Asymptotically Free Sketching and Applications in Ridge Regression

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MDS 2024





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Thanks to collaborators





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 $-\mathbf{S}^{\mathsf{T}}\mathbf{x}_{i}\|_{2} \leq (1+\epsilon)\|\mathbf{x}_{i}-\mathbf{x}_{i}\|_{2}$

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 - Use sum of one-hot encodings as features: $p \sim 10^7$, feasible \checkmark

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 - $S = X^{\top}$ or $S = Z^{\top}$ is determined by nature and may not be observed

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Q: How does sketching affect the result in machine learning?

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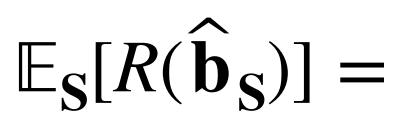
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Theorem (Lu et al. 2013). Let $r = rank(\mathbf{X})$ and **S** be SRHT. With high probability, $R(\hat{\mathbf{b}}_{\mathbf{S}}) - R(\hat{\mathbf{b}}) \le C \frac{r \log r}{q} R(\hat{\mathbf{b}}).$

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- Compare to ridge regression:

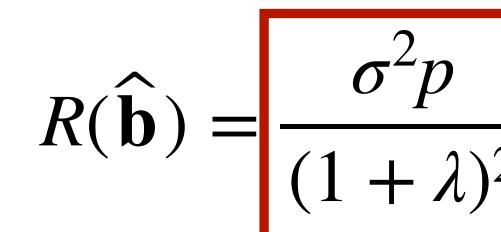
 $R(\hat{\mathbf{b}}) = \frac{1}{(1+\lambda)}$

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$$\frac{\lambda^2}{\lambda^2} + \|\mathbf{b}^*\|_2^2 \frac{\lambda^2}{(1+\lambda)^2}$$

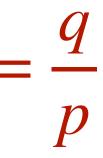
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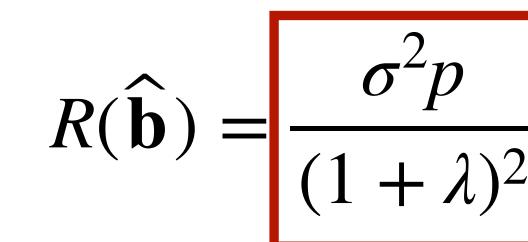
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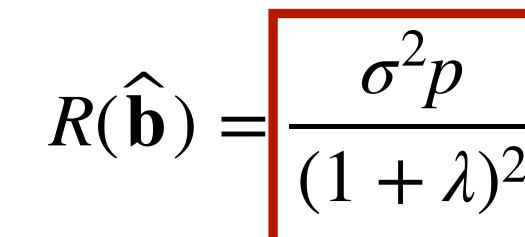
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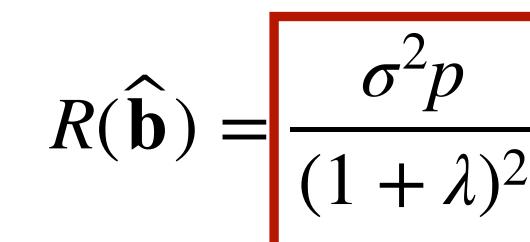
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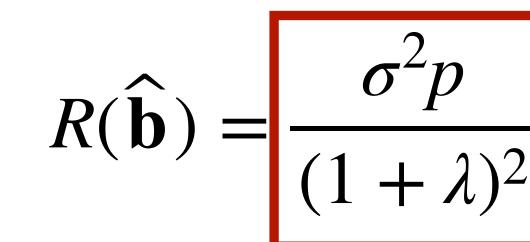




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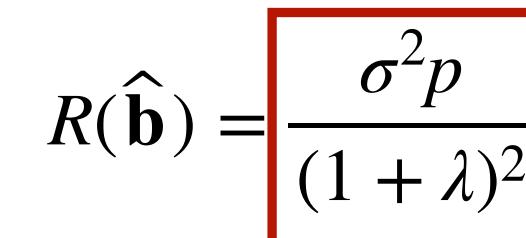




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Asymptotic equivalences admit a calculus (Dobriban and Sheng, 2021)

• Sum:
$$\mathbf{A}_n \simeq \mathbf{B}_n, \mathbf{C}_n \simeq \mathbf{D}_n \Longrightarrow$$

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 - Product: $\mathbf{A}_n \simeq \mathbf{B}_n$, $(\mathbf{A}_n, \mathbf{B}_n) \perp$
 - Elements: $\mathbf{A}_n \simeq \mathbf{B}_n \implies [\mathbf{A}_n]$

$$\mathbf{A}_{n} + \mathbf{C}_{n} \simeq \mathbf{B}_{n} + \mathbf{D}_{n}$$
$$(\mathbf{C}_{n}, \mathbf{D}_{n}) \Longrightarrow \mathbf{C}_{n} \mathbf{A}_{n} \mathbf{D}_{n} \simeq \mathbf{C}_{n} \mathbf{B}_{n} \mathbf{D}_{n}$$
$$|_{ij} - [\mathbf{B}_{n}]_{ij} \xrightarrow{\text{a.s.}} 0$$

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 - Derivative: $f(\mathbf{A}_n; z) \simeq g(\mathbf{B}_n; z)$

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$$\stackrel{ij}{=} [\mathbf{B}_{n}]_{ij} \stackrel{\text{a.s.}}{\longrightarrow} 0$$
$$\implies f'(\mathbf{A}_{n}; z) \simeq g'(\mathbf{B}_{n}; z)$$

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- - Sum: $\mathbf{A}_n \simeq \mathbf{B}_n, \mathbf{C}_n \simeq \mathbf{D}_n \Longrightarrow$
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- Not nonlinear ops: $A_n \simeq B_n \neq B_n$
 - Analogous: $\mathbb{E}[\mathbf{A}] = \mathbb{E}[\mathbf{B}] \implies$

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• Sketched ridge: $\hat{\mathbf{b}}_{\mathbf{S}} = \mathbf{S} \cdot \operatorname{argmin}_{\mathbf{b}} \{ \|\mathbf{y} - \mathbf{X}\mathbf{S}\mathbf{b}\|_{2}^{2} + \lambda \|\mathbf{b}\|_{2}^{2} \}$

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- \bullet $\mathbf{S} \in \mathbb{R}^{p \times q}$, its sketched pseudoinverse with regularization λ is

 $S(S^{T}AS)$

$$\left\{ \|\mathbf{y} - \mathbf{XSb}\|_2^2 + \lambda \|\mathbf{b}\|_2^2 \right\}$$

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 $\lambda \to 0$, it is the Moore–Penrose pseudoinverse of SS^TASS^T

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• **Definition.** Given a positive semidefinite matrix $\mathbf{A} \in \mathbb{R}^{p \times p}$ and sketching matrix

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• Called "pseudoinverse" because when \mathbf{S} has orthonormal columns and

• Proportional asymptotics, $\alpha = \frac{q}{p}$: $\lim_{p \to \infty} \alpha \in (0, \infty)$

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• Theorem (LeJeune, PP, et al., 2024). For A with uniformly bounded in operator norm independent of S and any $\lambda > -\lim \lambda_{\min}(S^{T}AS)$, $\mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{A}\mathbf{S} + \lambda\mathbf{I})$

where μ is the most positive solution to

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

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Orthogonal sketches

Orthogonal sketches

- columns. Then
 - $\mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_{a})$
 - where γ is the most positive solution to

$$\frac{1}{p} \operatorname{tr}[(\mathbf{A} + \mu \mathbf{I}_p)]$$

• Corollary (LeJeune, PP, et al., 2024). Let $\sqrt{\frac{p}{q}}$ S have orthonormal

$$(\mathbf{J})^{-1}\mathbf{S}^{\mathsf{T}} \simeq (\mathbf{A} + \gamma \mathbf{I}_p)^{-1},$$

 $\gamma^{-1}](\gamma - \alpha \lambda) = 1 - \alpha.$

Orthogonal sketches

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Less distortion: $\lambda < \gamma < \mu$ for i.i.d. sketch when $\mu > 0$ lacksquare

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• Example: A = diag(0, ..., 1, ..., 2, ...)

