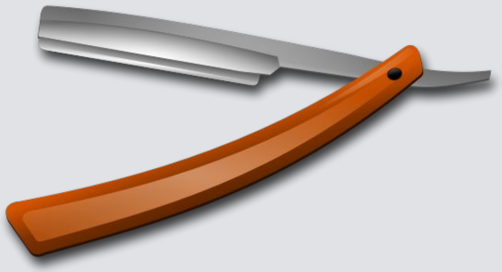
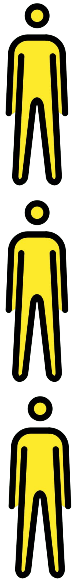






Occam's razor:
The true function should not be too complicated.



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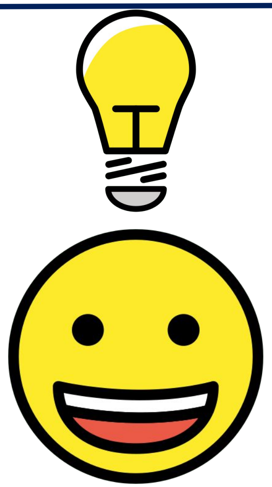

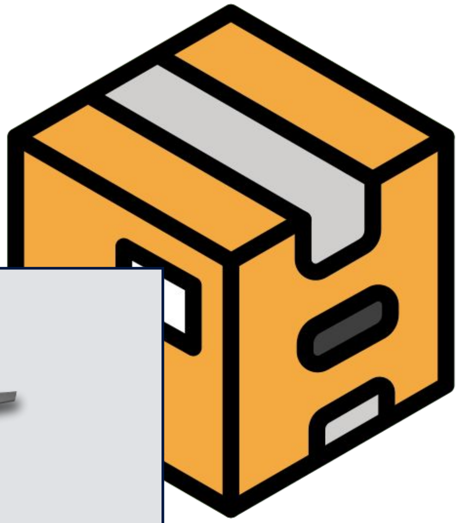

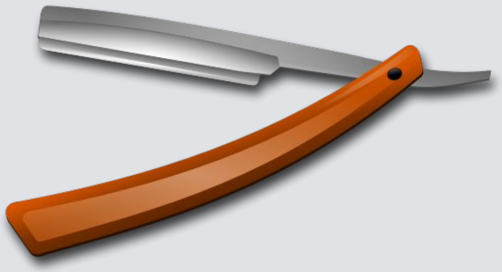

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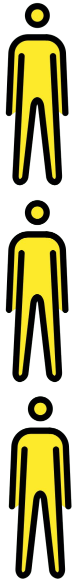

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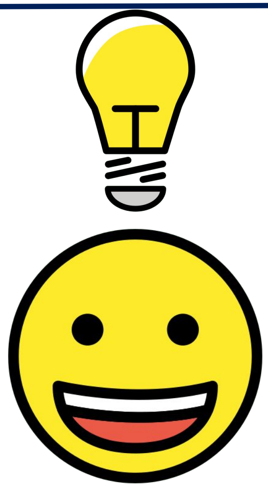

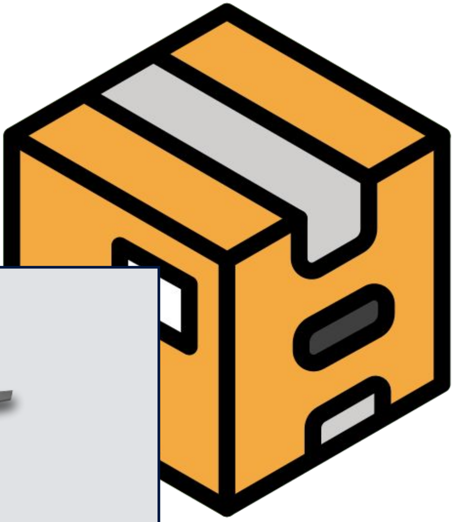

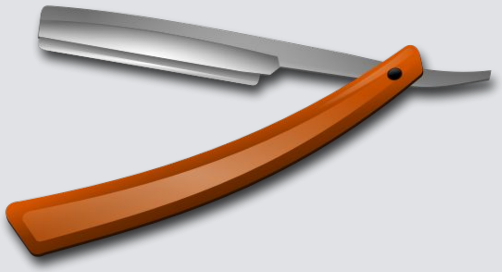

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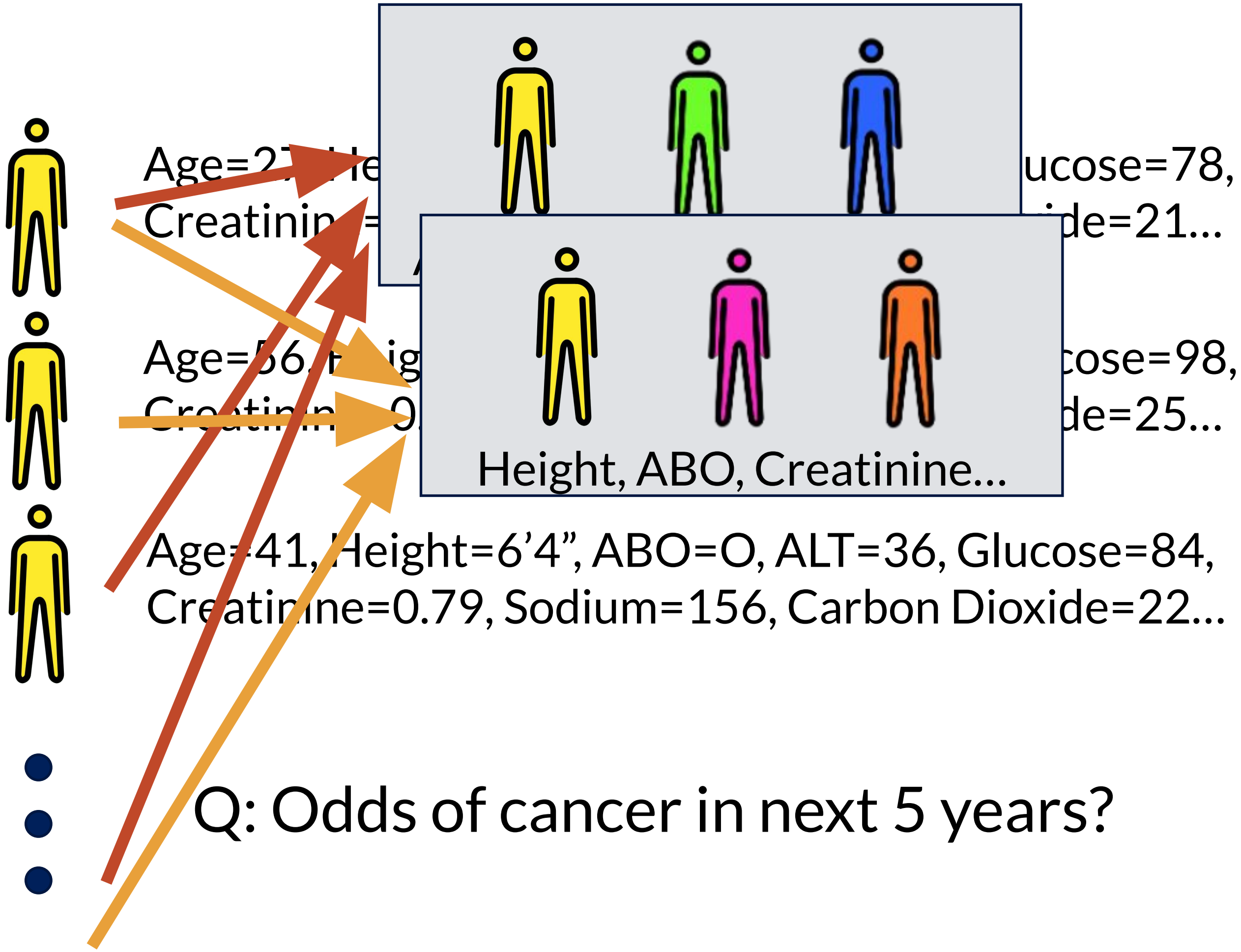

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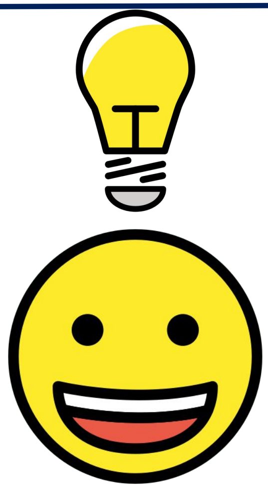

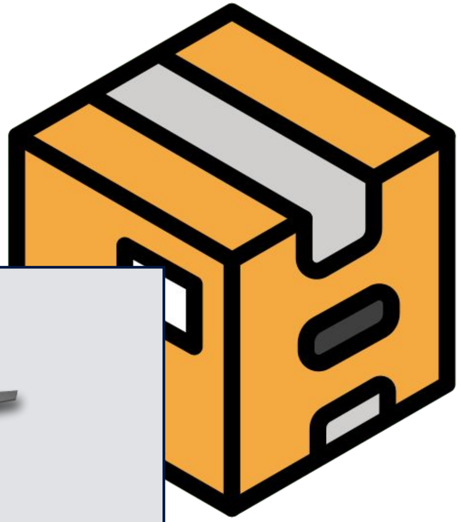

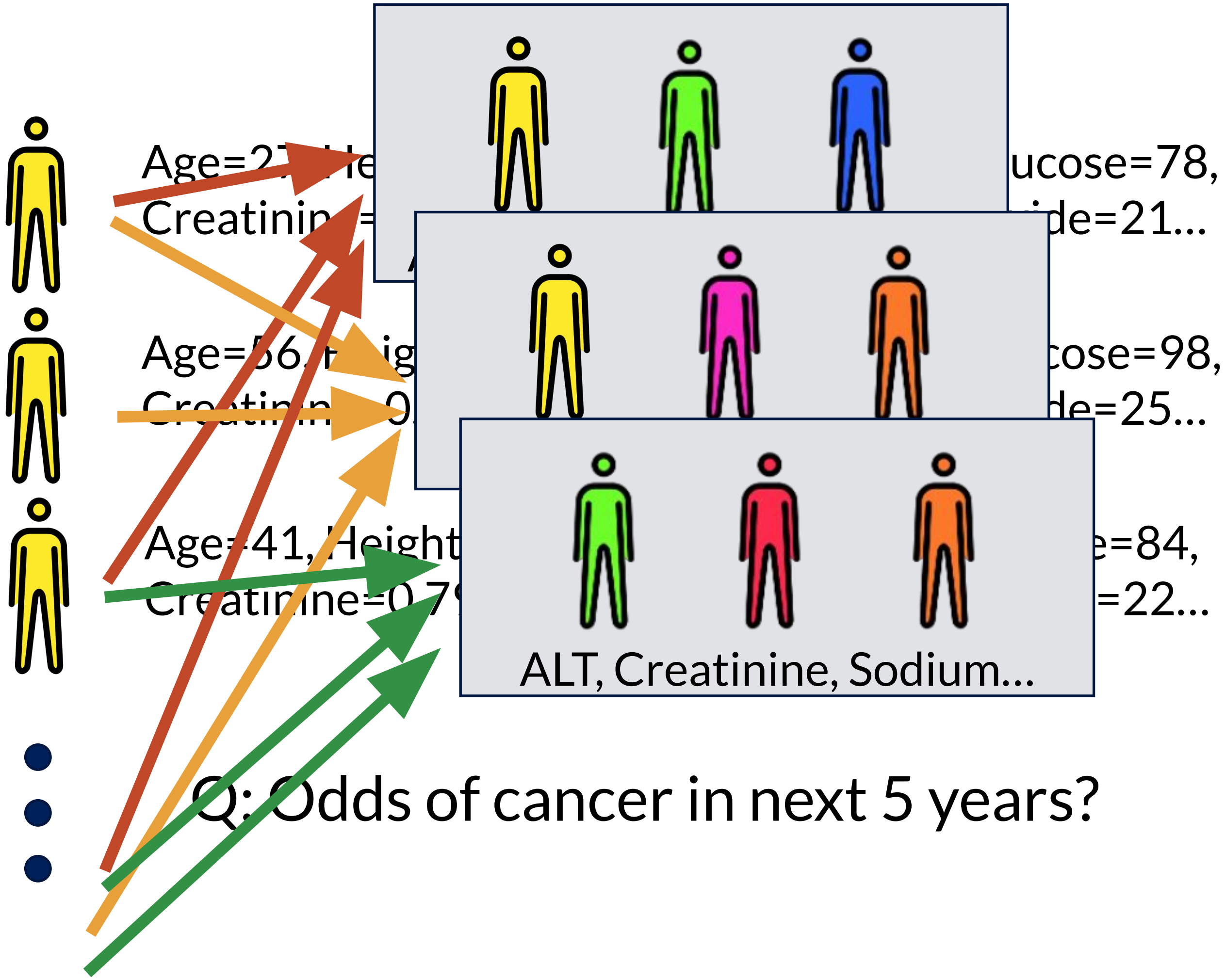

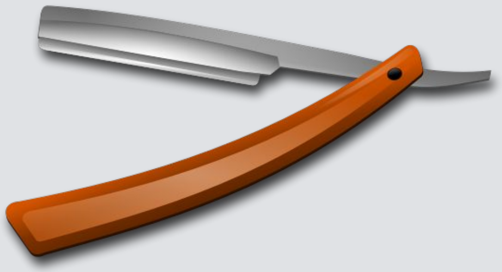

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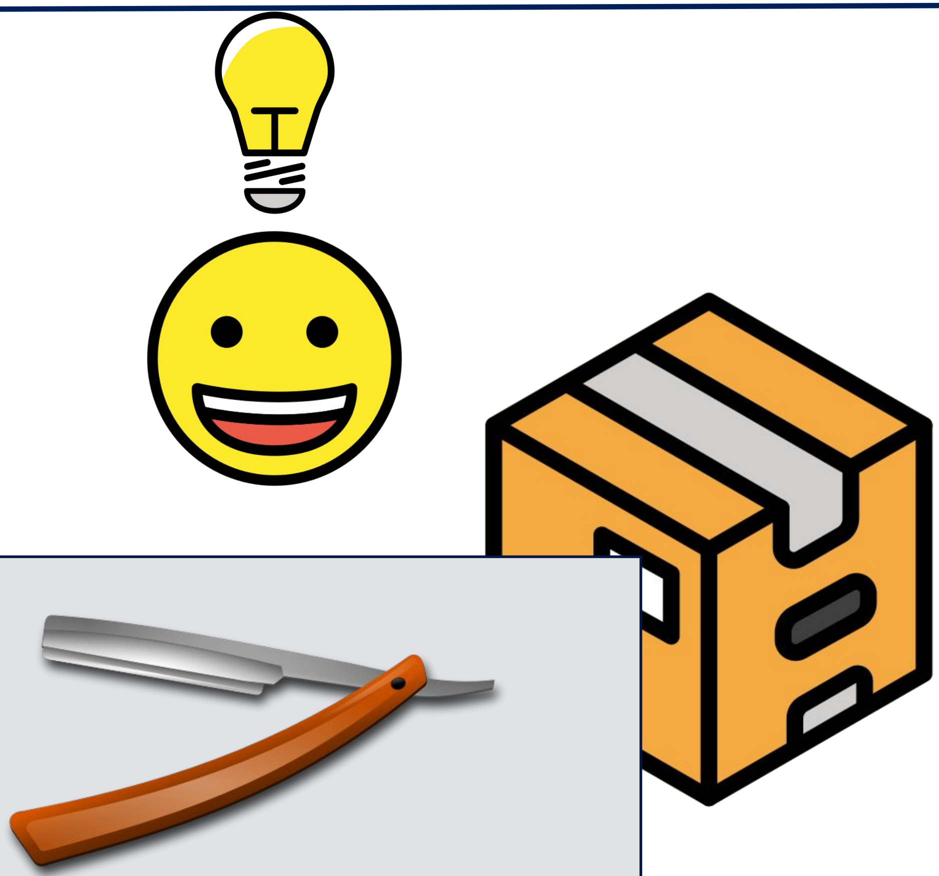