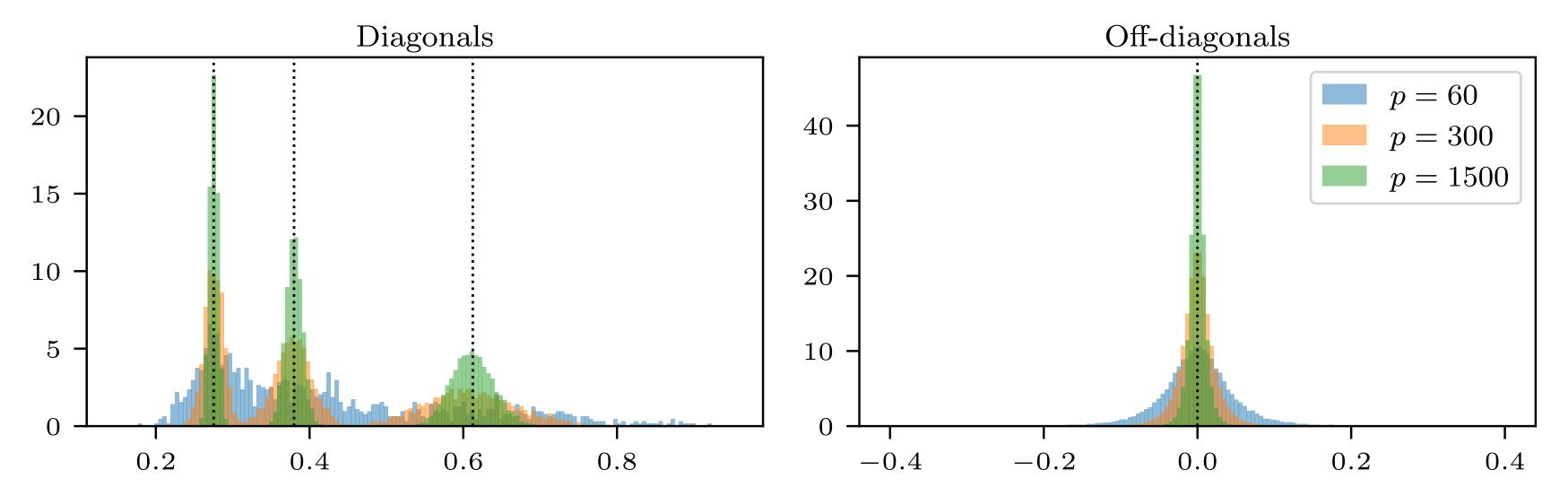
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Empirical concentration

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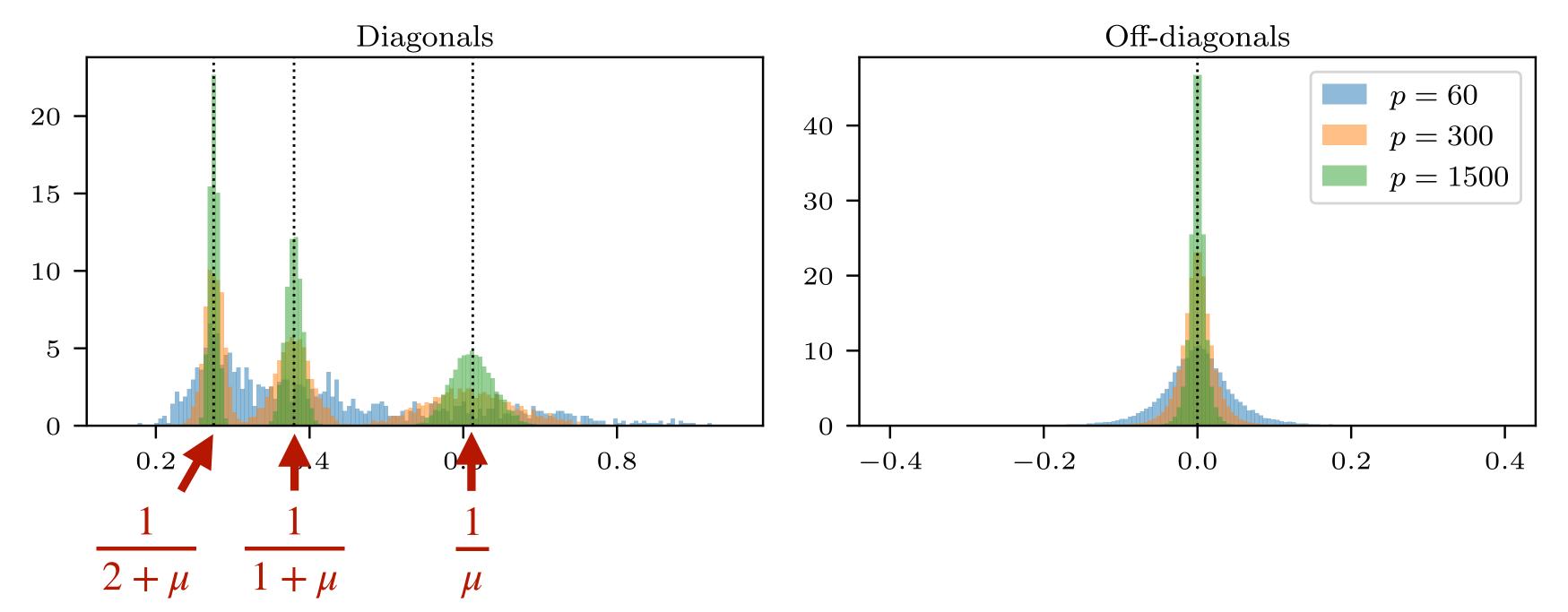
I.i.d. sketch