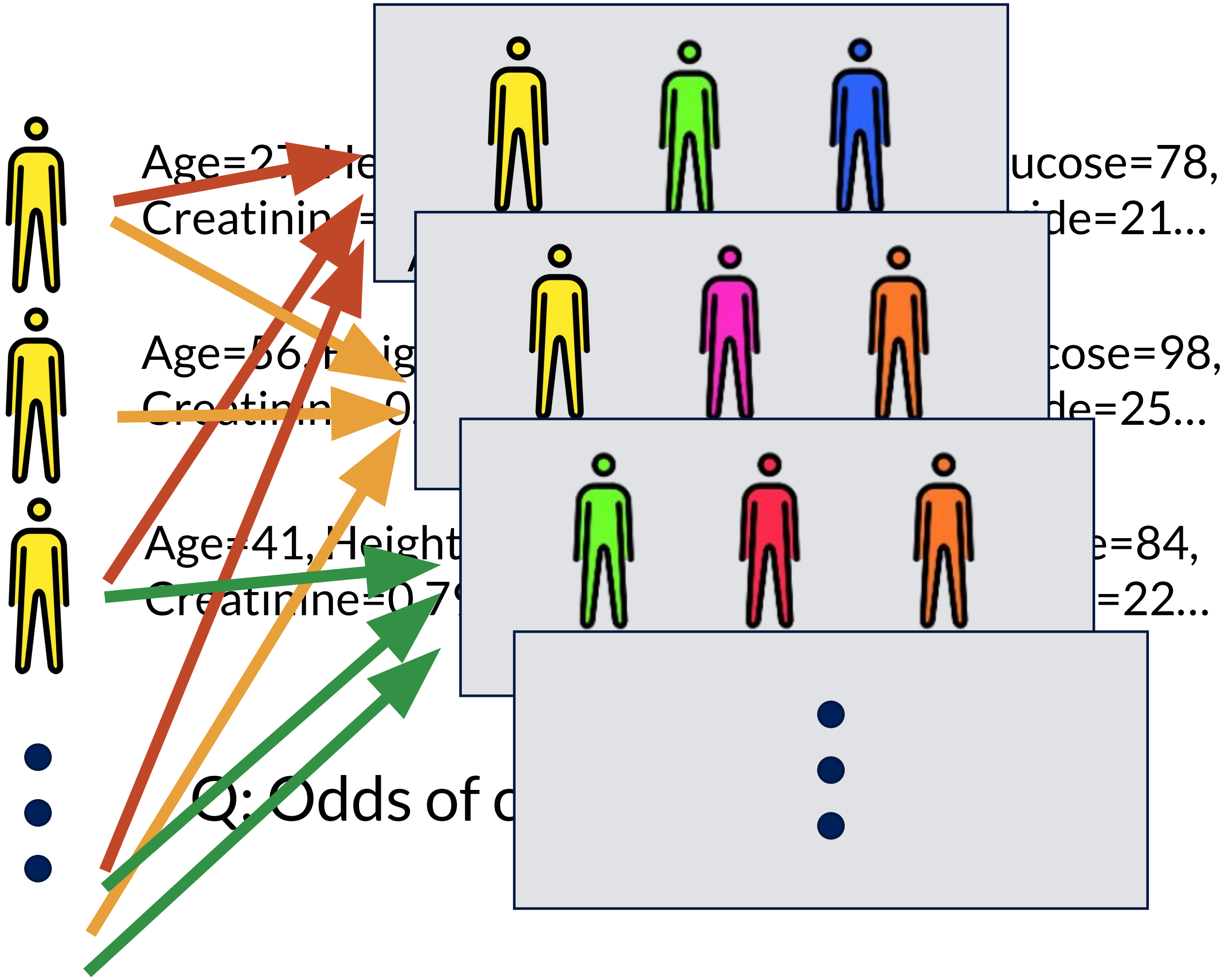

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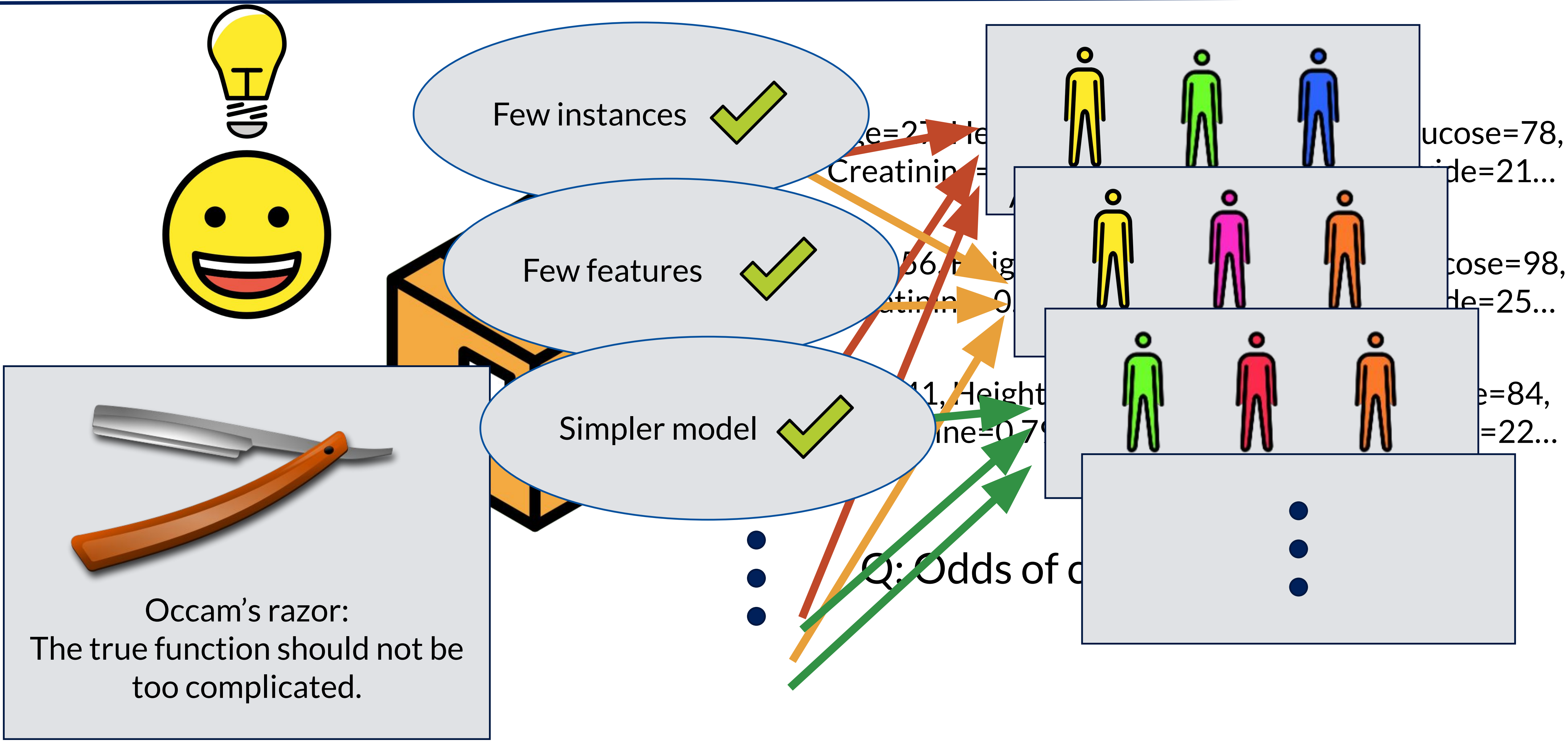
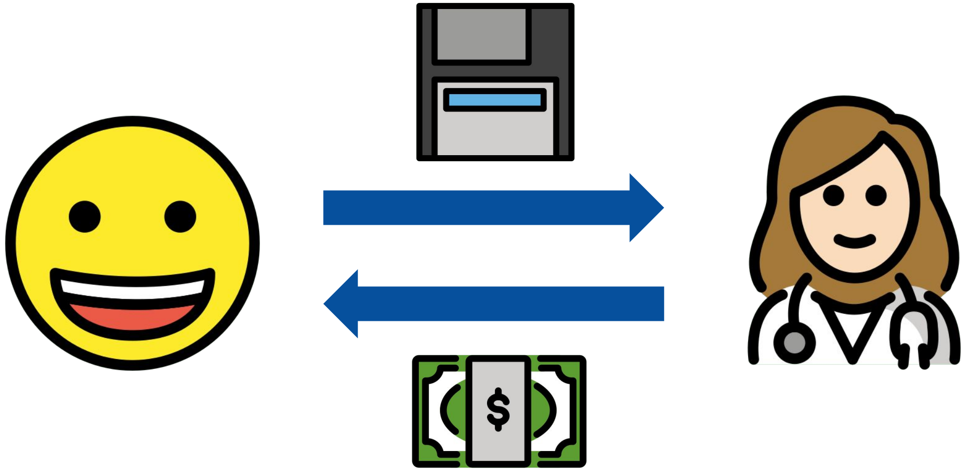
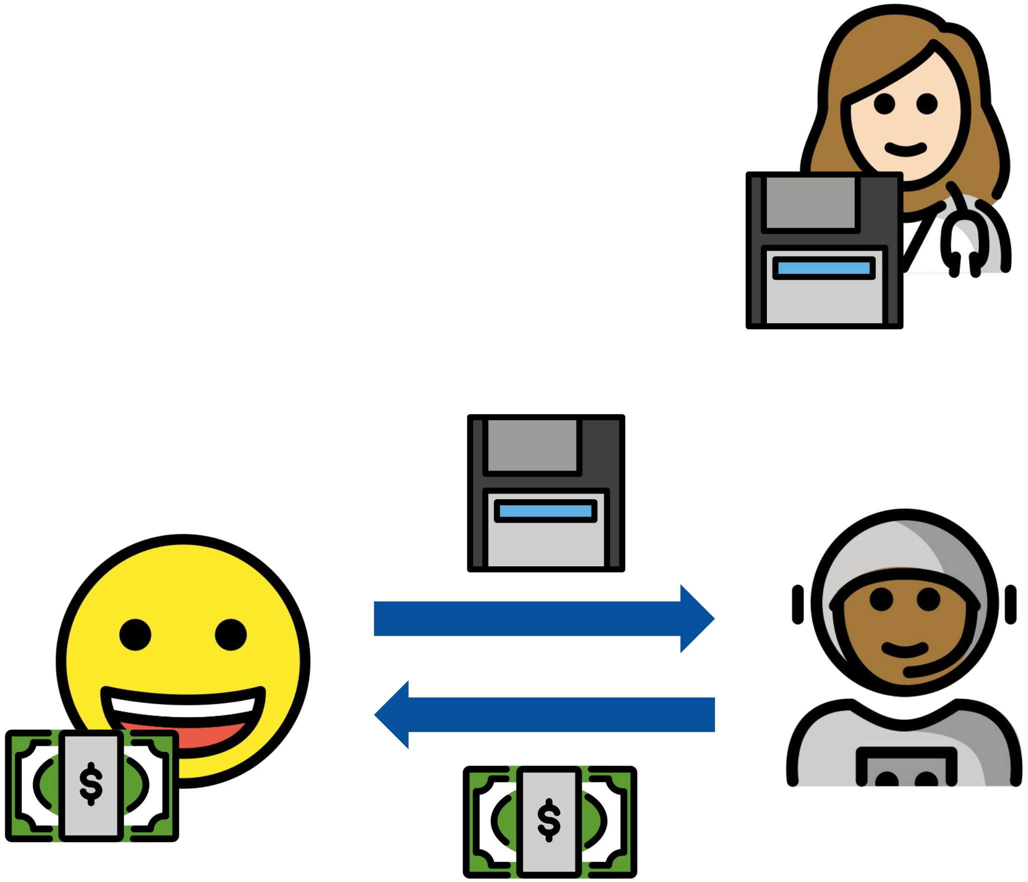
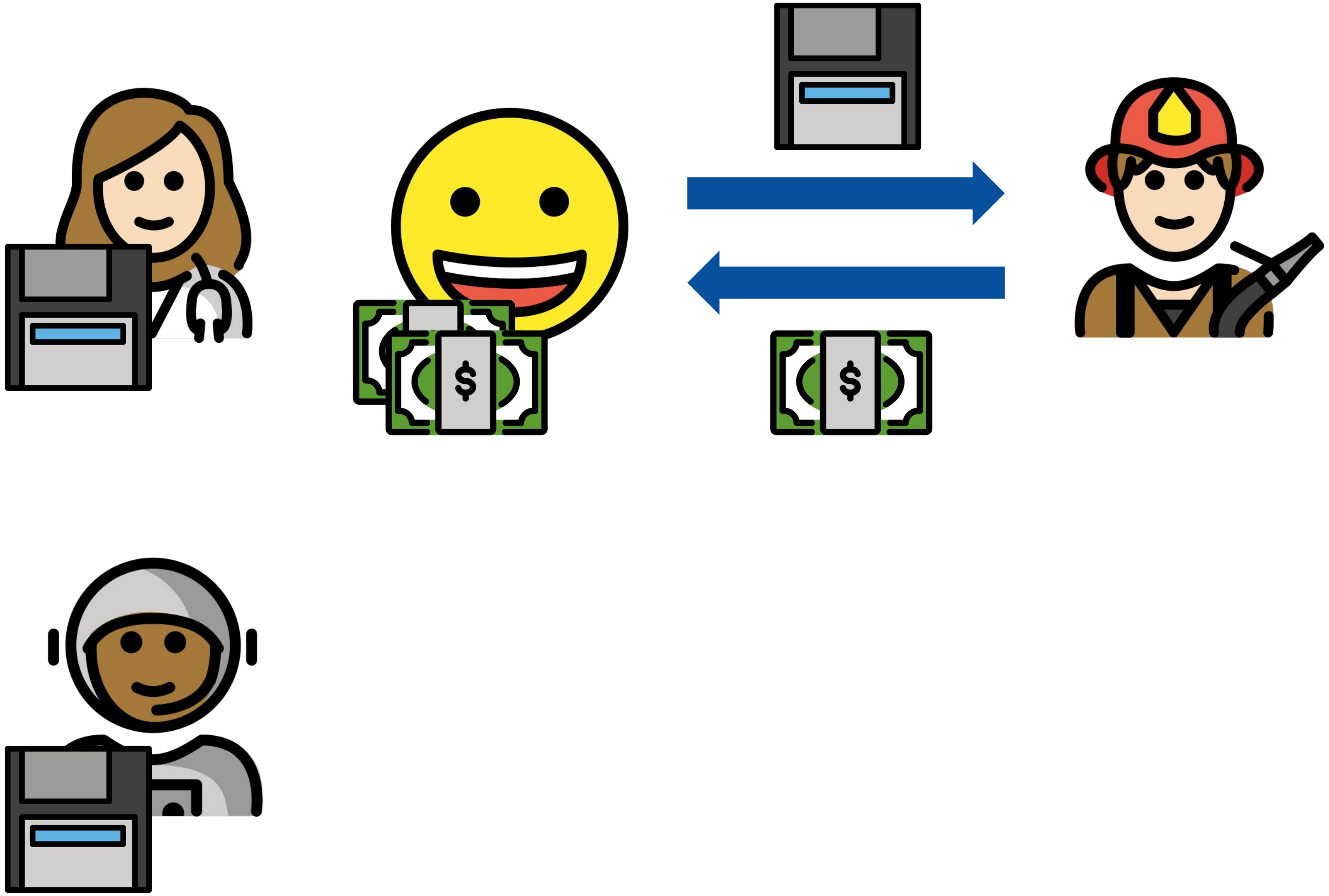
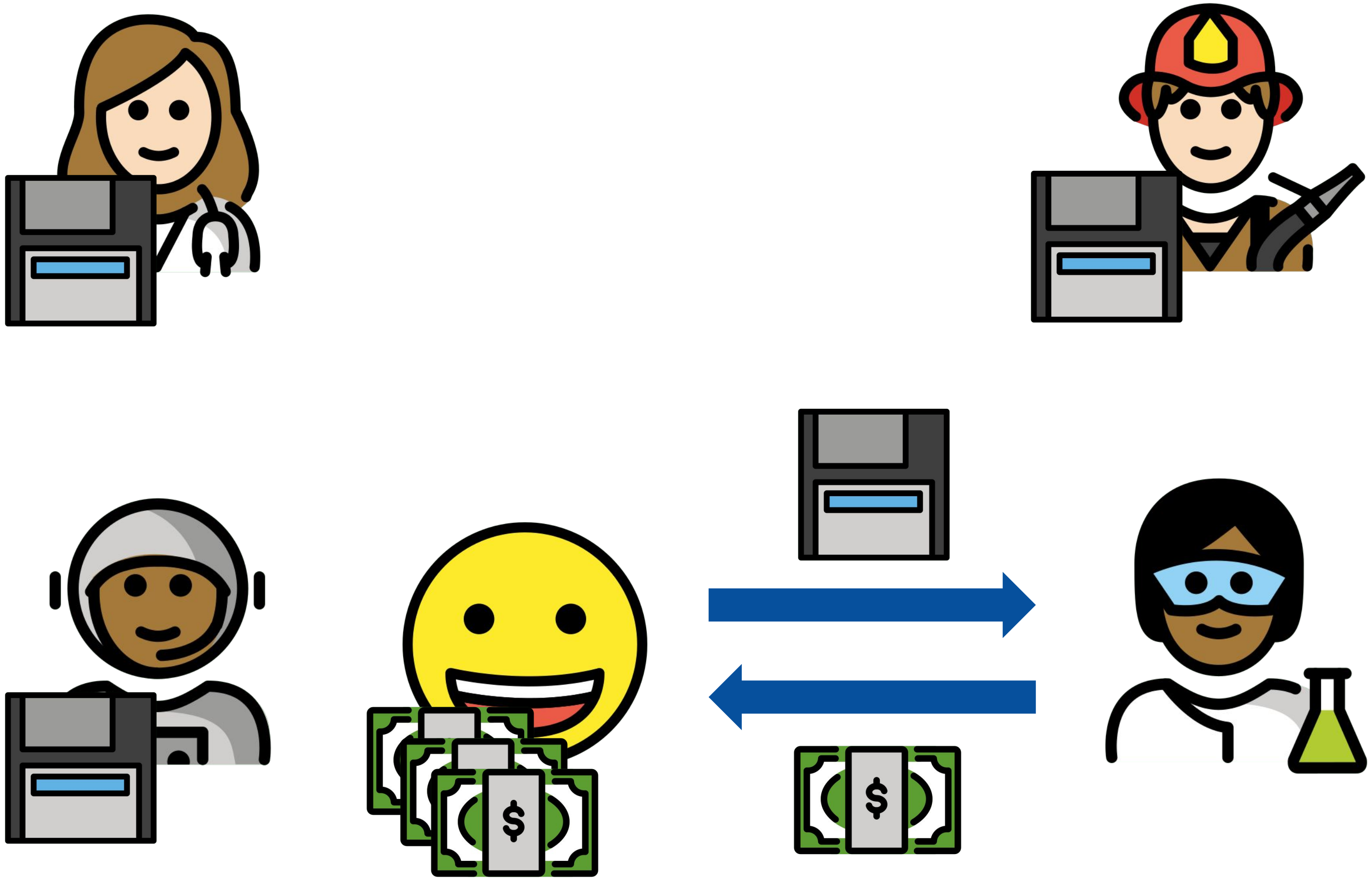