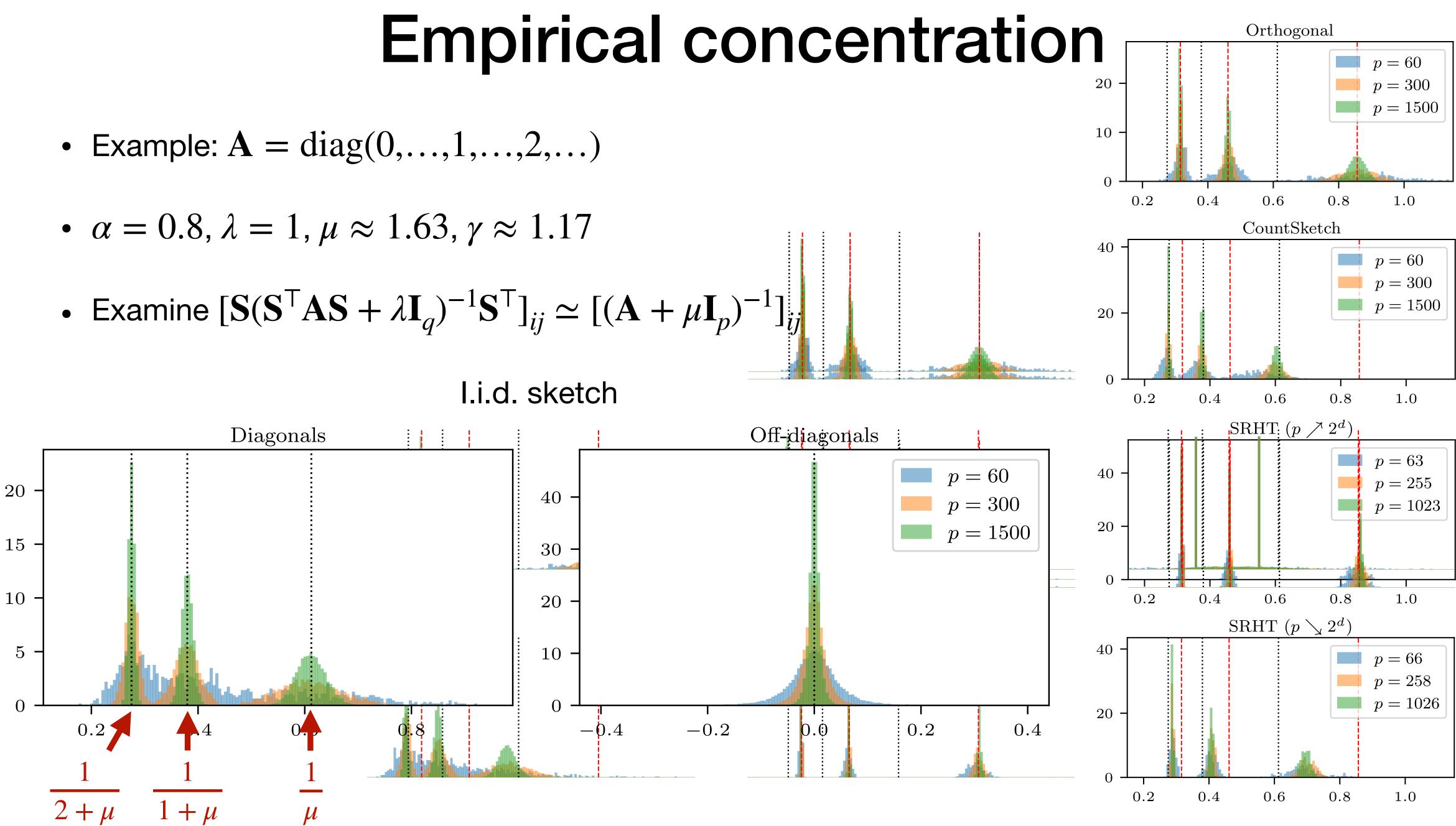


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I.i.d. sketch







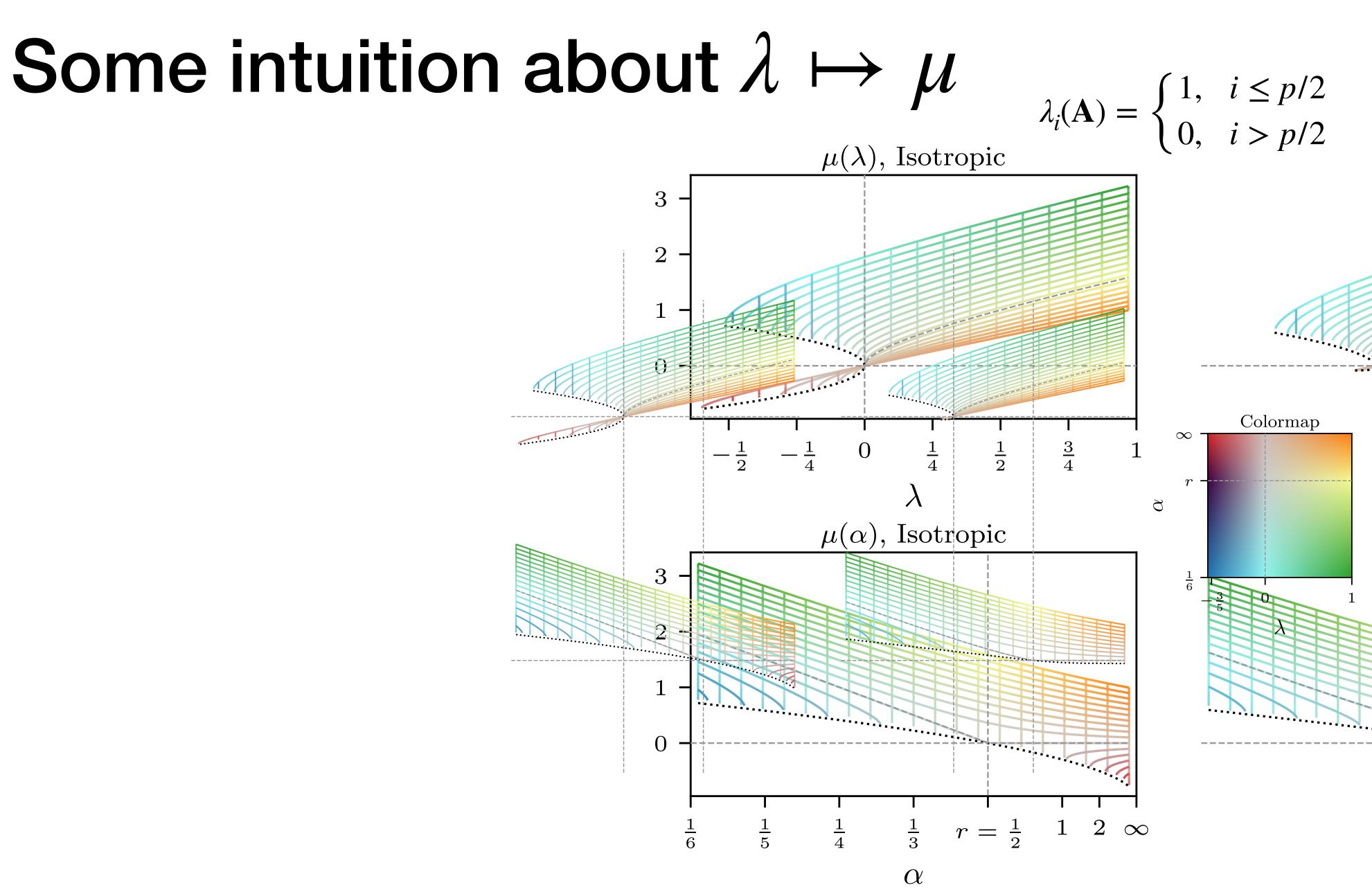




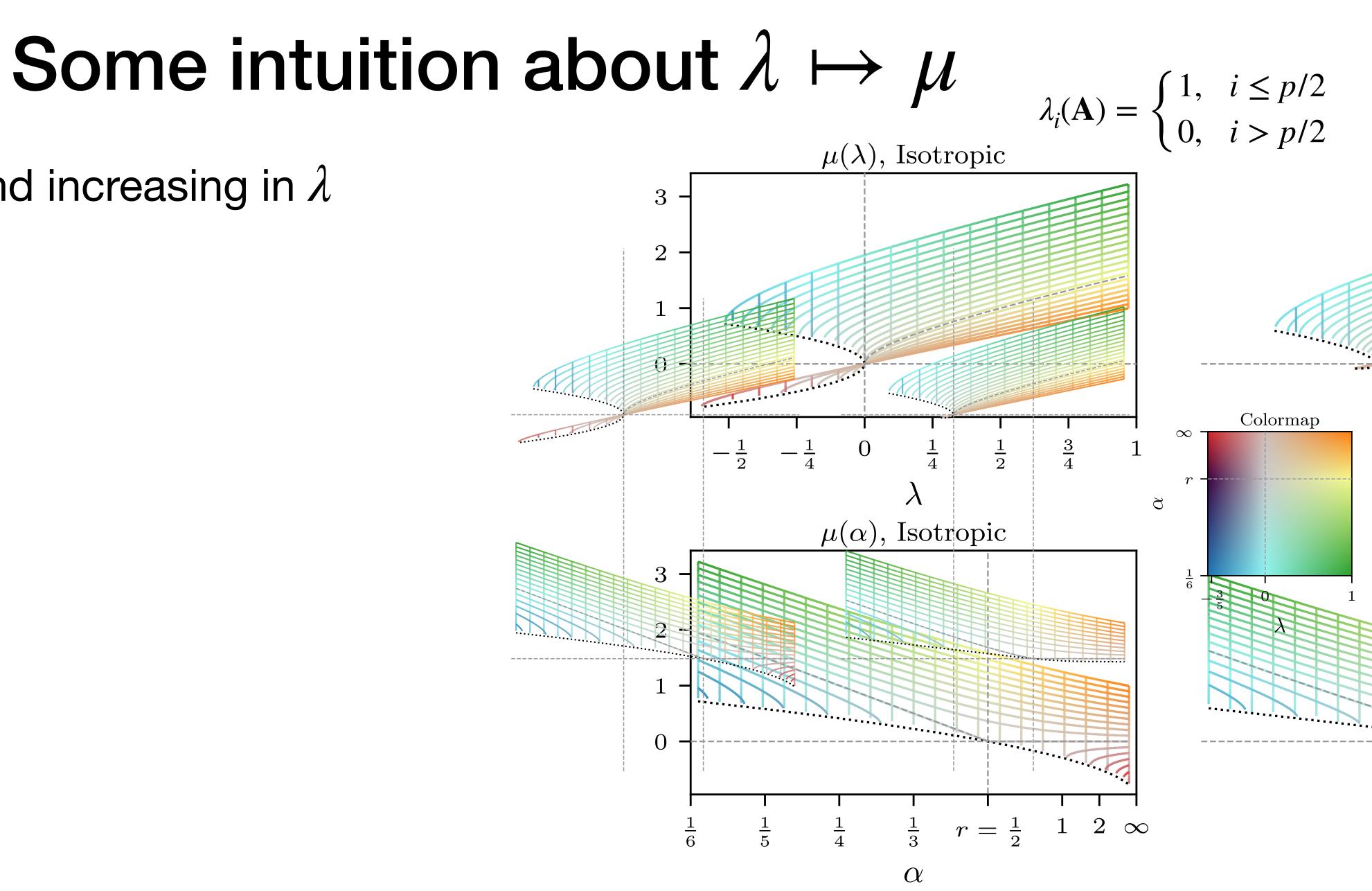




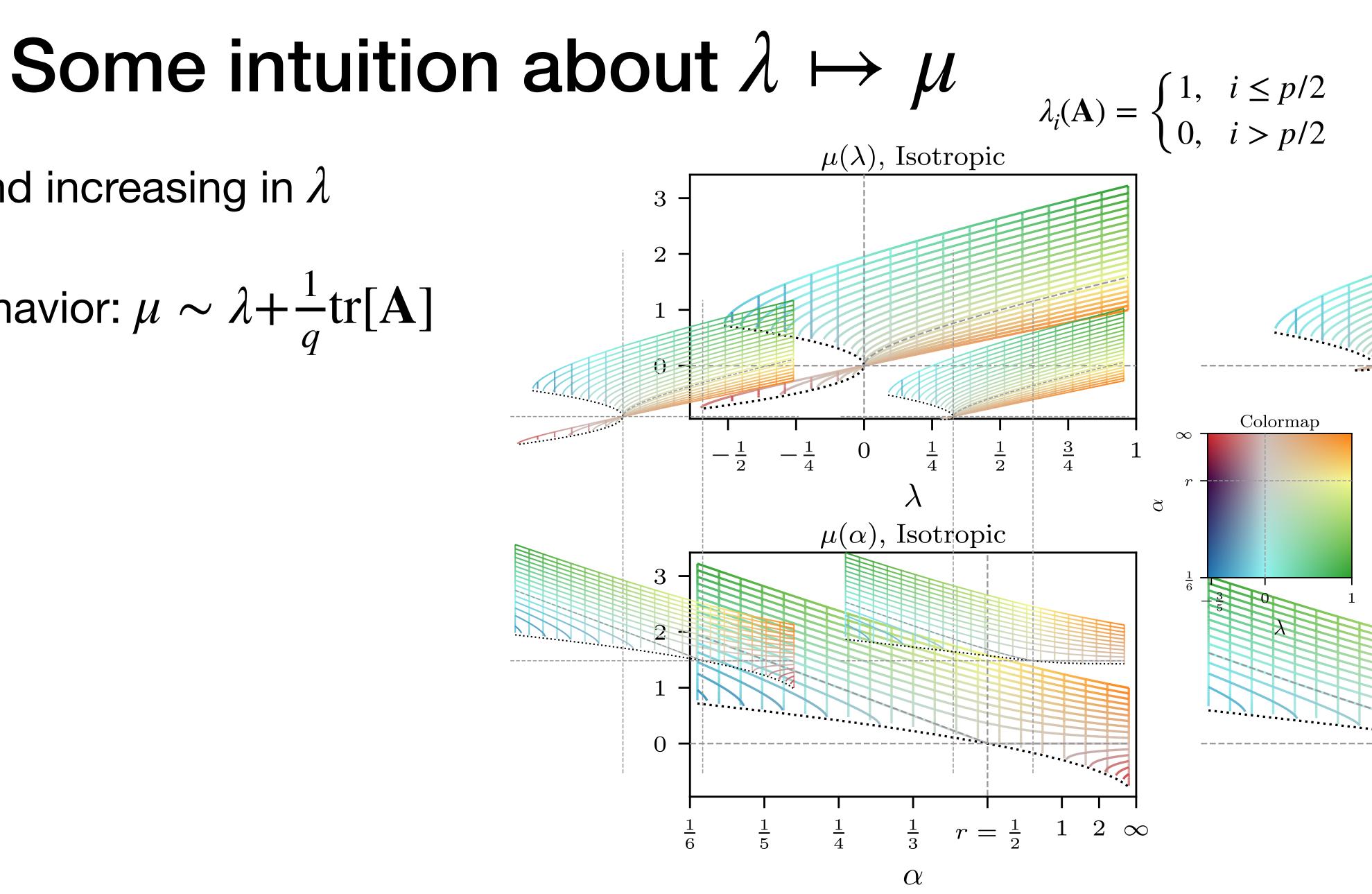
Some intuition about $\lambda \mapsto \mu$