The State of Data Science





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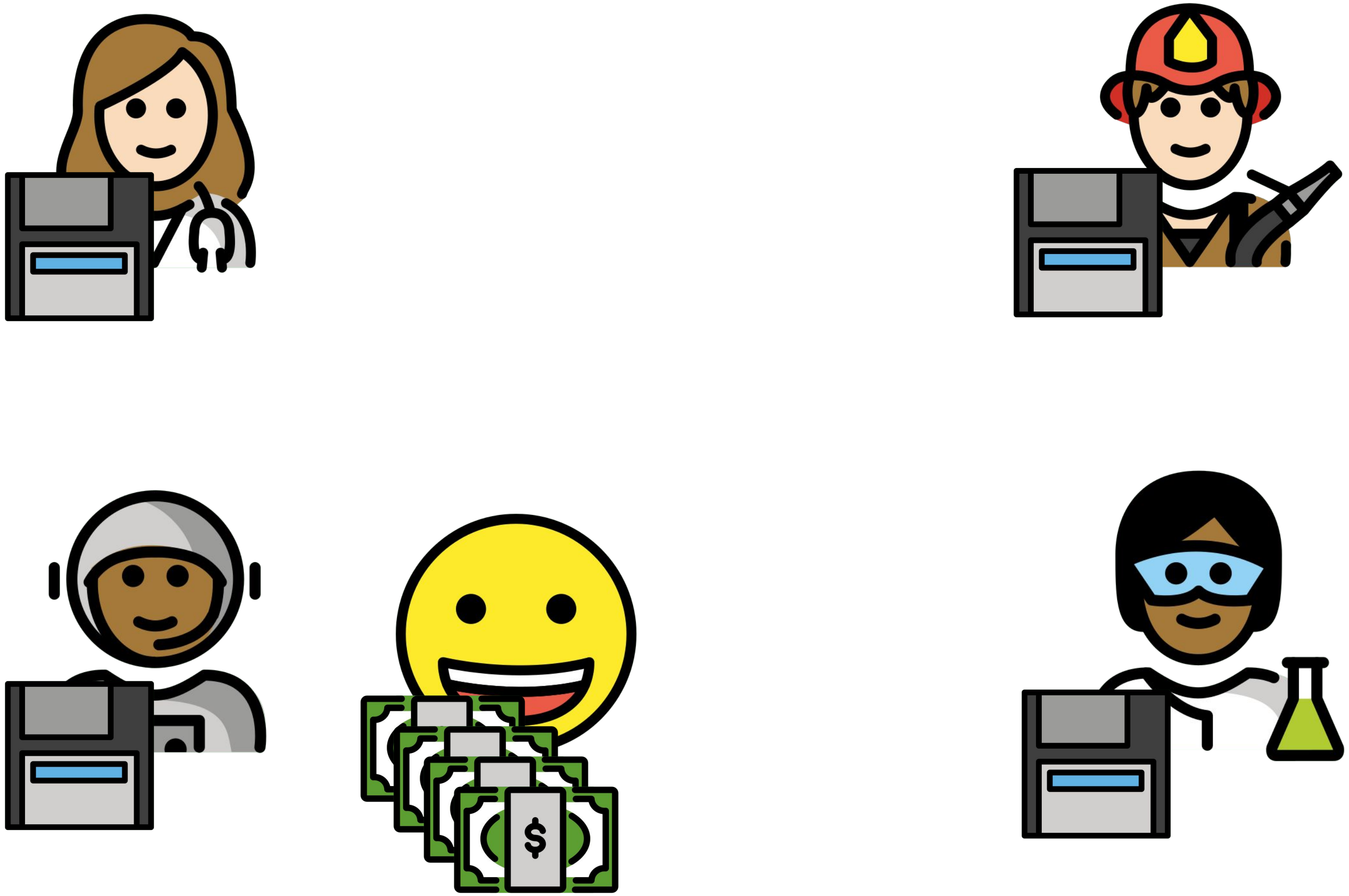

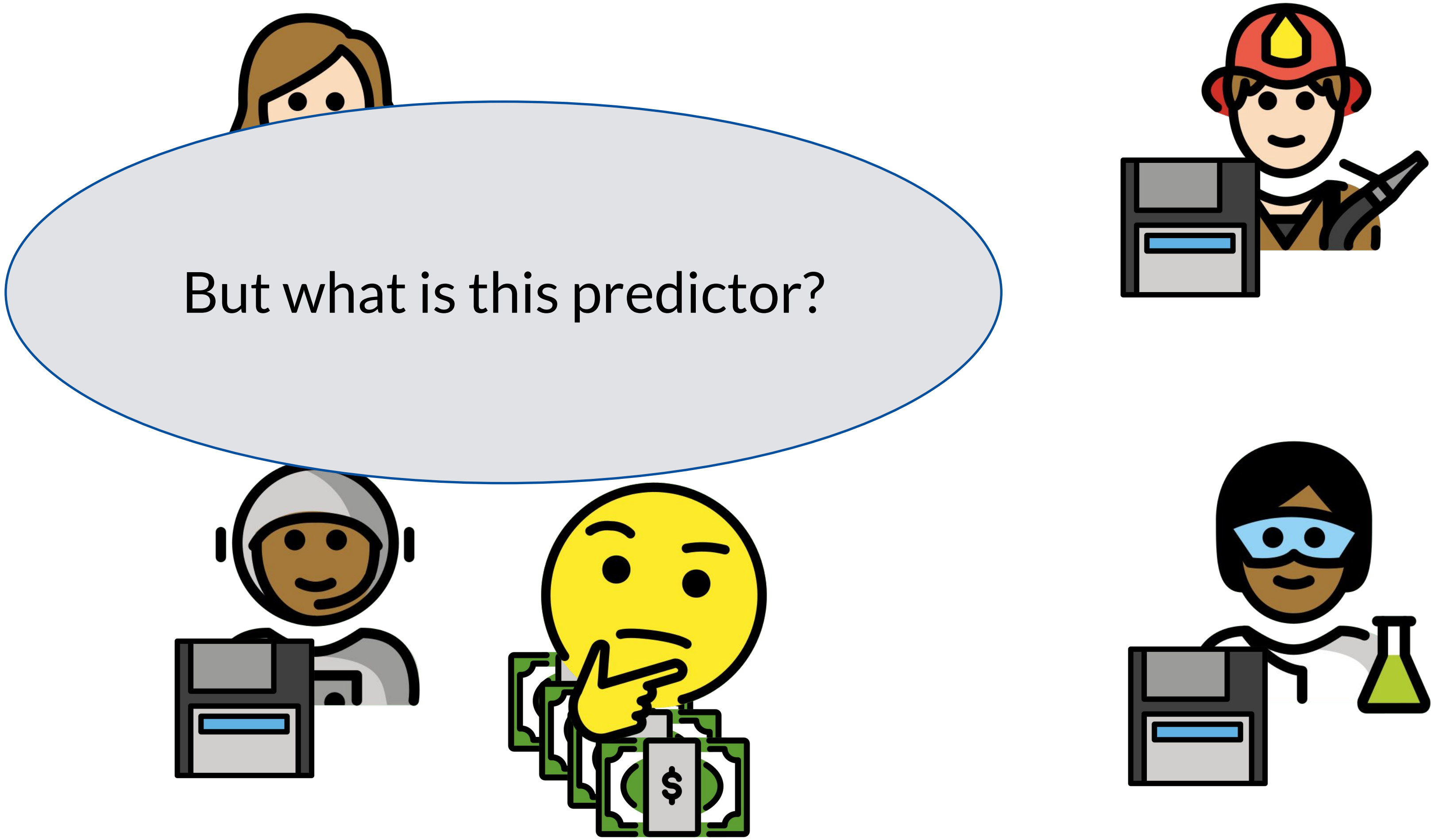
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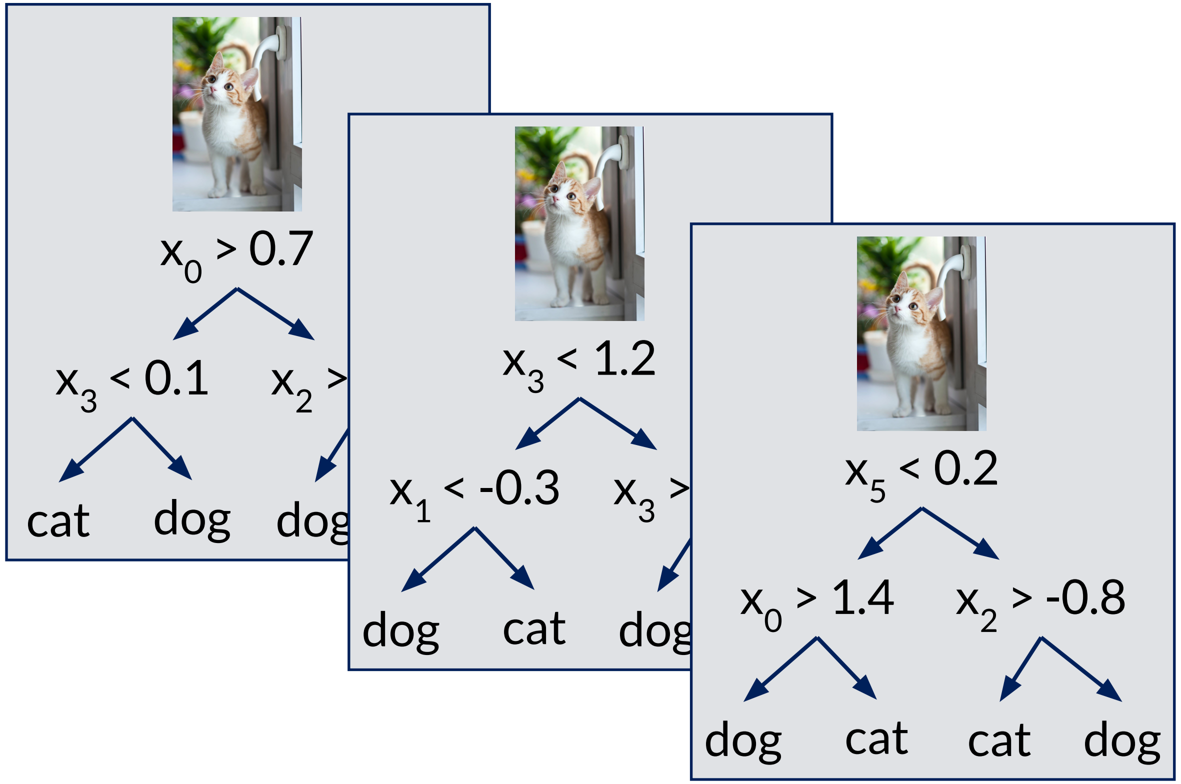
- Random forests [1]
  - Ensemble of decision trees
    - Trained on bootstrap samples
    - Branch on random feature subsets



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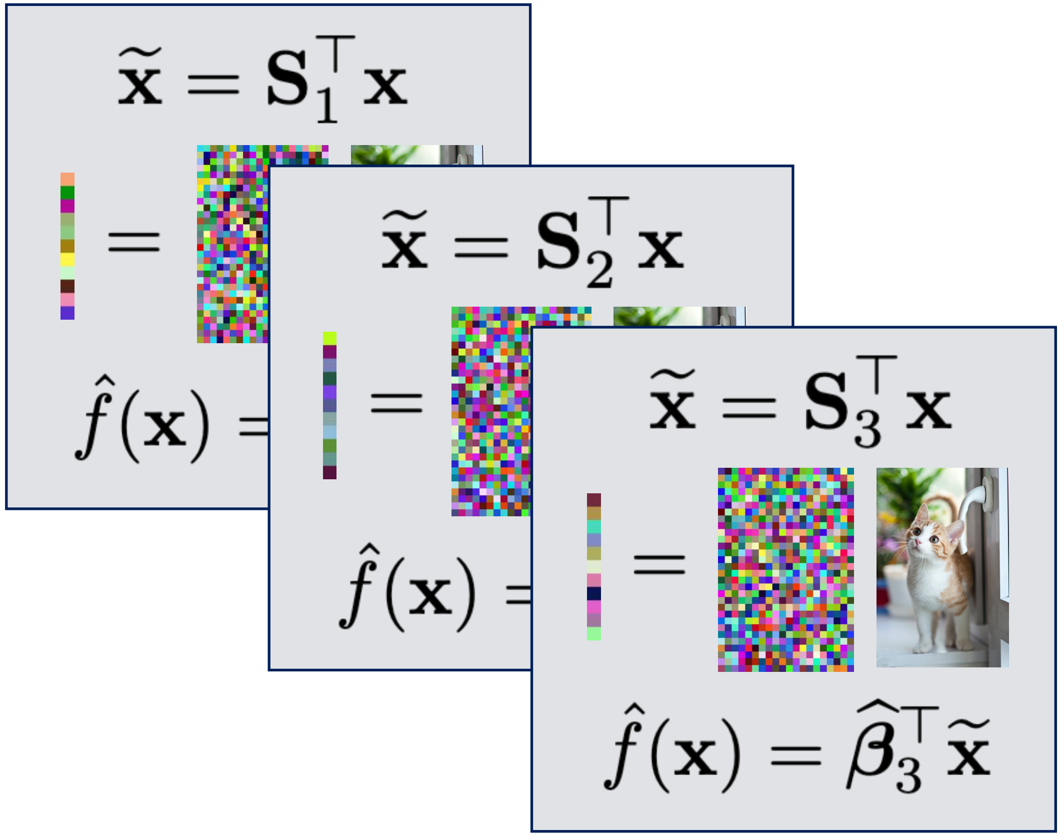
- Random projection ensembles [2]
    - Ensemble of sketched regressors
        - Randomly project observations
        - Randomly project features



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Existing Practice

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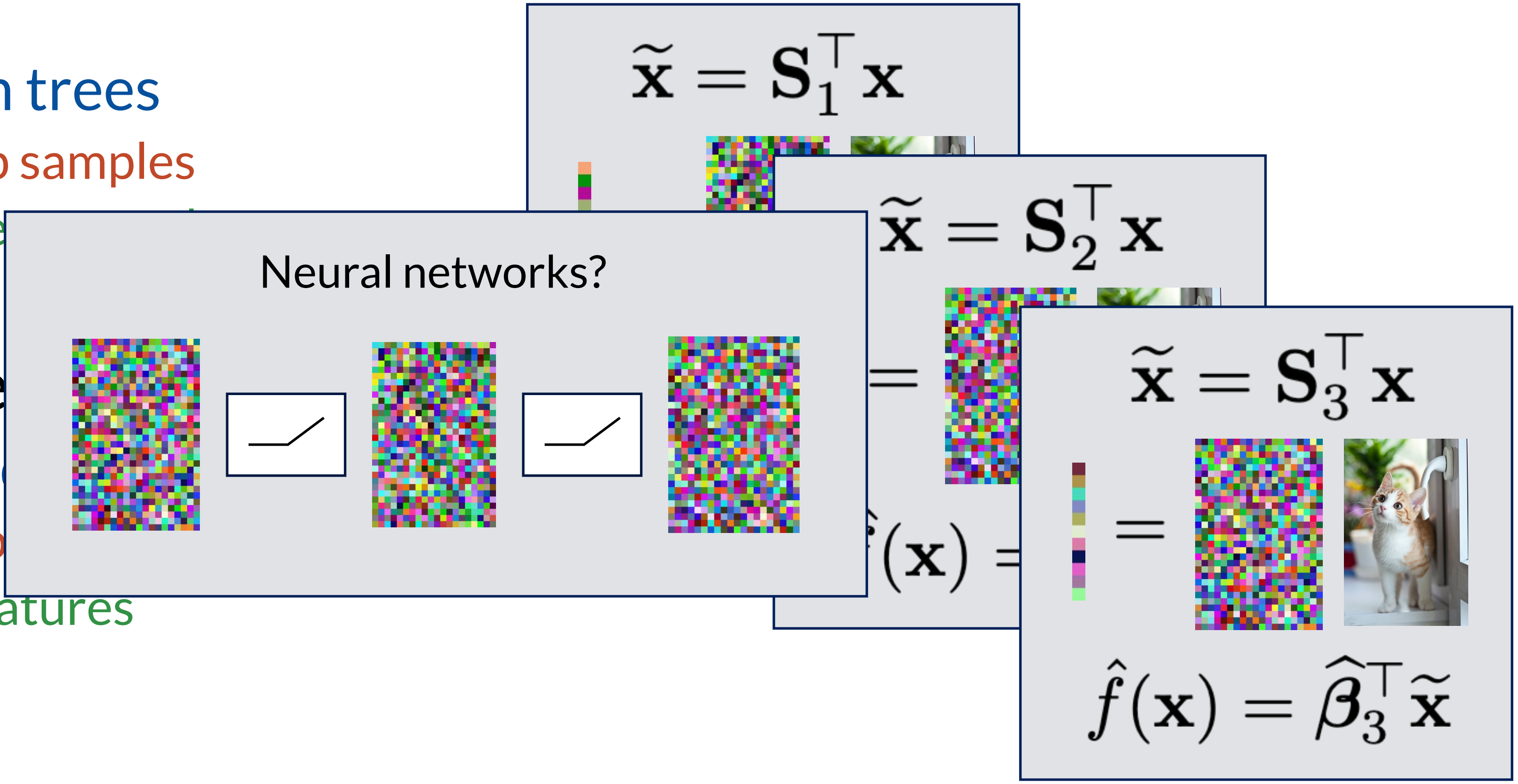

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Theoretical Questions

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  - Random forests are difficult to analyze
    - E.g., purely random forests [3] make analysis tractable
  - Simplified models [e.g., 2, 3] have proven upper bounds
    - Consistent estimation
    - Ensembles strictly better than individual models

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Spoiler:

Randomized least squares = ridge + noise

Randomized ensembles = ridge

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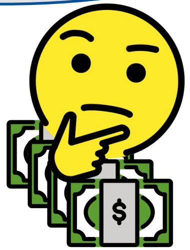