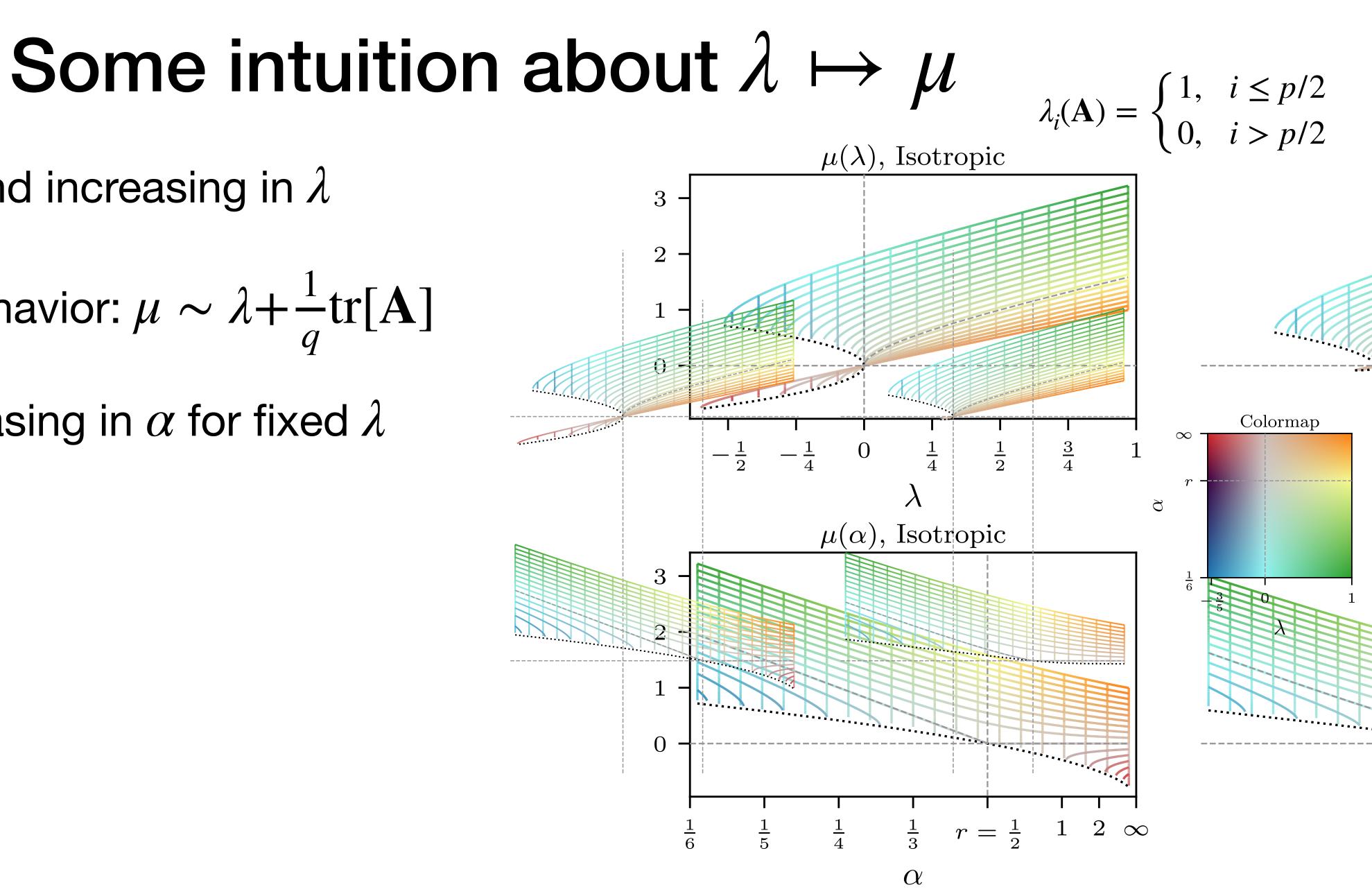
• Concave and increasing in λ



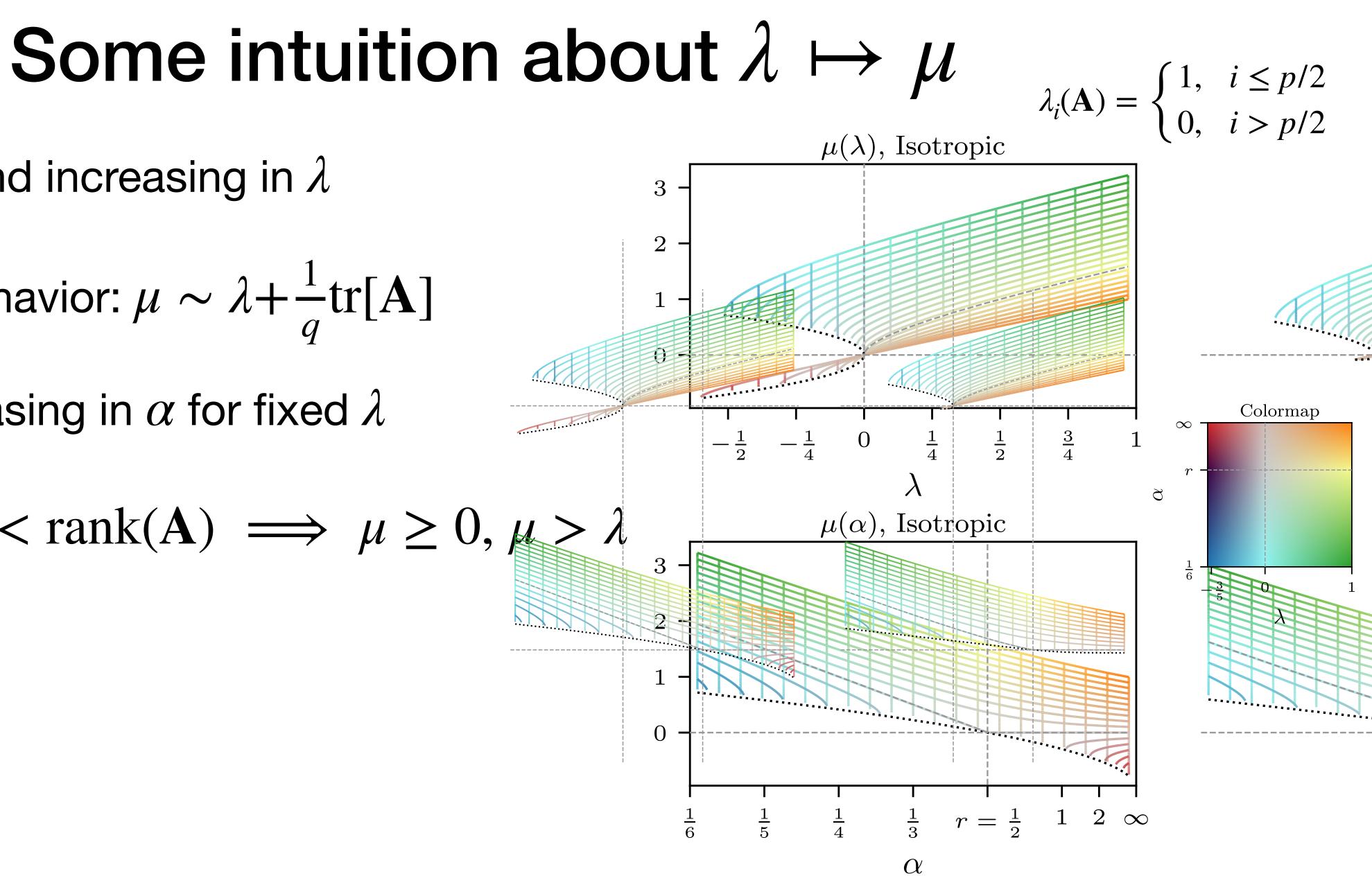
- Concave and increasing in λ
- Limiting behavior: $\mu \sim \lambda + \frac{1}{a} tr[\mathbf{A}]$



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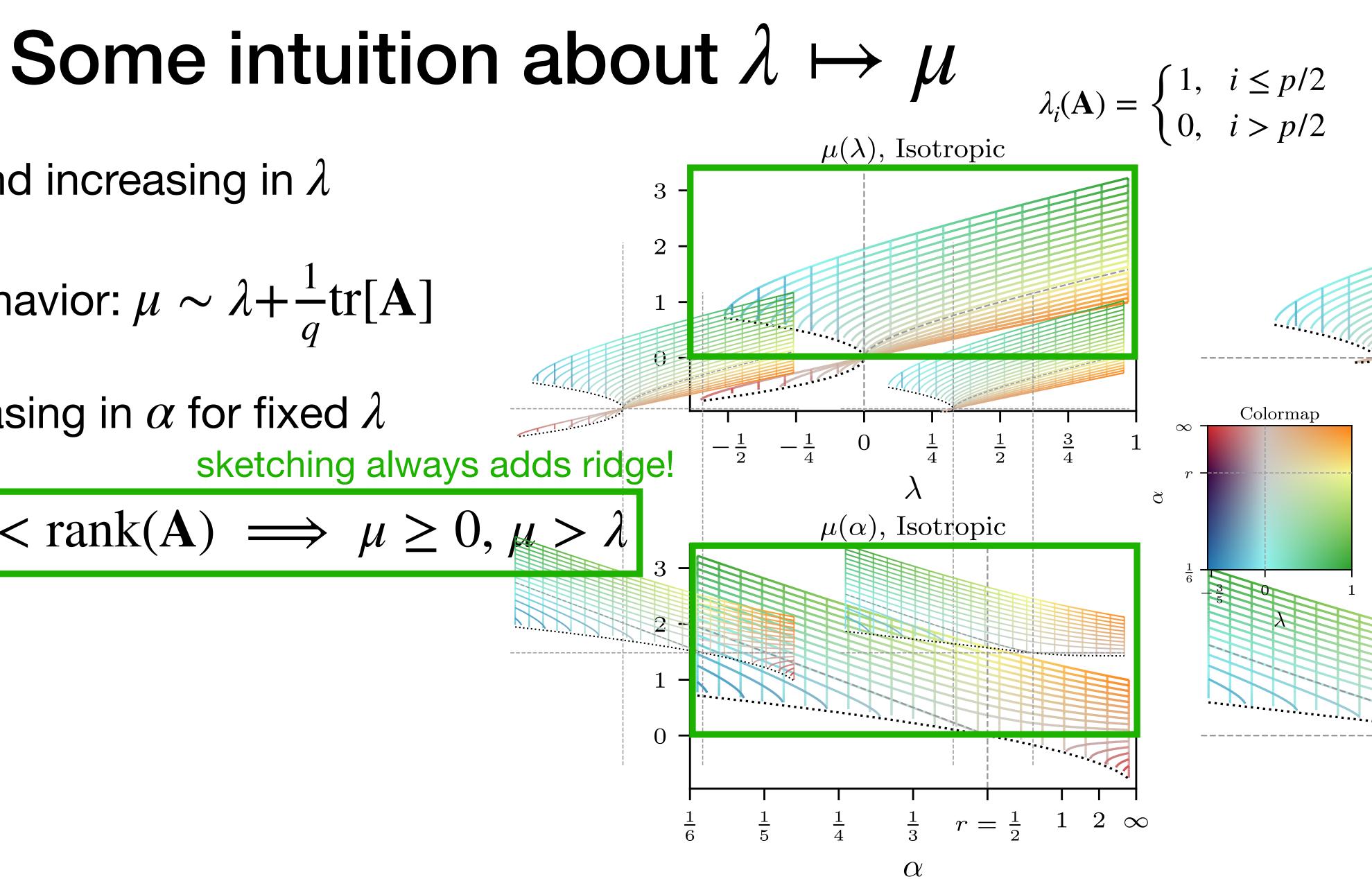