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Notation

- Ground truth function $f : \mathcal{X} \to \mathbb{R}$
- Ensemble of estimators $\hat{f}_1, \ldots, \hat{f}_K : \mathcal{X} \to \mathbb{R}$
- Squared error

$$R(\hat{f}_1, \ldots, \hat{f}_K) \triangleq \mathbb{E}\left[R(\hat{f}_1, \ldots, \hat{f}_K; x)\right]$$

$$R(\hat{f}_1, \ldots, \hat{f}_K; x) \triangleq \mathbb{E}\left[\left(\frac{1}{K}\sum_{k=1}^{K}\hat{f}_k(x) - f(x)\right)^2\right]$$

Early Work: Linear Regression Setting

- Training data: $\mathbf{X} = \left[\mathbf{x}_1 \ldots \mathbf{x}_n\right]^\top \in \mathbb{R}^{n \times p}$

$$\mathbf{y} = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$$

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- Data model: $\mathbf{x}_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$, $f(\mathbf{x}) = \boldsymbol{\beta}^{*\top}\mathbf{x}$, $\|\boldsymbol{\beta}^*\|_2 = 1$

$$y_i \sim \mathcal{N}\left(f(\mathbf{x}_i), \sigma^2\right)$$

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  $y_i \sim \mathcal{N}\left(f(\mathbf{x}_i), \sigma^2\right)$

- Estimators: $\hat{f}_k(\mathbf{x}) = \widehat{\boldsymbol{\beta}}_k^\top \mathbf{x}$

  $\widehat{\boldsymbol{\beta}}_k = \mathbf{S}_k \cdot \underset{\mathbf{b}}{\arg\min}\ \frac{1}{2} \left\| \mathbf{T}_k^\top \left(\mathbf{y} - \mathbf{X}\mathbf{S}_k \mathbf{b}\right) \right\|_2^2$

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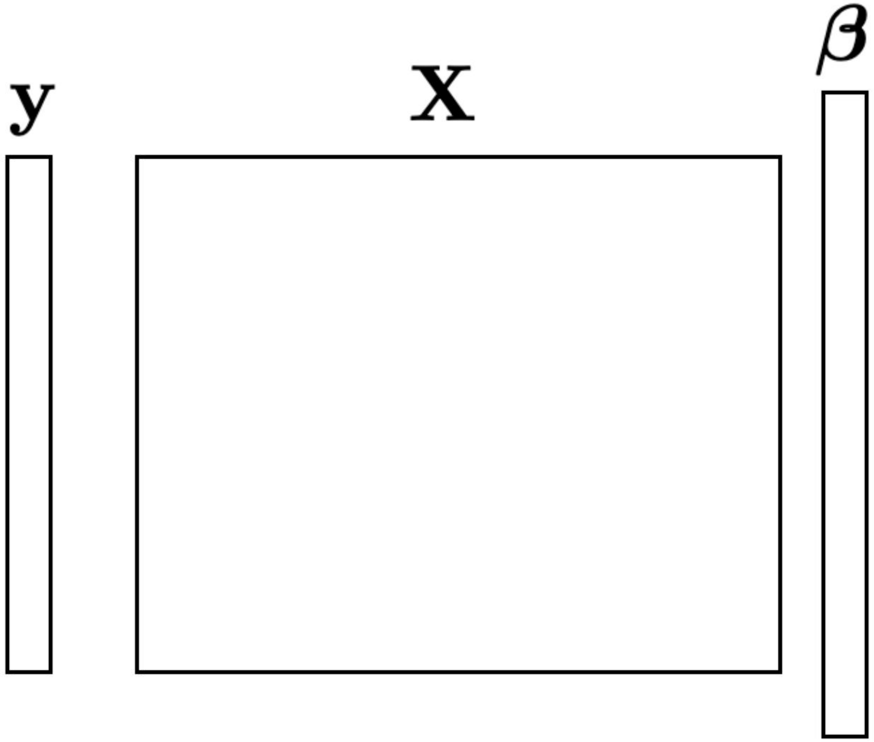
Random Subsampling

- Subsampling operators $\mathbf{S}_k \in \mathbb{R}^{p \times q}$, $\mathbf{T}_k \in \mathbb{R}^{n \times m}$, $m > q + 1$
  - Uniformly random columns of identity matrix



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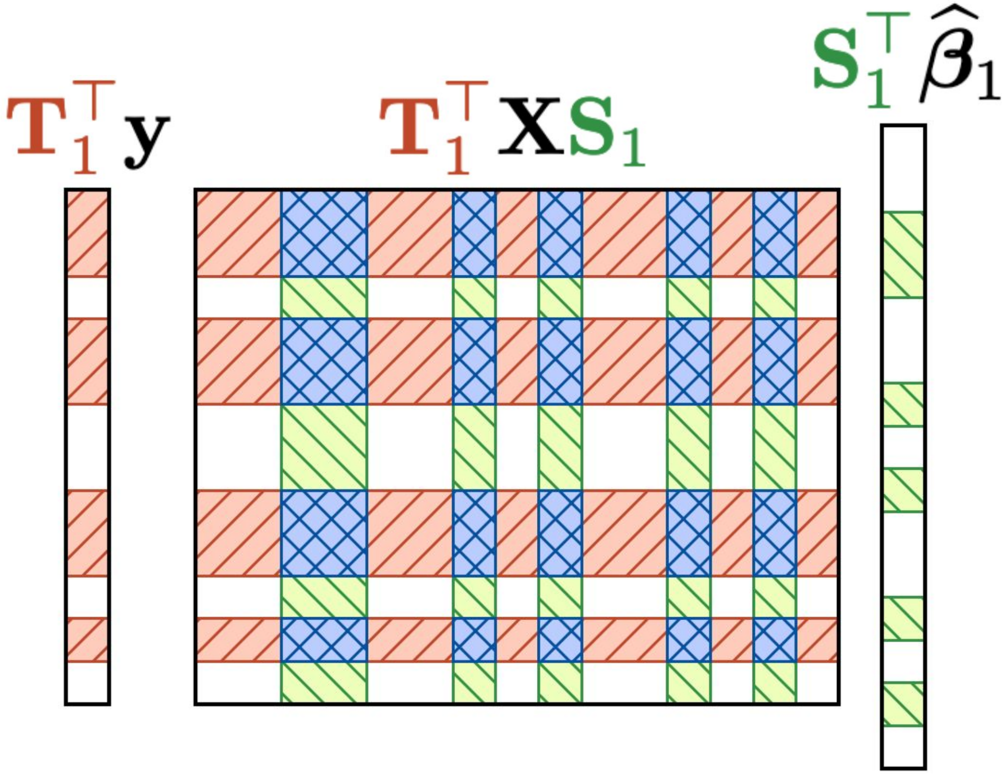

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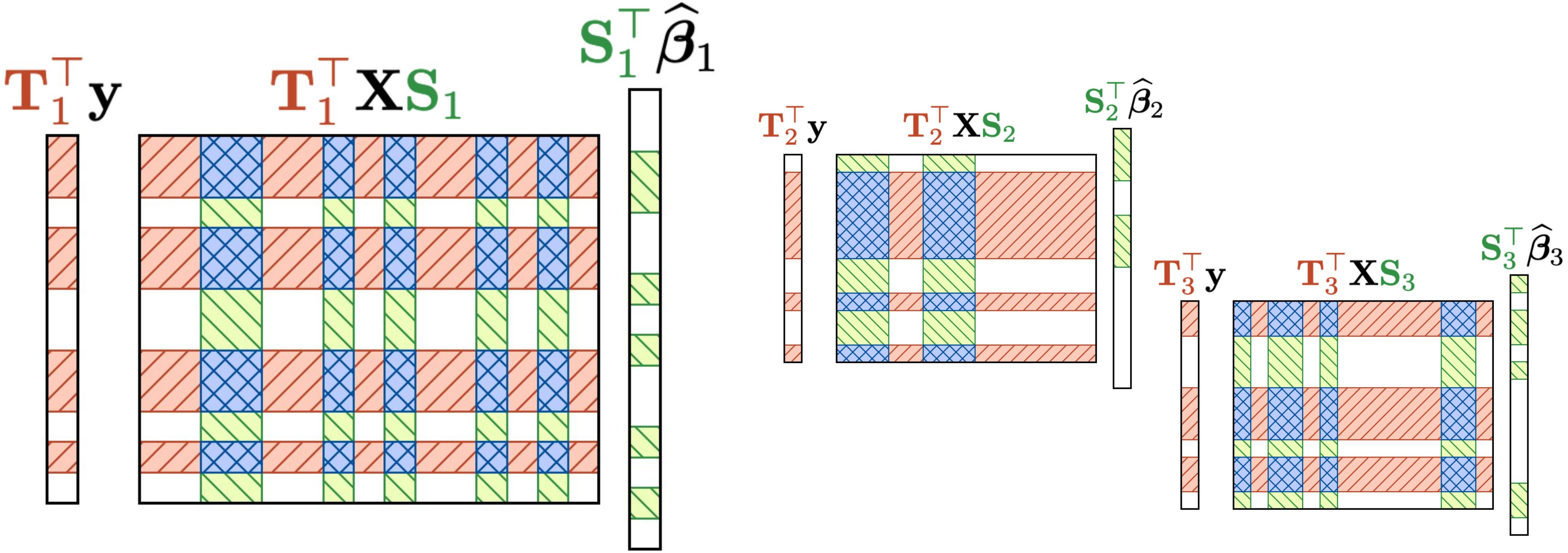

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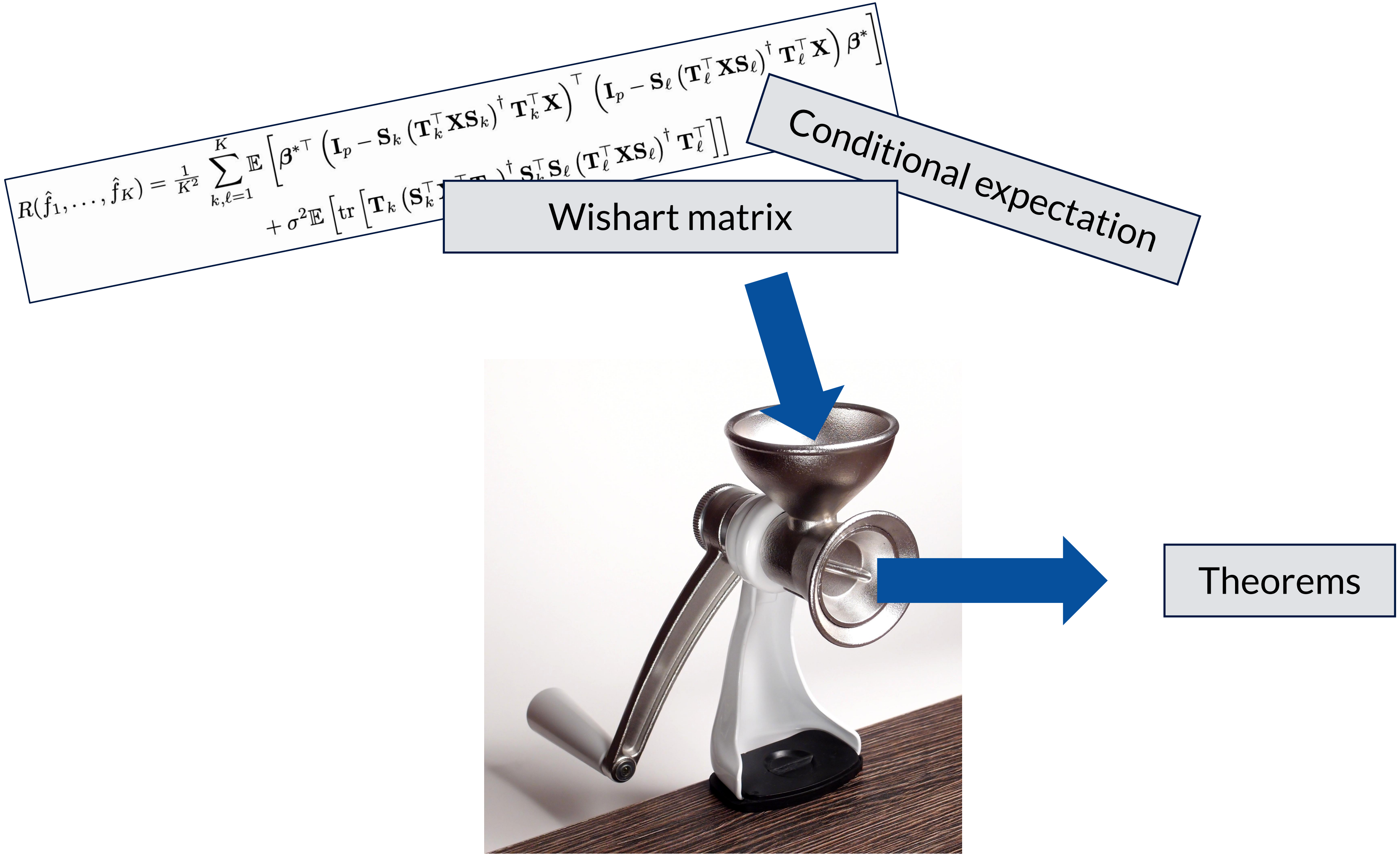
Turn the Crank...

$$R(\hat{f}_1, \ldots, \hat{f}_K) = \frac{1}{K^2} \sum_{k,\ell=1}^{K} \mathbb{E}\left[\boldsymbol{\beta}^{*\top} \left(\mathbf{I}_p - \mathbf{S}_k \left(\mathbf{T}_k^\top \mathbf{X} \mathbf{S}_k\right)^\dagger \mathbf{T}_k^\top \mathbf{X}\right)^\top \left(\mathbf{I}_p - \mathbf{S}_\ell \left(\mathbf{T}_\ell^\top \mathbf{X} \mathbf{S}_\ell\right)^\dagger \mathbf{T}_\ell^\top \mathbf{X}\right) \boldsymbol{\beta}^*\right]$$
$$+ \sigma^2 \mathbb{E}\left[\operatorname{tr}\left[\mathbf{T}_k \left(\mathbf{S}_k^\top \mathbf{X}^\top \mathbf{T}_k\right)^\dagger \mathbf{S}_k^\top \mathbf{S}_\ell \left(\mathbf{T}_\ell^\top \mathbf{X} \mathbf{S}_\ell\right)^\dagger \mathbf{T}_\ell^\top\right]\right]$$

Conditional expectation

Wishart matrix

Turn the Crank...



Error under Proportional Asymptotics

- Exact error expression for finite ensembles

Theorem 1. *In the limit as* $(n, p, m, q) \to \infty$ *with* $p/n \to \gamma$, $m/n \to \eta$, $q/p \to \alpha$, *if* $\eta > \alpha\gamma$,

$$R(\hat{f}_1, \ldots, \hat{f}_K) = \frac{K-1}{K}\left(\frac{(1-\alpha)^2 + \sigma^2\alpha^2\gamma}{1-\alpha^2\gamma}\right) + \frac{1}{K}\left(\frac{\eta(1-\alpha) + \sigma^2\alpha\gamma}{\eta - \alpha\gamma}\right).$$

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Error under Proportional Asymptotics

- Exact error expression for finite ensembles

Theorem 1. *In the limit as* $(n, p, m, q) \to \infty$ *with* $p/n \to \gamma$, $m/n \to \eta$, $q/p \to \alpha$, *if* $\eta > \alpha\gamma$,

$$R(\hat{f}_1, \ldots, \hat{f}_K) = \frac{K-1}{K}\left(\frac{(1-\alpha)^2 + \sigma^2\alpha^2\gamma}{1-\alpha^2\gamma}\right) + \frac{1}{K}\left(\frac{\eta(1-\alpha) + \sigma^2\alpha\gamma}{\eta - \alpha\gamma}\right).$$

- Infinite ensemble error depends only on feature subsampling

$$R_{\text{ens}}^{\infty}(\alpha) \triangleq \lim_{K\to\infty} R(\hat{f}_1, \ldots, \hat{f}_K) = \frac{(1-\alpha)^2 + \sigma^2\alpha^2\gamma}{1-\alpha^2\gamma}$$

[4] **DL**, H Javadi, RG Baraniuk. "The implicit regularization of ordinary least squares ensembles." AISTATS, 2020.

- Ridge regression: $\hat{f}_\lambda(\mathbf{x}) = \widehat{\boldsymbol{\beta}}_\lambda^\top \mathbf{x},\ \widehat{\boldsymbol{\beta}}_\lambda = \arg\min_{\mathbf{b}} \frac{1}{2n}\|\mathbf{y} - \mathbf{X}\mathbf{b}\|_2^2 + \frac{\lambda}{2}\|\mathbf{b}\|_2^2$

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- Tuning feature subsampling is optimal

Theorem 2. *Under the conditions of Theorem 1 and if* $\boldsymbol{\beta}^* \sim \mathcal{N}(\mathbf{0}, p^{-1}\mathbf{I})$,

$$\inf_{\alpha < \gamma^{-1}} R_{\text{ens}}^{\infty}(\alpha) = \inf_{\lambda > 0} R(\hat{f}_\lambda).$$

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Spoiler:

Randomized least squares = ridge + noise

Randomized ensembles = ridge

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- However, proof sheds little insight

$$\inf_{\alpha<\gamma^{-1}} R_{\text{ens}}^{\infty}(\alpha) = \frac{1}{2}\left(\frac{\gamma-1}{\gamma} - \sigma^2 + \sqrt{\left(\sigma^2 - \frac{\gamma-1}{\gamma}\right)^2 + 4\sigma^2}\right) = \inf_{\lambda>0} R(\hat{f}_\lambda)$$

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Interpretation of Results

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But what is this predictor?

- Infinite ensemble with only feature subsampling:

$$\hat{f}_{\text{ens}}^{\infty}(\mathbf{x}) = \lim_{K\to\infty} \frac{1}{K} \sum_{k=1}^{K} \widehat{\boldsymbol{\beta}}_k^\top \mathbf{x} = \mathbf{y}^\top \mathbf{X} \left(\lim_{K\to\infty} \frac{1}{K} \sum_{k=1}^{K} \mathbf{S}_k \left(\mathbf{S}_k^\top \mathbf{X}^\top \mathbf{X} \mathbf{S}_k \right)^{-1} \mathbf{S}_k^\top \right) \mathbf{x}$$

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- Determinantal Point Process pseudoinverse [7]:

Theorem (Mutny et al. 2020). *If* $\mathbf{M} \succ \mathbf{0}$ *and* $\mathbf{S} \sim \mathcal{DPP}(\frac{1}{\lambda}\mathbf{M})$,

$$\mathbb{E}\left[\mathbf{S}\left(\mathbf{S}^\top \mathbf{M} \mathbf{S}\right)^{-1} \mathbf{S}^\top\right] = (\mathbf{M} + \lambda \mathbf{I})^{-1},$$

where λ *is the solution to* $\mathbb{E}\left[\frac{q_{\mathrm{S}}}{p}\right] = \mathrm{tr}(\mathbf{M}(\mathbf{M}+\lambda\mathbf{I})^{-1})$.

[5] M Mutny, M Dereziński, A Krause. "Convergence analysis of block coordinate algorithms with determinantal sampling." AISTATS, 2020.

Moving to Sketched Ensembles

- Problem: strict isotropic assumption on data
  - Solution: let subsampling operators be isotropic sketches instead

$$[\mathbf{S}]_{ij} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \tfrac{1}{q}), \; [\mathbf{T}]_{ij} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \frac{1}{m})$$

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Asymptotic Equivalences

- Asymptotic equivalences [6]:

Definition. *Two sequences of matrices* $\mathbf{A}_n, \mathbf{B}_n$ *are* ***asymptotically equivalent****, written* $\mathbf{A}_n \simeq \mathbf{B}_n$*, if for every sequence* $\boldsymbol{\Theta}_n$ *having uniformly bounded trace norm, almost surely*

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- Admits a calculus:
  - Addition $\mathbf{A}_n \simeq \mathbf{B}_n,\ \mathbf{C}_n \simeq \mathbf{D}_n \implies \mathbf{A}_n + \mathbf{C}_n \simeq \mathbf{B}_n + \mathbf{D}_n$
  - Multiplication $\mathbf{A}_n \simeq \mathbf{B}_n \implies \mathbf{C}_n\mathbf{A}_n\mathbf{D}_n \simeq \mathbf{C}_n\mathbf{B}_n\mathbf{D}_n$
  - Elements $\mathbf{A}_n \simeq \mathbf{B}_n \implies [\mathbf{A}_n]_{ij} - [\mathbf{B}_n]_{ij} \xrightarrow{\text{a.s.}} 0$
  - Differentiation [7] $f(\mathbf{A}_n; z) \simeq g(\mathbf{B}_n; z) \implies f'(\mathbf{A}_n; z) \simeq g'(\mathbf{B}_n; z)$

[6] E Dobriban, Y Sheng. "Distributed linear regression by averaging." Annals of Statistics, 2021.
[7] E Dobriban, Y Sheng. "WONDER: Weighted one-shot distributed ridge regression in high dimensions." JMLR, 2020.

An Asymptotic Equivalence of Resolvents

Theorem (Rubio & Mestre 2011). *Let* $\mathbf{Z} \in \mathbb{C}^{n\times p}$ *be a random matrix consisting of i.i.d. random variables that have mean 0, variance 1, and finite absolute moment of order* $8+\delta$ *for some* $\delta > 0$. *Let* $\boldsymbol{\Sigma} \in \mathbb{C}^{p\times p}$ *be a positive semidefinite matrix with operator norm uniformly bounded in* p, *and let* $\mathbf{X} = \mathbf{Z}\boldsymbol{\Sigma}^{1/2}$. *Then, for* $z \in \mathbb{C}^+$, *as* $n, p \to \infty$ *such that* $0 < \liminf \frac{p}{n} \leq \limsup \frac{p}{n} < \infty$, *we have*

$$\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} - z\mathbf{I}_p\right)^{-1} \simeq \left(c(z)\boldsymbol{\Sigma} - z\mathbf{I}_p\right)^{-1}, \tag{32}$$

where $c(z)$ *is the unique solution in* $\mathbb{C}^-$ *to the fixed point equation*

$$\frac{1}{c(z)} - 1 = \tfrac{1}{n}\mathrm{tr}\left[\boldsymbol{\Sigma}\left(c(z)\boldsymbol{\Sigma} - z\mathbf{I}_p\right)^{-1}\right]. \tag{33}$$

Furthermore, $\frac{1}{p}\mathrm{tr}\left[\boldsymbol{\Sigma}(c(z)\boldsymbol{\Sigma} - z\mathbf{I}_p)^{-1}\right]$ *is a Stieltjes transform of a certain positive measure on* $\mathbb{R}_{\geq 0}$ *with total mass* $\frac{1}{p}\mathrm{tr}[\boldsymbol{\Sigma}]$.

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What about real arguments?

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Analytic continuation →

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Limits of negative regularization

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Reparameterization

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Then, for each $z \in \mathbb{R}$ *satisfying* $z < \liminf z_0$*, as* $n, p \to \infty$ *such that* $0 < \liminf \frac{p}{n} \leq \limsup \frac{p}{n} < \infty$*, we have*

$$z\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} - z\mathbf{I}_p\right)^{-1} \simeq \zeta\left(\mathbf{\Sigma} - \zeta\mathbf{I}_p\right)^{-1}, \tag{35}$$

where $\zeta \in \mathbb{R}$ *is the unique solution in* $(-\infty$

Explicit form of implicit value

$$z = \zeta\left(1 - \tfrac{1}{n}\mathrm{tr}\left[\mathbf{\Sigma}\left(\mathbf{\Sigma} - \zeta\mathbf{I}_p\right)^{-1}\right]\right). \tag{36}$$

Furthermore, as $n, p \to \infty$, $|\zeta + \frac{1}{v(z)}| \xrightarrow{\text{a.s.}} 0$, *where* $v(z)$ *is the companion Stieltjes transform of the spectrum of* $\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}$ *given by*

$$v(z) = \tfrac{1}{n}\mathrm{tr}\left[\left(\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} - z\mathbf{I}_n\right)^{-1}\right]$$

and $|z_0 - \lambda^+_{\min}(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X})| \xrightarrow{\text{a.s.}} 0$.

Obtaining a Sketching Equivalence

$$z\left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} - z\mathbf{I}_p\right)^{-1} \simeq \zeta\left(\mathbf{\Sigma} - \zeta\mathbf{I}_p\right)^{-1}$$

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$$\mathbf{I}_p - \lambda\left(\mathbf{A}^{1/2}\mathbf{S}\mathbf{S}^{\mathsf{H}}\mathbf{A}^{1/2} + \lambda\mathbf{I}_p\right)^{-1} \simeq \mathbf{I}_p - \mu\left(\mathbf{A} + \mu\mathbf{I}_p\right)^{-1}$$

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Uniform convergence

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$$\hat{f}_{\mathrm{ens}}(\mathbf{x}) = \mathbf{y}^{\top}\mathbf{X}\left(\frac{1}{K}\sum_{k=1}^{K}\mathbf{S}_k\left(\mathbf{S}_k^{\top}\mathbf{X}^{\top}\mathbf{X}\mathbf{S}_k\right)^{-1}\mathbf{S}_k^{\top}\right)\mathbf{x}$$

First-order Sketching Equivalence

Theorem 4. *For each* $\lambda > \limsup \lambda_0$, *as* $q, p \to \infty$,

$$\mathbf{S}\left(\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_q\right)^{-1}\mathbf{S}^{\mathsf{H}} \simeq \left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1},$$

where μ *is the unique solution in* (μ_0, ∞) *to the fixed point equation*

$$\lambda = \mu\left(1 - \tfrac{1}{q}\operatorname{tr}\left[\mathbf{A}\left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1}\right]\right).$$

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$$\mathbb{E}\left[\frac{q_{\mathcal{S}}}{p}\right] = \mathrm{tr}(\mathbf{M}\left(\mathbf{M} + \mu\mathbf{I}\right)^{-1})$$

Same as DPP when $\lambda = 0$

- That is, sketching + ridge = another ridge without sketching.

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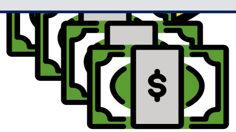
- That is, sketching + ketching.

Spoiler:

Randomized least squares = ridge + noise

Randomized ensembles = ridge



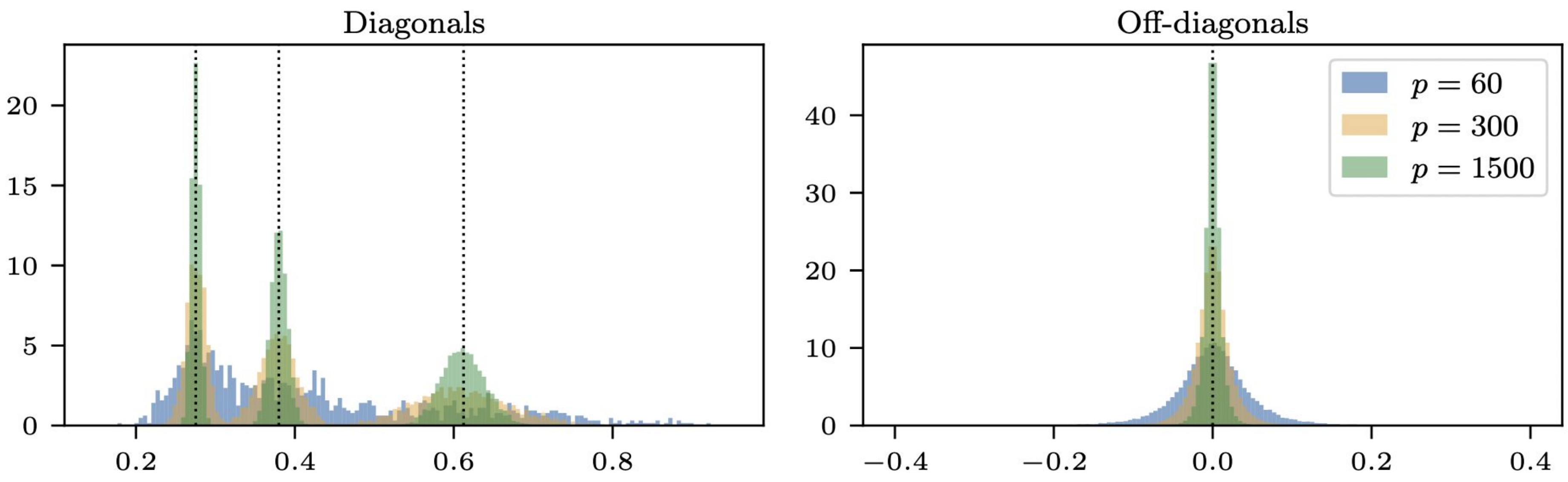
Element-wise Convergence

$\mathbf{A} = \mathrm{diag}(0\ldots,1\ldots,2\ldots)$

$\alpha = 0.8$

$\lambda = 1$

$\mu \approx 1.63$



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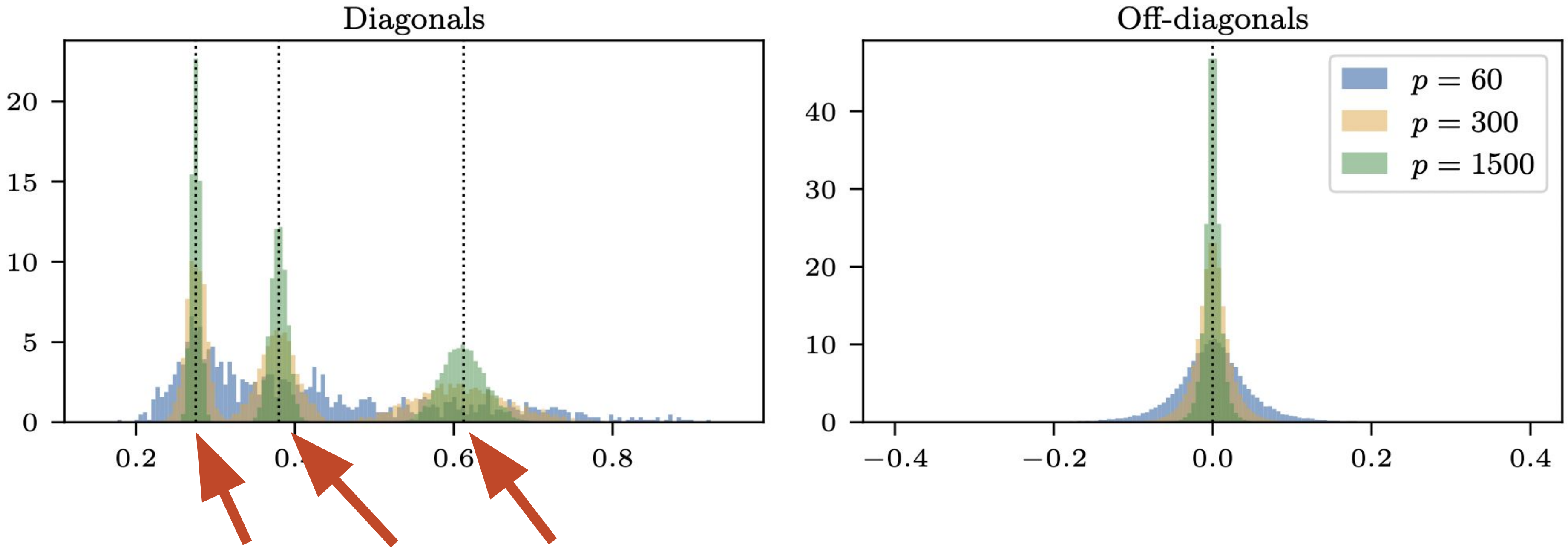

$$\frac{1}{a+\mu} = \frac{1}{3.63}, \quad \frac{1}{2.63}, \quad \frac{1}{1.63}$$

A Blurring Analogy

Original Image

256x256

A Blurring Analogy

$\mathbf{S}^{\mathrm{H}}\mathbf{AS}$
Downsample

Original Image

256x256

64x64

32x32

16x16

A Blurring Analogy

Original Image

256x256

	$\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S}$ Downsample	$\left(\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_q\right)^{-1}$ Blur (1.6%)
64x64		
32x32		
16x16		

A Blurring Analogy

Original Image

256x256

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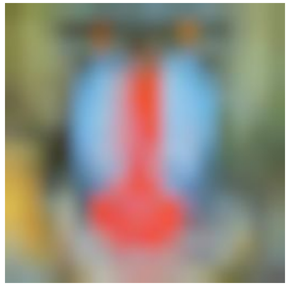
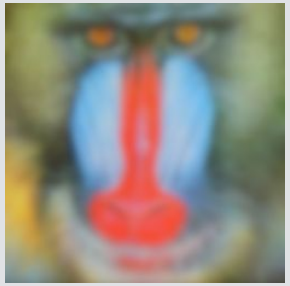
16x16			

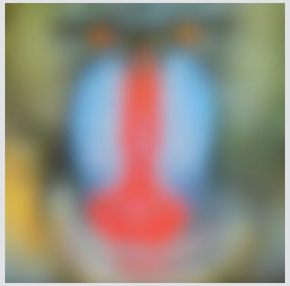
$(\mathbf{A} + \mu\mathbf{I}_p)^{-1}$

Original Image

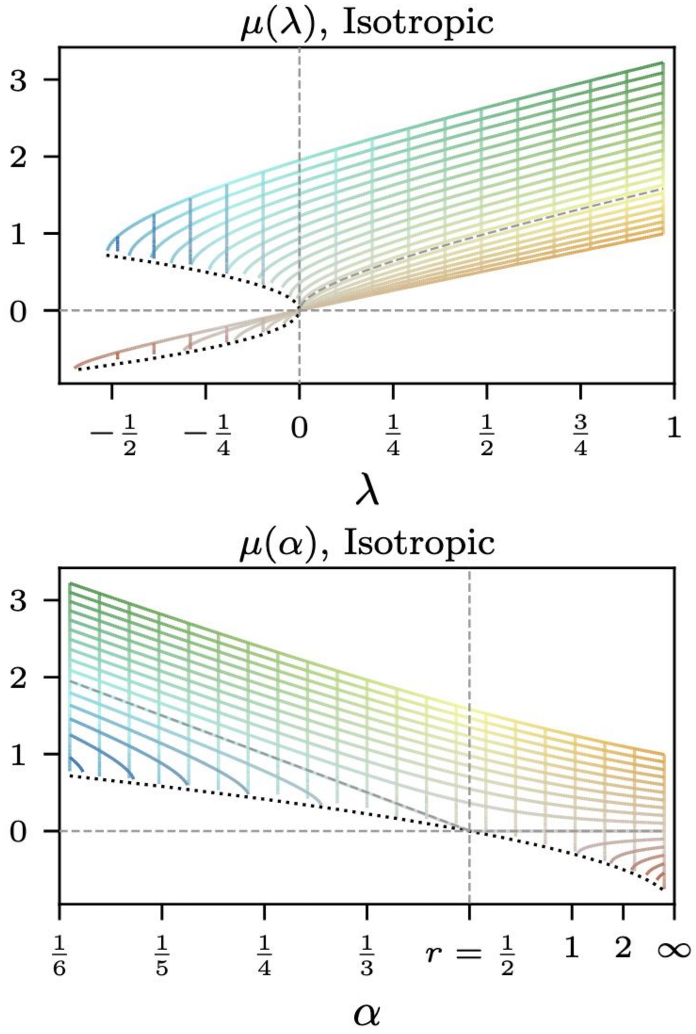
Blur (1.6%)



Blur (3.1%)