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- $\lambda > 0$ or $q < \operatorname{rank}(\mathbf{A}) \implies \mu \ge 0, \mu > \lambda$



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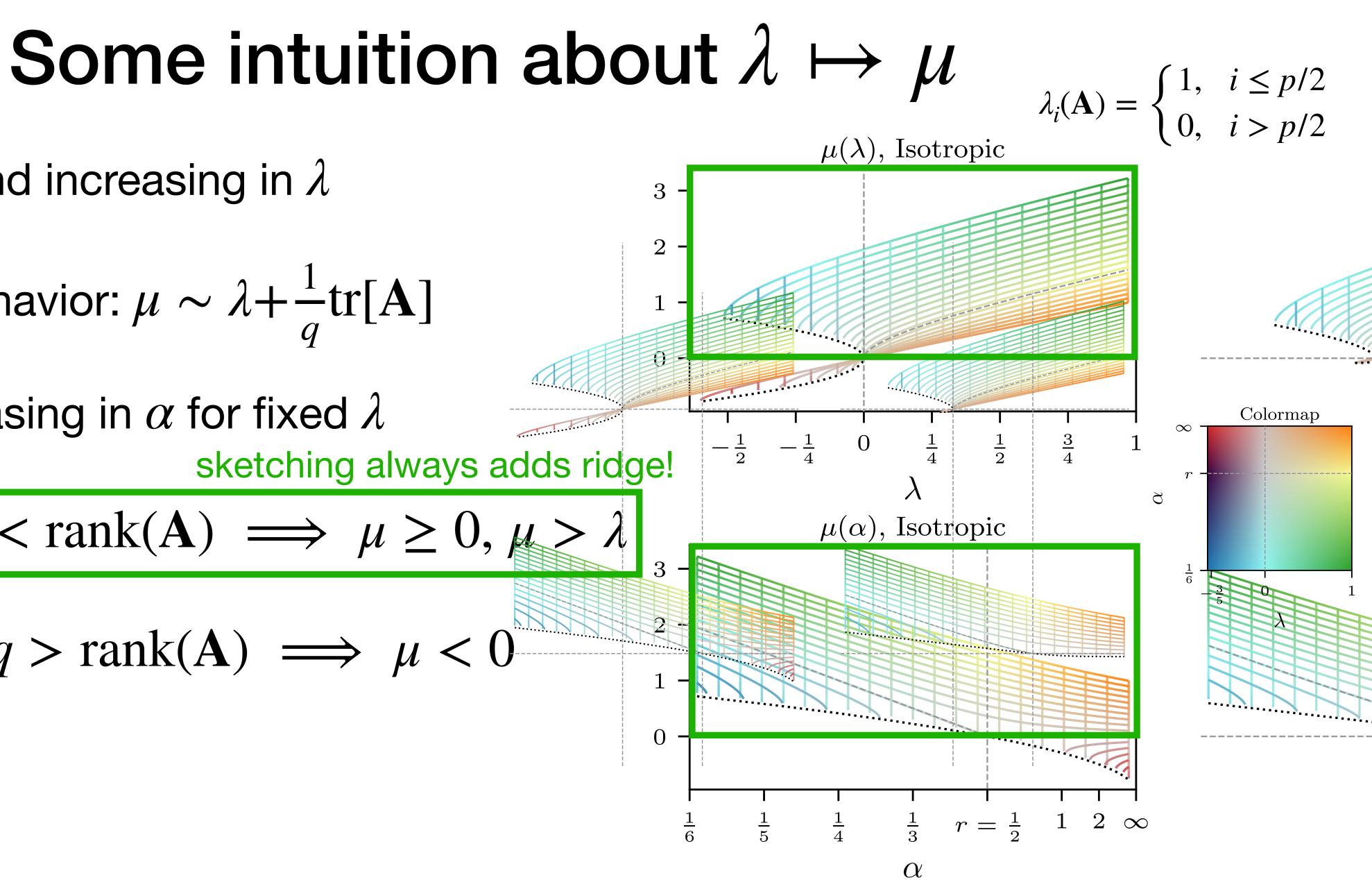
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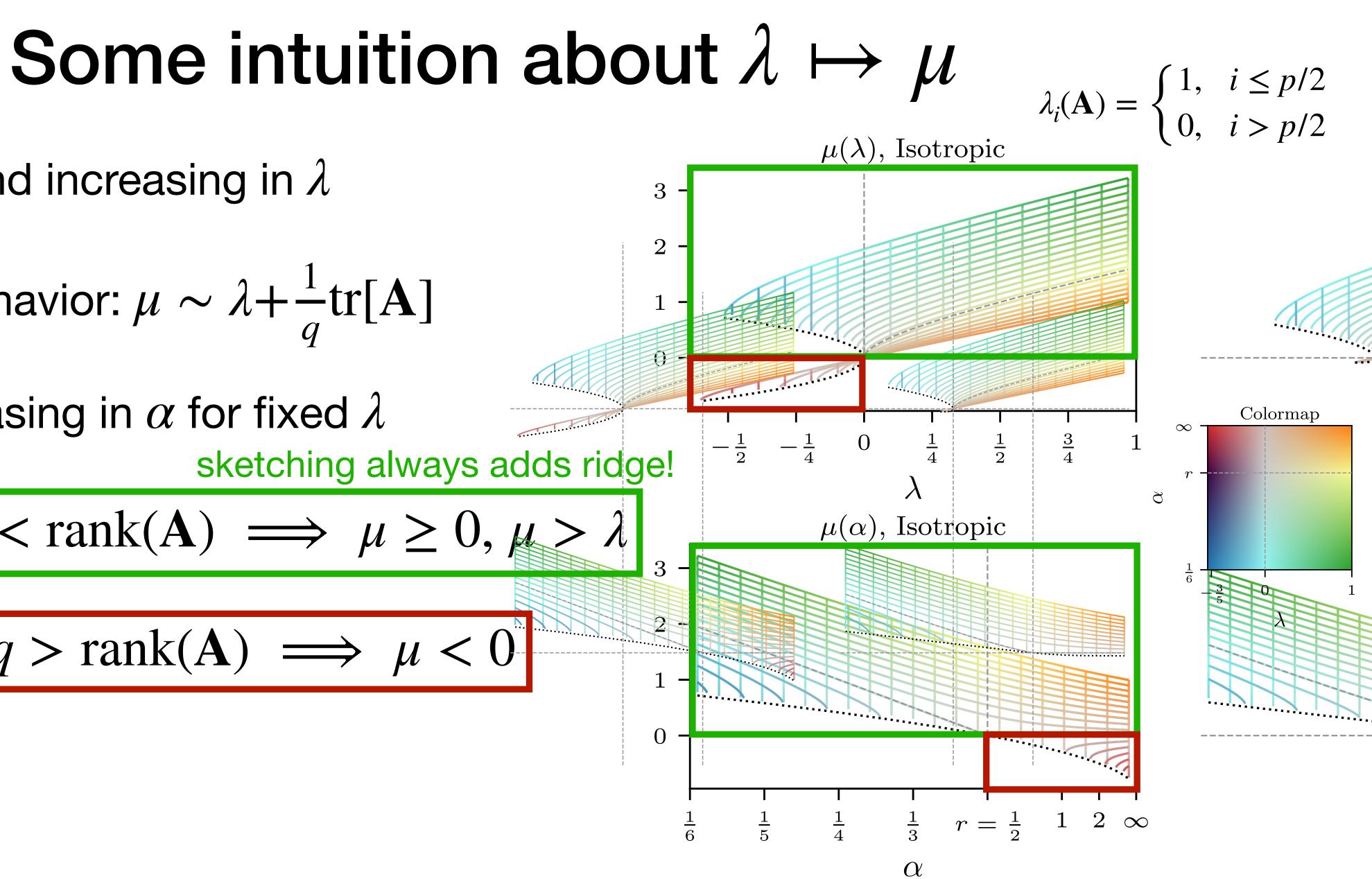
• $\lambda < 0$ and $q > \operatorname{rank}(\mathbf{A}) \implies \mu < 0$