Implicit Regularization Behavior



- Example: isotropic spectrum with $r(\mathbf{A}) = \frac{1}{2}$

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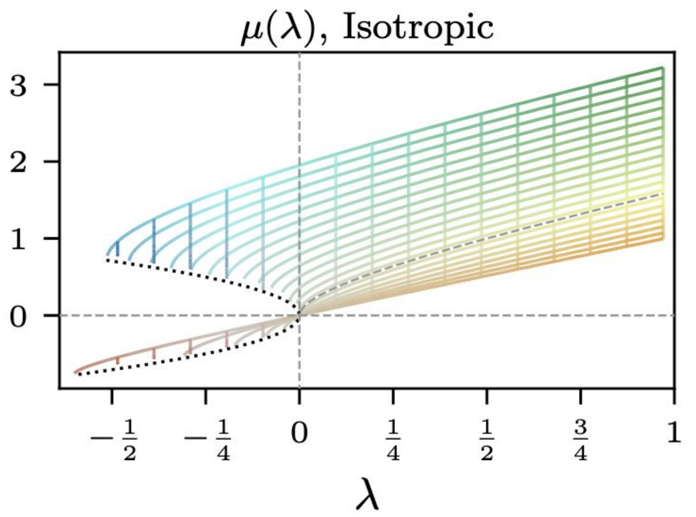

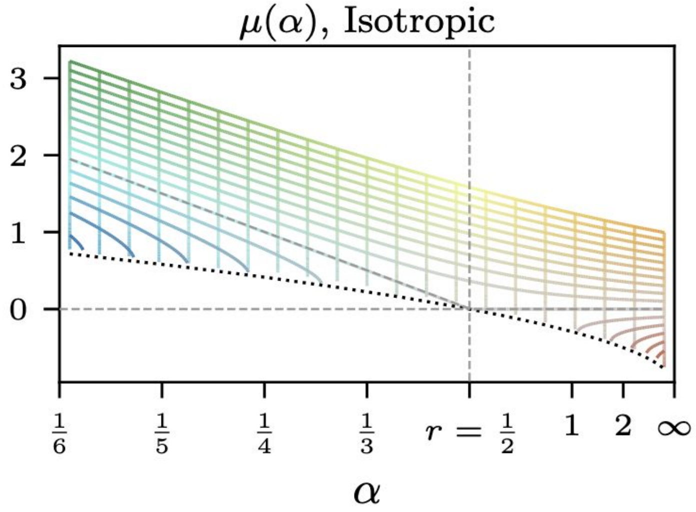

- Example: isotropic spectrum with $r(\mathbf{A}) = \frac{1}{2}$
- $\lambda \mapsto \mu$ is increasing and concave
- $\alpha \mapsto \mu$ is decreasing unless $\alpha > r(\mathbf{A})$ and $\lambda < 0$

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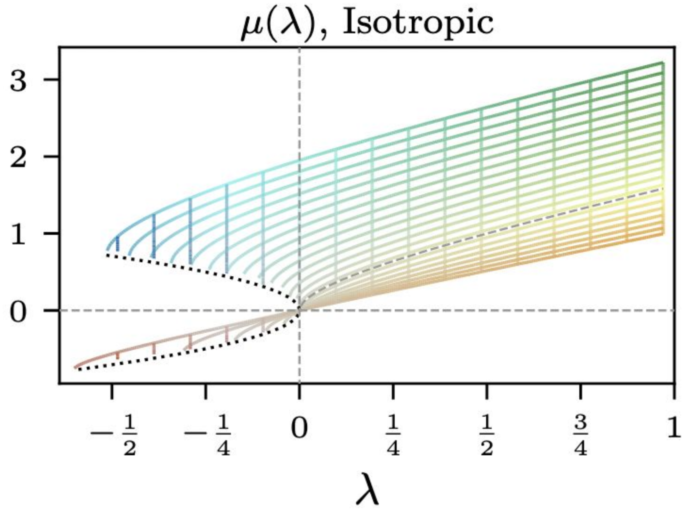

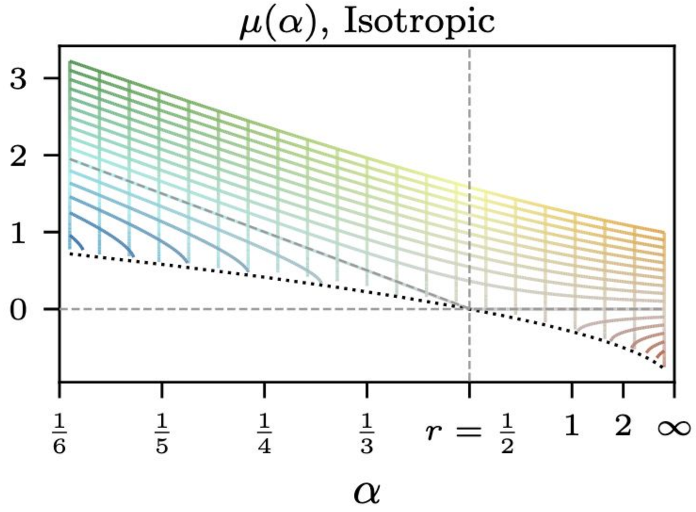

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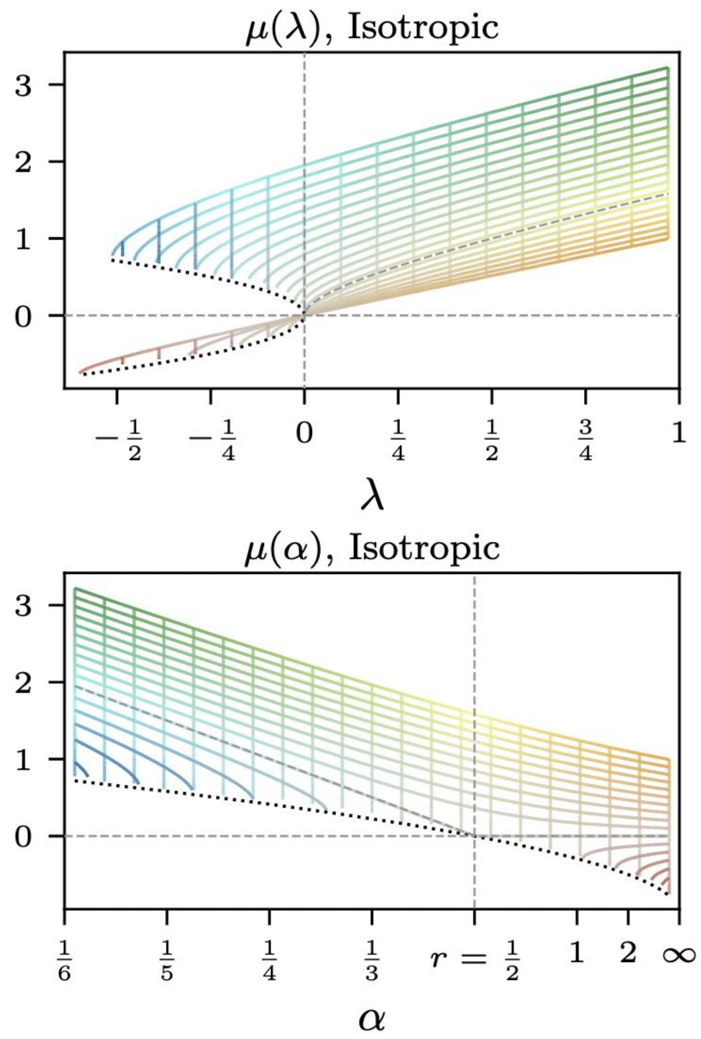

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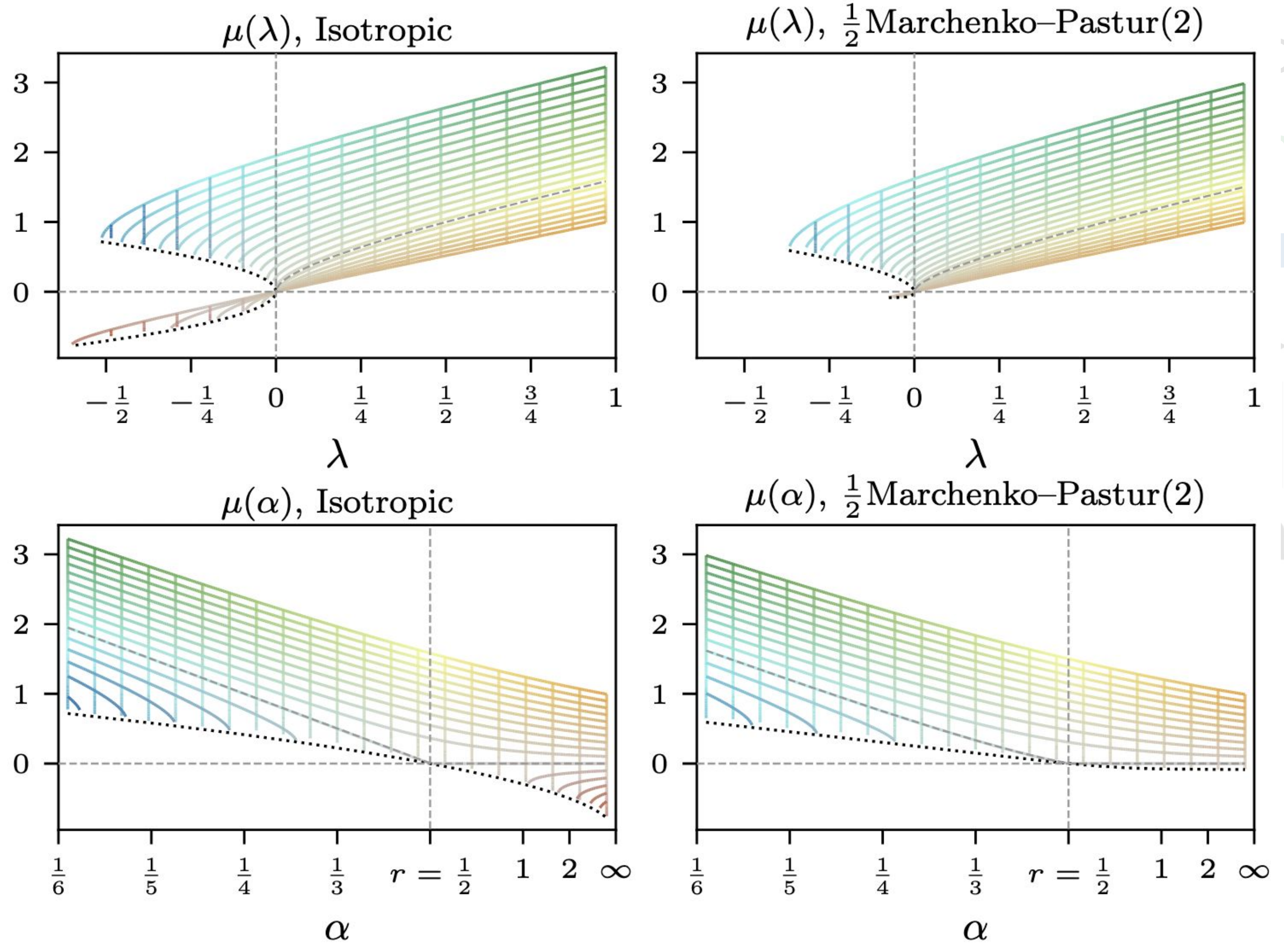
- $\mathrm{sign}(\mu) = \mathrm{sign}(\lambda)$ if $\alpha > r(\mathbf{A})$
- else $\mu \geq 0$

Implicit Regularization Behavior



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$r(\mathbf{A})$ and $\lambda < 0$

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- Similarly, products of equivalences do not compose if not independent
- Solution: derivative rule of asymptotic equivalence

$$\frac{d}{dz}\left(\mathbf{A} - z\mathbf{I}\right)^{-1} = -\left(\mathbf{A} - z\mathbf{I}\right)^{-2}$$

Second-order Sketching Equivalence

Theorem 5. *If $\mathbf{\Psi} \in \mathbb{C}^{p \times p}$ is a deterministic or random positive semidefinite matrix independent of $\mathbf{S}$ with $\|\mathbf{\Psi}\|_{\text{op}}$ uniformly bounded in p, then*

$$\mathbf{S}\big(\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_q\big)^{-1}\mathbf{S}^{\mathsf{H}}\mathbf{\Psi}\mathbf{S}\big(\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_q\big)^{-1}\mathbf{S}^{\mathsf{H}} \simeq \left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1}\left(\mathbf{\Psi} + \mu' \mathbf{I}_p\right)\left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1},$$

where

$$\mu' = \frac{\frac{1}{q}\operatorname{tr}\left[\mu^3\left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1}\mathbf{\Psi}\left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-1}\right]}{\lambda + \frac{1}{q}\operatorname{tr}\left[\mu^2 \mathbf{A}\left(\mathbf{A} + \mu \mathbf{I}_p\right)^{-2}\right]} \geq 0.$$

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- Depends significantly on the choice of $\boldsymbol{\Psi}$

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Spoiler:

Randomized least squares = ridge + noise

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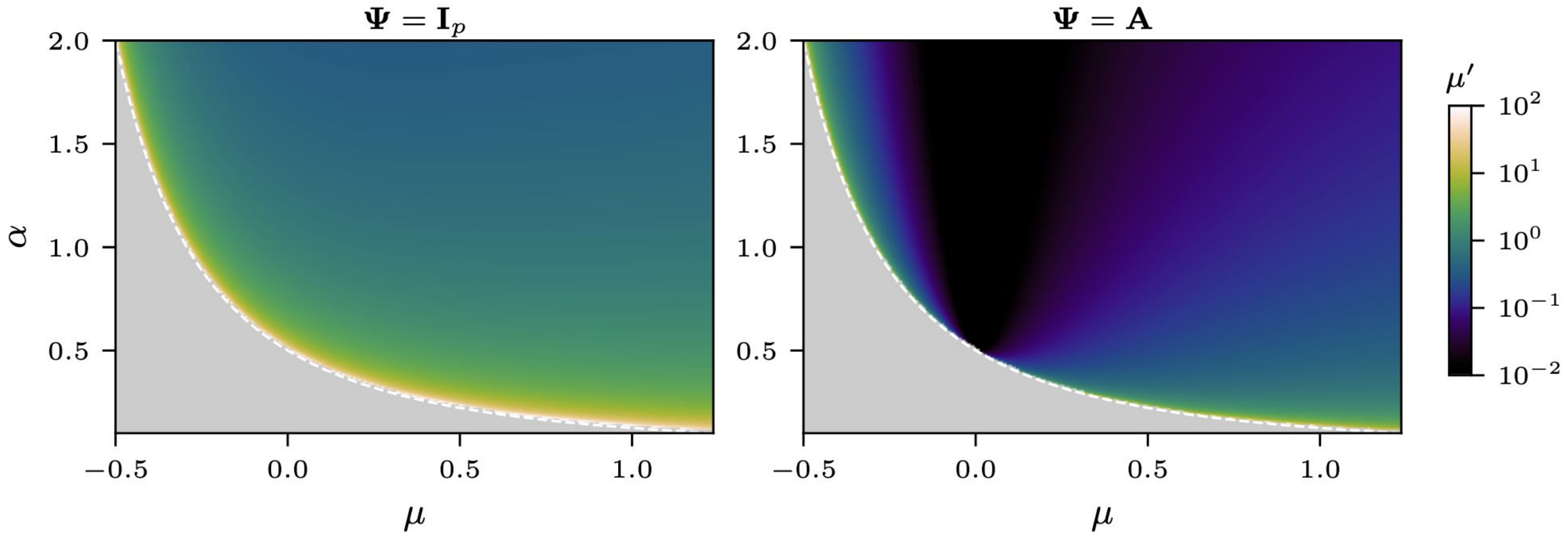
- Example: isotropic spectrum with $r(\mathbf{A}) = \frac{1}{2}$



One Incredible Regime

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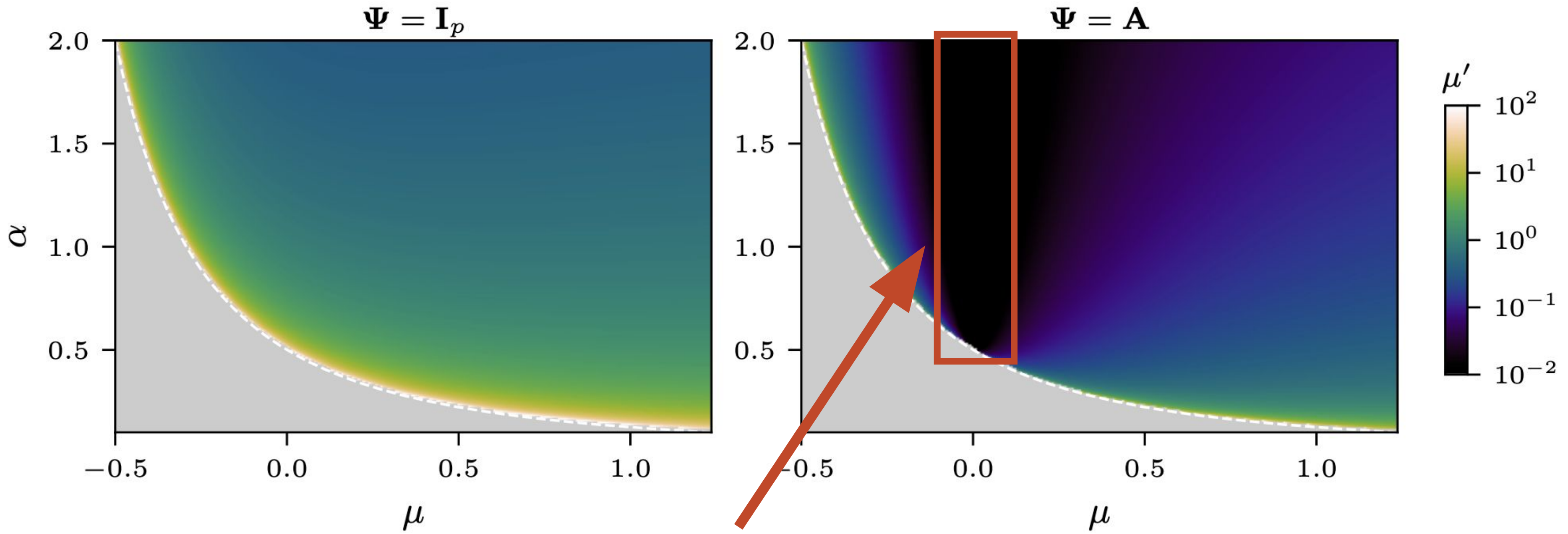


- If $\mathbf{\Psi} \in \mathrm{Range}(\mathbf{A})$, $\alpha > r(\mathbf{A})$, and $\mu = \lambda = 0$, there is no inflation
  - Agrees with classical sketching results: sketch larger than rank
  - Sketching is ideal for benign overfitting

Application: Ridge Regression

How about a machine
learning problem?

- Primal (observations) and dual (features) sketching:

$$\widehat{\boldsymbol{\beta}}_P \triangleq \arg\min_{\mathbf{b}} \frac{1}{n}\left\|\mathbf{T}^\top(\mathbf{y} - \mathbf{X}\mathbf{b})\right\|_2^2 + \lambda\|\mathbf{b}\|_2^2$$

$$\widehat{\boldsymbol{\beta}}_D \triangleq \mathbf{S} \cdot \arg\min_{\mathbf{b}} \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{S}\mathbf{b}\|_2^2 + \lambda\|\mathbf{b}\|_2^2$$

$$\widehat{\boldsymbol{\beta}}_{PD} \triangleq \mathbf{S} \cdot \arg\min_{\mathbf{b}} \frac{1}{n}\left\|\mathbf{T}^\top(\mathbf{y} - \mathbf{X}\mathbf{S}\mathbf{b})\right\|_2^2 + \lambda\|\mathbf{b}\|_2^2$$

Preparing for Equivalences

- Express in terms of the sketched pseudoinverse:

$$\widehat{\boldsymbol{\beta}}_\psi = \frac{1}{\sqrt{n}}\mathbf{X}_\psi^\ddagger \mathbf{y},\ \psi \in \{P, D, PD\}$$

$$\mathbf{X}_P^\ddagger \triangleq \frac{1}{\sqrt{n}}\left(\frac{1}{n}\mathbf{X}^\top\mathbf{T}\mathbf{T}^\top\mathbf{X} + \lambda\mathbf{I}\right)^{-1}\mathbf{X}^\top\mathbf{T}\mathbf{T}^\top$$

$$\mathbf{X}_D^\ddagger \triangleq \frac{1}{\sqrt{n}}\mathbf{S}\left(\frac{1}{n}\mathbf{S}^\top\mathbf{X}^\top\mathbf{X}\mathbf{S} + \lambda\mathbf{I}\right)^{-1}\mathbf{S}^\top\mathbf{X}^\top$$

$$\mathbf{X}_{PD}^\ddagger \triangleq \frac{1}{\sqrt{n}}\mathbf{S}\left(\frac{1}{n}\mathbf{S}^\top\mathbf{X}^\top\mathbf{T}\mathbf{T}^\top\mathbf{X}\mathbf{S} + \lambda\mathbf{I}\right)^{-1}\mathbf{S}^\top\mathbf{X}^\top\mathbf{T}\mathbf{T}^\top$$

First-order Data Pseudoinverse Equivalence

Theorem 6. *If* $\left\|\frac{1}{\sqrt{n}}\mathbf{X}\right\|_{\mathrm{op}}$ *is uniformly bounded in* p*, then as* $m, n, q, p \to \infty$*,*

$$\mathbf{X}_{\psi}^{\ddagger} \simeq \frac{1}{\sqrt{n}}\left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_{\psi}\mathbf{I}\right)^{-1}\mathbf{X}^{\mathsf{H}},$$

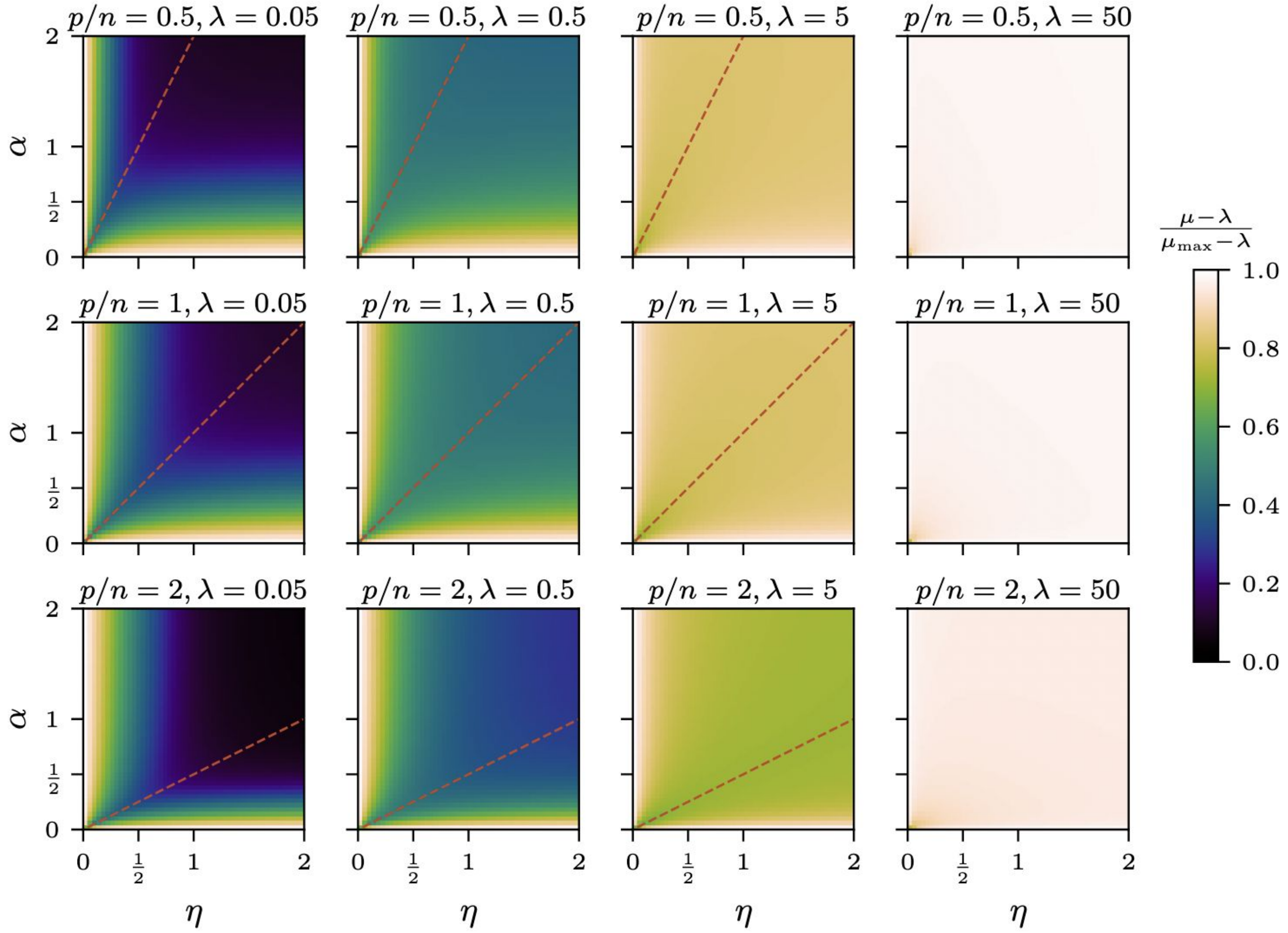
where μ_{ψ} *are is the most positive solutions to the equations*

$$\lambda = \mu_{P}\left(1 - \frac{1}{m}\mathrm{tr}\left[\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}\left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_{P}\mathbf{I}\right)^{-1}\right]\right),$$

$$\lambda = \mu_{D}\left(1 - \frac{1}{q}\mathrm{tr}\left[\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}\left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_{D}\mathbf{I}\right)^{-1}\right]\right),$$

$$\frac{\lambda}{\theta} - 1 = \frac{m}{q}\left(\frac{\theta}{\mu_{PD}} - 1\right), \quad \theta = \mu_{PD}\left(1 - \frac{1}{m}\mathrm{tr}\left[\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}\left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_{PD}\mathbf{I}\right)^{-1}\right]\right).$$

Sharp Phase Transition for Joint Sketching



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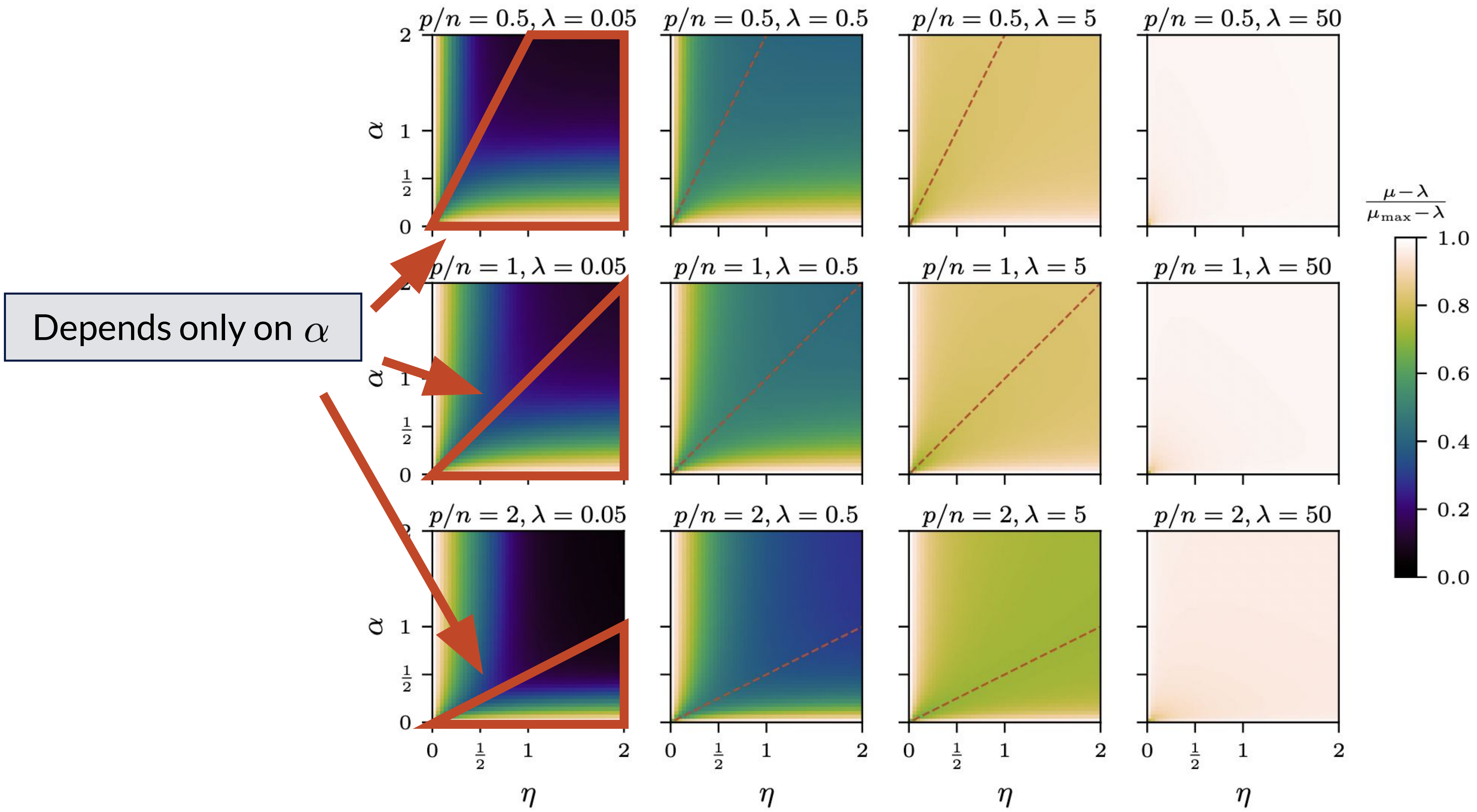

Sketching Makes Same Predictions as Ridge

Corollary 7. *If* $\|\frac{1}{\sqrt{n}}\mathbf{y}\|_2$ *is uniformly bounded in* p *and* $\mathbf{w} \in \mathbb{C}^p$ *is independent of* $\mathbf{S}$ *and* $\mathbf{T}$ *such that* $\|\mathbf{w}\|_2$ *is uniformly bounded in* p*, then for any continuous function* $f : \mathbb{C} \to \mathbb{C}$*, as* $p \to \infty$,

$$f(\mathbf{w}^{\mathsf{H}} \widehat{\boldsymbol{\beta}}_{\psi}) - f(\mathbf{w}^{\mathsf{H}} \widehat{\boldsymbol{\beta}}^{\mathrm{ridge}}_{\mu_\psi}) \xrightarrow{\mathrm{a.s.}} 0.$$

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$$f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}_{\psi}) - f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}^{\mathrm{ridge}}_{\mu_\psi}) \xrightarrow{\text{a.s.}} 0.$$

- Sketching asymptotically makes the same prediction as the equivalent ridge on any single test point

Sketching Makes Same Predictions as Ridge

Corollary 7. *If* $\|\frac{1}{\sqrt{n}}\mathbf{y}\|_2$ *is uniformly bounded in* p *and* $\mathbf{w} \in \mathbb{C}^p$ *is independent of* $\mathbf{S}$ *and* $\mathbf{T}$ *such that* $\|\mathbf{w}\|_2$ *is uniformly bounded in* p*, then for any continuous function* $f\colon \mathbb{C} \to \mathbb{C}$*, as* $p \to \infty$*,*

$$f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}_{\psi}) - f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}^{\mathrm{ridge}}_{\mu_\psi}) \xrightarrow{\text{a.s.}} 0.$$

- Sketching asymptotically makes the same prediction as the equivalent ridge on any single test point

Why this qualifier?

Sketching Makes Same Predictions as Ridge

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$$f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}_{\psi}) - f(\mathbf{w}^{\mathsf{H}}\widehat{\boldsymbol{\beta}}^{\mathrm{ridge}} \ldots$$

- Sketching asymptoticall… prediction as the equivalent ridge on any sin…

Pointwise convergence does not imply uniform convergence

Why this qualifier?

Quadratic Metrics of Sketched Ensembles

- Ensemble of independent sketches: $\widehat{\boldsymbol{\beta}}_{\psi}^{\mathrm{ens}} = \frac{1}{K} \sum_{k=1}^{K} \widehat{\boldsymbol{\beta}}_{\psi}^{(k)}$
- Quadratic error metrics: $\mathcal{E}_{\boldsymbol{\Psi}}\left(\boldsymbol{\beta}, \boldsymbol{\beta}'\right) = \left(\boldsymbol{\beta} - \boldsymbol{\beta}'\right)^{\mathsf{H}} \boldsymbol{\Psi} \left(\boldsymbol{\beta} - \boldsymbol{\beta}'\right)$
  - Includes test risk

Quadratic Metrics of Sketched Ensembles

Theorem 8. *If $\boldsymbol{\Psi} \in \mathbb{C}^{p \times p}$ is a positive semidefinite matrix and $\boldsymbol{\beta}' \in \mathbb{C}^p$ a vector such that $\|\boldsymbol{\Psi}\|_{\mathrm{op}}$ and $\|\boldsymbol{\beta}'\|_2$ are uniformly bounded in p and $(\boldsymbol{\Psi}, \boldsymbol{\beta})$ is independent of $(\mathbf{S}_k, \mathbf{T}_k)_{k=1}^K$, then for $\psi \in \{P, D\}$,*

$$\mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_P^{\mathrm{ens}}, \boldsymbol{\beta}'\right) - \left(\mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_{\mu_P}^{\mathrm{ridge}}, \boldsymbol{\beta}'\right) + \frac{\mu_P'}{Kn}\mathbf{y}^{\mathsf{H}}\left(\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P\mathbf{I}\right)^{-2}\mathbf{y}\right) \xrightarrow{\text{a.s.}} 0,$$

$$\mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_D^{\mathrm{ens}}, \boldsymbol{\beta}'\right) - \left(\mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_{\mu_D}^{\mathrm{ridge}}, \boldsymbol{\beta}'\right) + \frac{\mu_D'}{Kn}\mathbf{y}^{\mathsf{H}}\mathbf{X}\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D\mathbf{I}\right)^{-2}\mathbf{X}^{\mathsf{H}}\mathbf{y}\right) \xrightarrow{\text{a.s.}} 0,$$

where

$$\mu_P' = \frac{\frac{1}{m}\mathrm{tr}\left[\mu_P^3\left(\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P\mathbf{I}\right)^{-1}\tfrac{1}{n}\mathbf{X}\boldsymbol{\Psi}\mathbf{X}^{\mathsf{H}}\left(\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P\mathbf{I}\right)^{-1}\right]}{\lambda + \frac{1}{m}\mathrm{tr}\left[\mu_P^2\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}}\left(\tfrac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P\mathbf{I}\right)^{-2}\right]},$$

$$\mu_D' = \frac{\frac{1}{q}\mathrm{tr}\left[\mu_D^3\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D\mathbf{I}\right)^{-1}\boldsymbol{\Psi}\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D\mathbf{I}\right)^{-1}\right]}{\lambda + \frac{1}{q}\mathrm{tr}\left[\mu_D^2\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}\left(\tfrac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D\mathbf{I}\right)^{-2}\right]}.$$

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where

$$\mu'_P = \frac{\frac{1}{m}\mathrm{tr}\left[\mu_P^3 \left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P \mathbf{I}\right)^{-1} \frac{1}{n}\mathbf{X}\boldsymbol{\Psi}\mathbf{X}^{\mathsf{H}} \left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P \mathbf{I}\right)^{-1}\right]}{\lambda + \frac{1}{m}\mathrm{tr}\left[\mu_P^2 \frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} \left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P \mathbf{I}\right)^{-2}\right]},$$

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$$\mathcal{E}_{\Psi}\left(\widehat{\beta}^{\mathrm{ens}}_{\psi}, \beta'\right) \xrightarrow{\text{a.s.}} \mathcal{E}_{\Psi}\left(\widehat{\beta}^{\mathrm{ridge}}_{\mu_\psi}, \beta'\right) + O\left(\frac{\mu'_\psi}{K}\right)$$

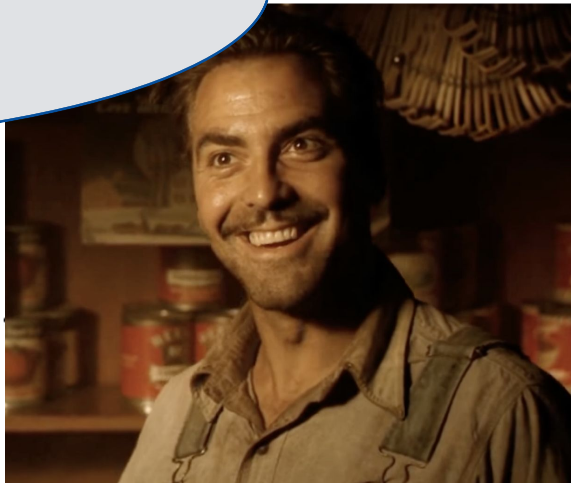
where

Well, ain't this a geometrical oddity.