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•
$$\lambda < 0$$
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Ridge regression risk?

Ridge regression risk? • Bias: $\hat{\mathbf{b}}_{\mathbf{S}} = \mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{S} + \lambda \mathbf{I}_{q})^{-1}\mathbf{S}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{y} \simeq (\mathbf{X}^{\mathsf{T}}\mathbf{X} + \mu \mathbf{I}_{q})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y} = \hat{\mathbf{b}}_{\mu}$

Ridge regression risk?

- What about risk? lacksquare

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- What about risk? \bullet
 - Problem: $\hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu} \iff \hat{\mathbf{b}}_{\mathbf{S}}^{\mathsf{T}} \hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu}^{\mathsf{T}} \hat{\mathbf{b}}_{\mu}$

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- What about risk? lacksquare
 - Problem: $\hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu} \iff \hat{\mathbf{b}}_{\mathbf{S}}^{\mathsf{T}} \hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu}^{\mathsf{T}} \hat{\mathbf{b}}_{\mu}$
 - Just like $\mathbb{E}[X] = \mathbb{E}[Y] \implies \mathbb{E}[X^2] = \mathbb{E}[Y^2]$

Ridge regression risk? • Bias: $\hat{\mathbf{b}}_{\mathbf{S}} = \mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{S} + \lambda \mathbf{I}_{a})^{-1}\mathbf{S}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{y} \simeq (\mathbf{X}^{\mathsf{T}}\mathbf{X} + \mu \mathbf{I}_{a})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y} = \hat{\mathbf{b}}_{u}$

- What about risk?
 - Problem: $\hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu} \iff \hat{\mathbf{b}}_{\mathbf{S}}^{\mathsf{T}} \hat{\mathbf{b}}_{\mathbf{S}} \simeq \hat{\mathbf{b}}_{\mu}^{\mathsf{T}} \hat{\mathbf{b}}_{\mu}$
 - Just like $\mathbb{E}[X] = \mathbb{E}[Y] \implies \mathbb{E}[X^2] = \mathbb{E}[Y^2]$
 - We need a second order equivalence to work out variance

 $\mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_{a})^{-1}\mathbf{S}^{\mathsf{T}}\mathbf{\Psi}\mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{A}\mathbf{S} + \lambda \mathbf{I}_{a})$

where

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

• Theorem (LeJeune, PP, et al., 2024). For any Ψ with uniformly bounded operator norm independent of S and the previous conditions, for i.i.d. S,

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• Proof idea: $\frac{\partial}{\partial z} (\mathbf{A} - z\mathbf{I})^{-1} = (\mathbf{A} - z\mathbf{I})^{-2}$ with carefully placed Ψ

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$$\frac{\Psi(\mathbf{A} + \mu \mathbf{I}_p)^{-2}]}{2^2 \mathbf{A}(\mathbf{A} + \mu \mathbf{I}_p)^{-2}]} \ge 0.$$

Ridge regression risk

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• Consider quadratic functional $R(\hat{\mathbf{b}}_{\mathbf{S}}) = \hat{\mathbf{b}}_{\mathbf{S}}^{\mathsf{T}} \Psi \hat{\mathbf{b}}_{\mathbf{S}} + \mathbf{h}^{\mathsf{T}} \hat{\mathbf{b}}_{\mathbf{S}} + c$

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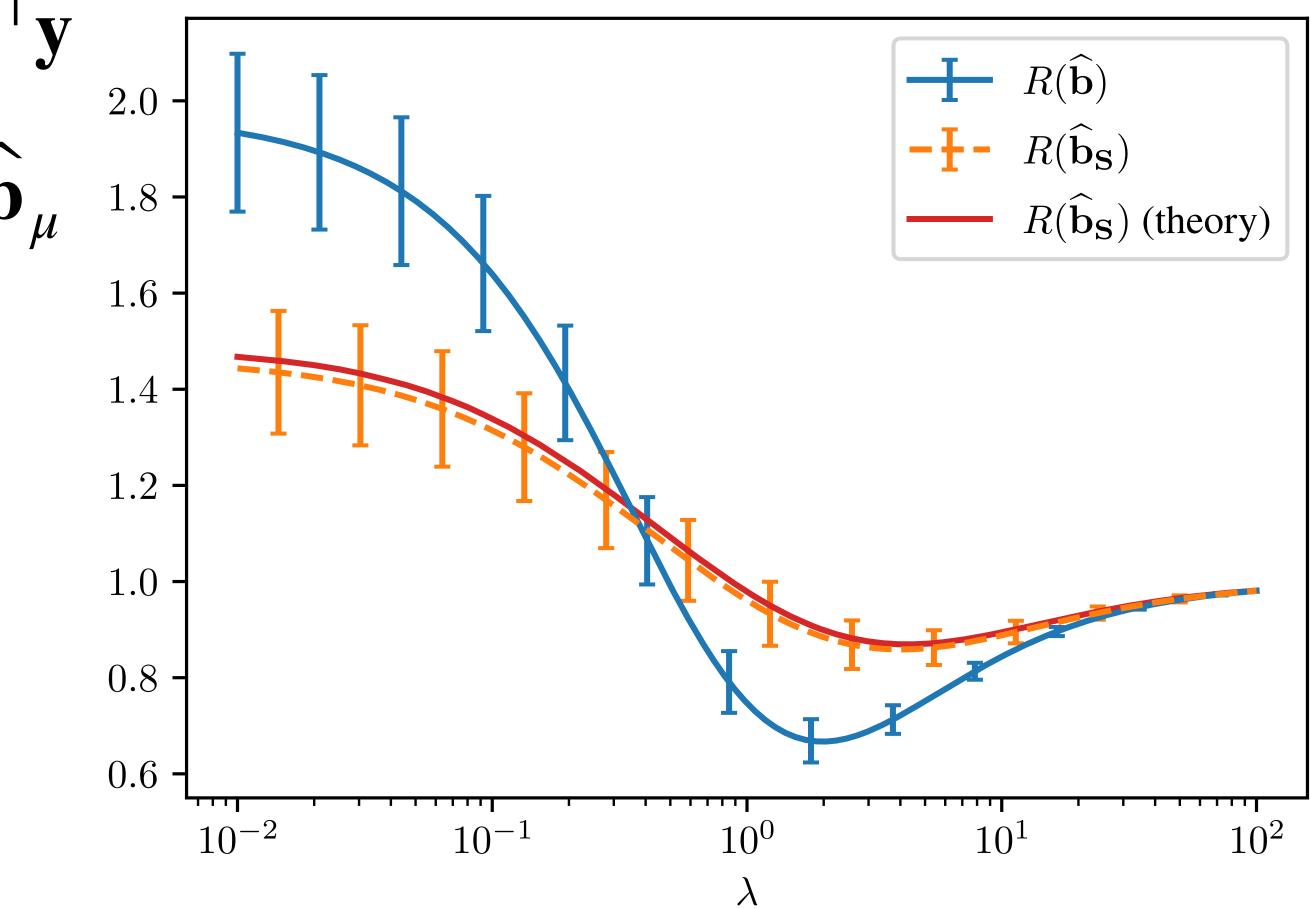
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$$\frac{1}{q} \operatorname{tr}[\mu^{2} \Psi(\mathbf{A} + \mu \mathbf{I}_{p})^{-2}] \frac{\partial \mu}{\partial \lambda}$$

$$\geq C \text{ if}$$

$$\operatorname{rank}(\Psi) > \operatorname{rank}(\mathbf{A}) \geq 1$$

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 - unless $\mu = 0$ and range(Ψ) \subseteq range(\mathbf{A})!