$O\left(\frac{\mu'_\psi}{K}\right)$ from everywhere!

$$\mu'_P = \frac{\frac{1}{m}\mathrm{tr}\left[\mu_P^3 \left(\frac{1}{n}\mathbf{X}\mathbf{X}\cdots\right.\right.}{\lambda + \frac{1}{m}\mathrm{tr}\left[\mu_P^2 \frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} \left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{H}} + \mu_P \mathbf{I}\right)\cdots\right]}$$

$$\mu'_D = \frac{\frac{1}{q}\mathrm{tr}\left[\mu_D^3 \left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D \mathbf{I}\right)^{-1} \Psi \left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D \mathbf{I}\right)^{-1}\right]}{\lambda + \frac{1}{q}\mathrm{tr}\left[\mu_D^2 \frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} \left(\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X} + \mu_D \mathbf{I}\right)^{-2}\right]}$$



Quadratic Conclusions

$$\mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_{\psi}^{\mathrm{ens}}, \boldsymbol{\beta}'\right) \xrightarrow{\text{a.s.}} \mathcal{E}_{\boldsymbol{\Psi}}\left(\widehat{\boldsymbol{\beta}}_{\mu_\psi}^{\mathrm{ridge}}, \boldsymbol{\beta}'\right) + O\left(\frac{\mu_\psi'}{K}\right)$$

- For infinite K, sketched ensemble = ridge

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Spoiler:

Randomized least squares = ridge + noise

Randomized ensembles = ridge

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- For finite K, sketched ensemble is worse than ridge

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- For infinite K, sketched ensemble = ridge
- For finite K, sketched ensemble is worse than ridge
  - Unless $\boldsymbol{\Psi} \in \mathrm{Range}(\mathbf{A})$, $\alpha > r(\mathbf{A})$, and $\mu = \lambda = 0$!

A Sketched Ensemble Efficiency Experiment

- Setup: fixed $O(p^2 n)$ budget ensembles with $K = \lfloor \frac{1}{\alpha^2} \rfloor$, $r(\mathbf{\Sigma}) = \frac{1}{2}$

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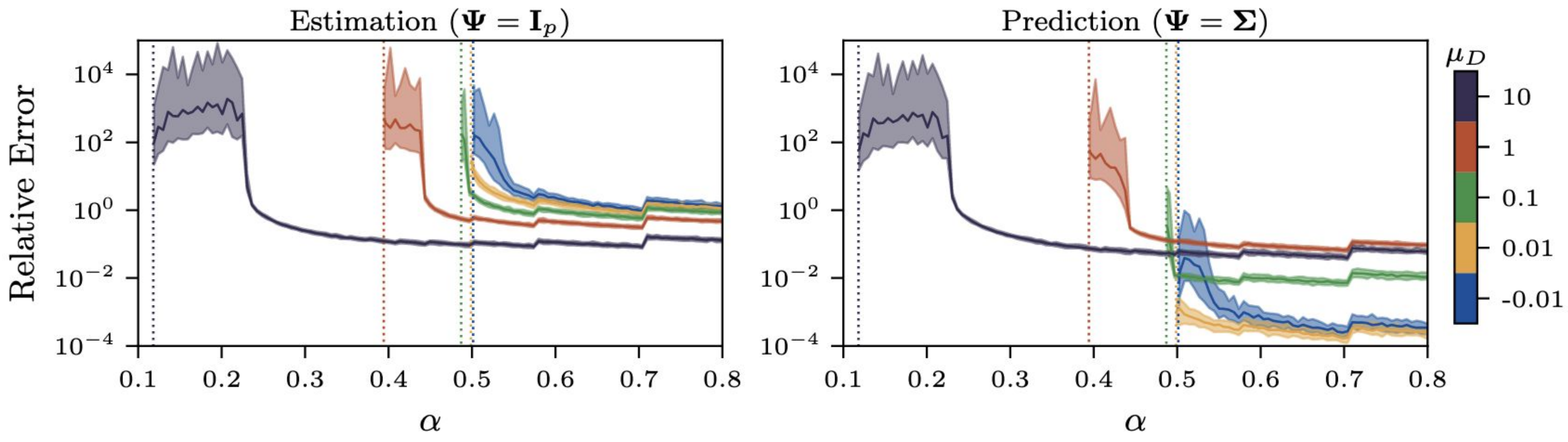

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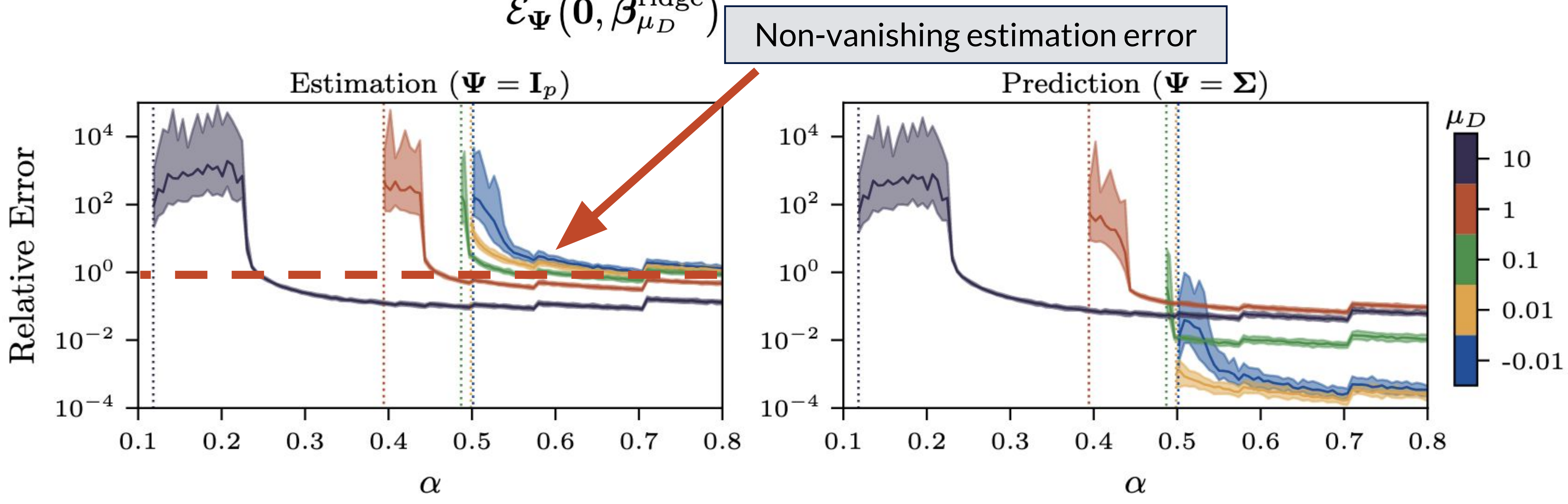

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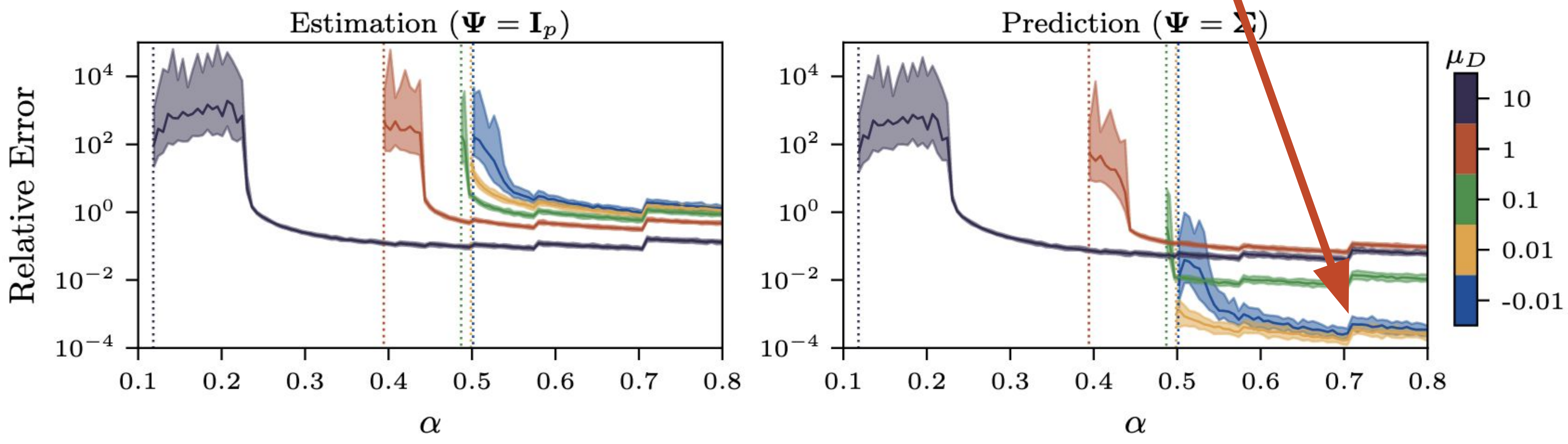
Vanishing prediction error!



Better Sketches?

What if I use a better/faster
sketch than i.i.d.?

A Free Sketching Conjecture

Conjecture 9. *Let* $\mathbf{S} \in \mathbb{C}^{p \times q}$ *be a norm-preserving sketch such that* $\mathbf{S}\mathbf{S}^{\mathsf{H}}$ *and* $\mathbf{A}$ *converge almost surely to operators that are free with respect to the average trace* $\frac{1}{p}\mathrm{tr}[\cdot]$. *Then there exists a monotonic mapping* $\lambda \mapsto \gamma$ *such that*

$$\mathbf{S}\big(\mathbf{S}^{\mathsf{H}}\mathbf{A}\mathbf{S} + \lambda\mathbf{I}_q\big)^{-1}\mathbf{S}^{\mathsf{H}} \simeq \big(\mathbf{A} + \gamma\mathbf{I}_p\big)^{-1}.$$

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- Includes i.i.d. sketching and more
  - Orthogonal sketching
  - Efficient sketches like CountSketch, FJLT, SRHT?

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Conjecture 10. *For* $q \leq p$ *let* $\sqrt{\frac{q}{p}}\mathbf{Q} \in \mathbb{C}^{p \times q}$ *be a Haar-distributed matrix with orthonormal columns. Then*

$$\mathbf{Q}\left(\mathbf{Q}^{\mathsf{H}}\mathbf{A}\mathbf{Q} + \lambda\mathbf{I}_q\right)^{-1}\mathbf{Q}^{\mathsf{H}} \simeq \left(\mathbf{A} + \gamma\mathbf{I}_p\right)^{-1},$$

where γ *is the most positive solution to*

$$\frac{1}{p}\mathrm{tr}\left[\left(\mathbf{A} + \gamma\mathbf{I}_p\right)^{-1}\right](\gamma - \alpha\lambda) = 1 - \alpha.$$

Furthermore, for $\mu > 0$ *applied to the same* $(\mathbf{A}, \alpha, \lambda)$*, we have* $\gamma < \mu$.

Orthogonal Sketching

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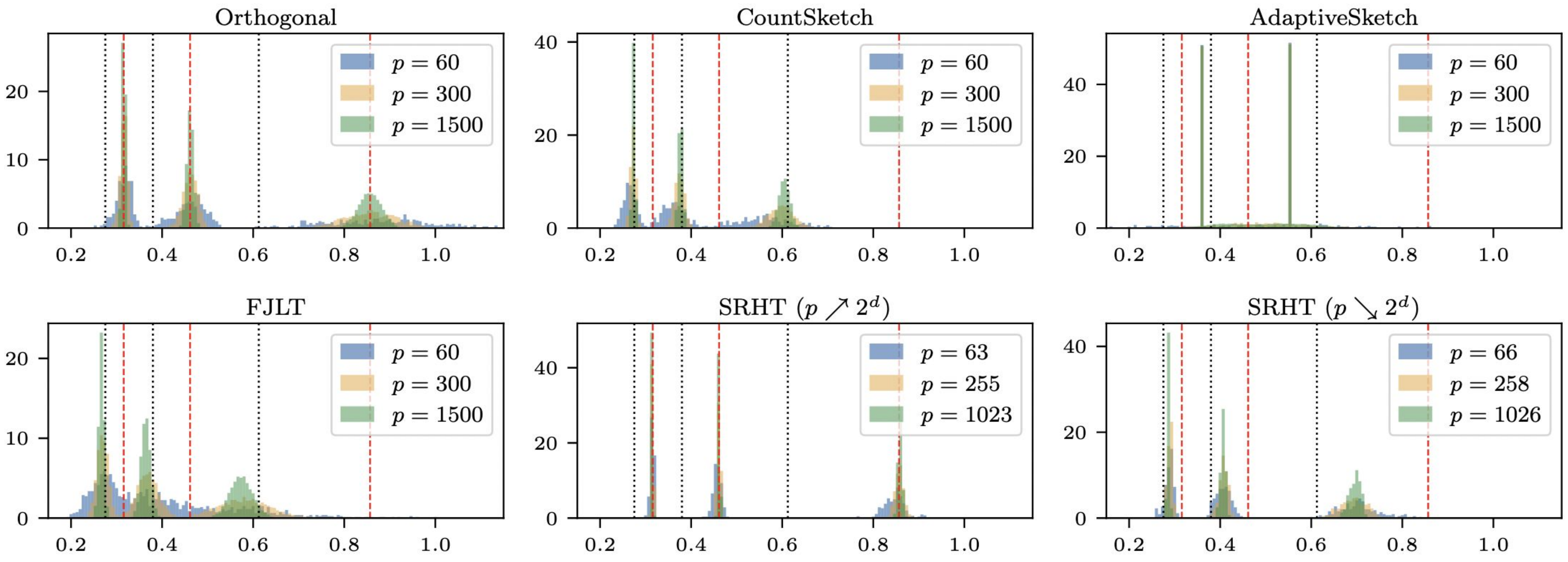
- Same form as i.i.d. sketching, but with less regularization

Equivalence for Sketches Used in Practice?



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- Future work:
  - More asymptotic equivalences
    - Generalized cross-validation with sketching
    - General linear models via leave-one-dimension-out
    - Asymptotics of PCA

Questions?

Corollary 11. *Let* $\mathbf{W}$ *be an invertible* $p \times p$ *positive semidefnite matrix, either deterministic or random but independent of* $\mathbf{S}$ *with* $\limsup \|\mathbf{W}\|_{\mathrm{op}} < \infty$*. Let* $\widetilde{\mathbf{S}} = \mathbf{W}^{1/2}\mathbf{S}$*. Then for each* $\lambda > -\liminf \lambda_{\min}^{+}(\widetilde{\mathbf{S}}^\top \mathbf{A} \widetilde{\mathbf{S}})$ *as* $p, q \to \infty$ *such that* $0 < \liminf \frac{q}{p} \leq \limsup \frac{q}{p} < \infty$,

$$\widetilde{\mathbf{S}}\big(\widetilde{\mathbf{S}}^\top \mathbf{A} \widetilde{\mathbf{S}} + \lambda \mathbf{I}_q\big)^{-1} \widetilde{\mathbf{S}}^\top \simeq \big(\mathbf{A} + \mu \mathbf{W}^{-1}\big)^{-1},$$

where μ *most positive solution to*

$$\lambda = \mu \left(1 - \tfrac{1}{q} \mathrm{tr}\left[\mathbf{A}\left(\mathbf{A} + \mu \mathbf{W}^{-1}\right)^{-1}\right]\right).$$

Theorem 12. *Let* $\mathbf{X} = \mathbf{Z}\mathbf{\Sigma}^{1/2}$ *and* $\mathbf{\Sigma} \in \mathbb{C}^{p \times p}$ *have eigenvalue decomposition* $\mathbf{U}\mathbf{D}\mathbf{U}^{\mathsf{H}}$*, and let* $\mathbf{\Pi}_{\mathcal{A}}$ *be the projection operator of the principal eigenspace corresponding to a set of eigenvalues* $\mathcal{A}$ *of the matrix* $\frac{1}{n}\mathbf{X}^{\mathsf{H}}\mathbf{X}$*. Then there exists a family of measures* μ_{σ^2} *for all* $\sigma^2 \geq 0$ *such that for any* $\mathcal{A} \subseteq \mathbb{R}_{\geq 0}$*, in the limit as* $p \to \infty$*,*

$$\mathbf{\Pi}_{\mathcal{A}} \simeq \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathsf{H}},$$

where $\mathbf{\Lambda}$ *is a diagonal matrix defined for by*

$$[\mathbf{\Lambda}]_{ii} = \mu_{[\mathbf{\Sigma}]_{ii}}(\mathcal{A}).$$