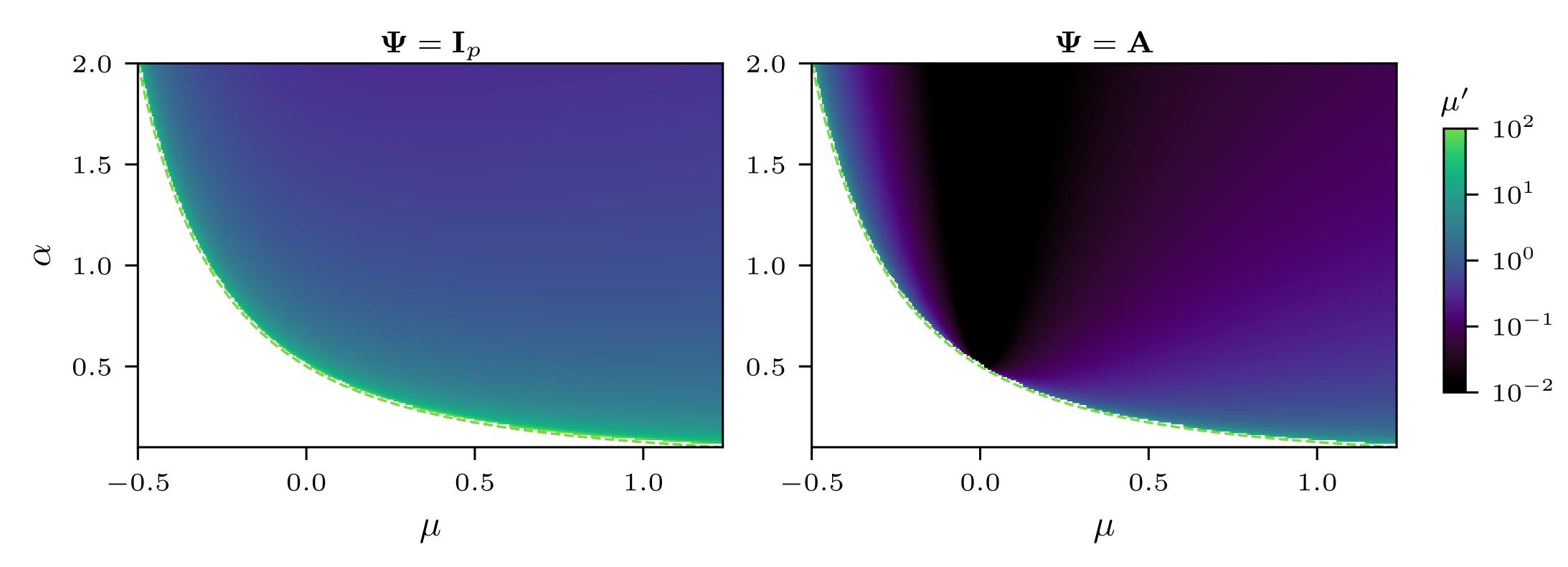
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 $\geq C \text{ if}$
 $\operatorname{rank}(\Psi) > \operatorname{rank}(\mathbf{A}) \geq 1$

When is sketching good/useful?

- When both $R(\hat{\mathbf{b}}_{\mu})$ and $\mu' \hat{\mathbf{b}}_{\mu}^{\top} \hat{\mathbf{b}}_{\mu}$ are small
 - $R(\hat{\mathbf{b}}_{\mu})$: λ should be less than μ =
 - μ' : consider alternate form $\mu' =$
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 - unless $\mu = 0$ and range(Ψ) \subseteq range(\mathbf{A})!
 - requires $\lambda = 0$ and $q > \operatorname{rank}(\mathbf{A})$

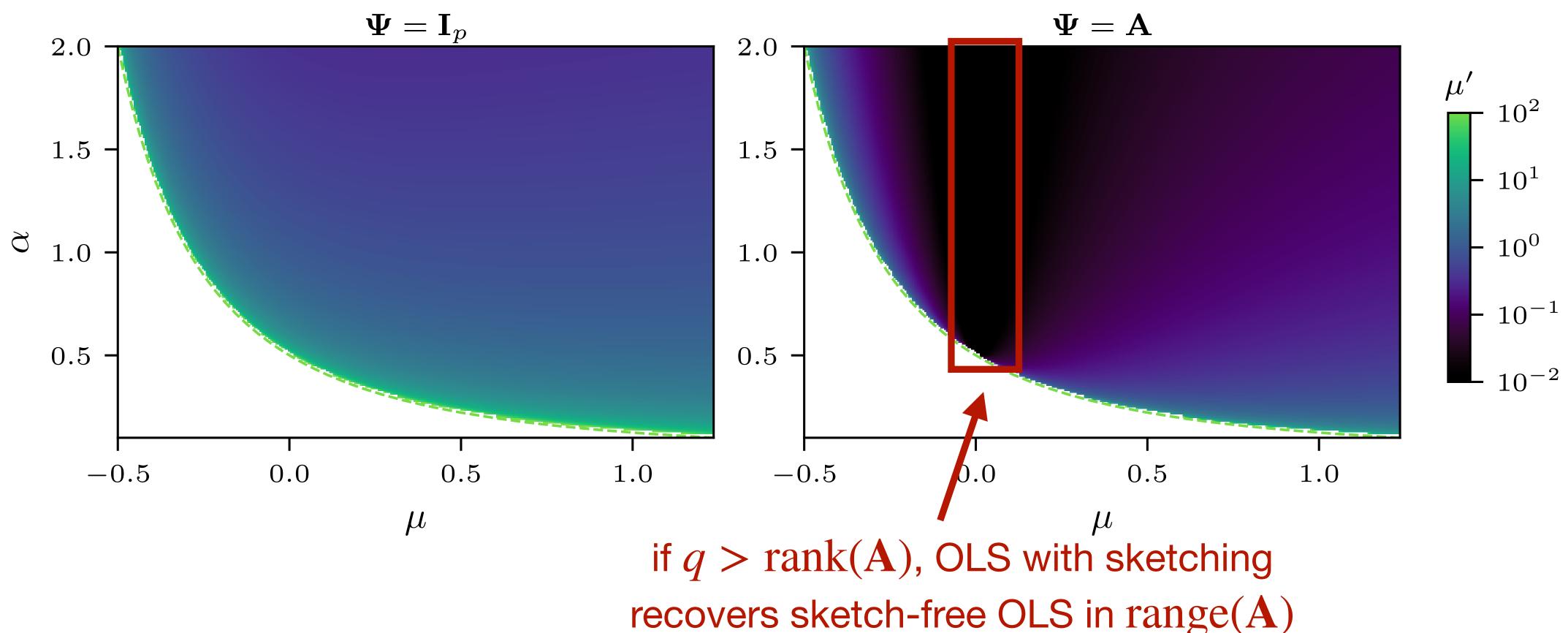
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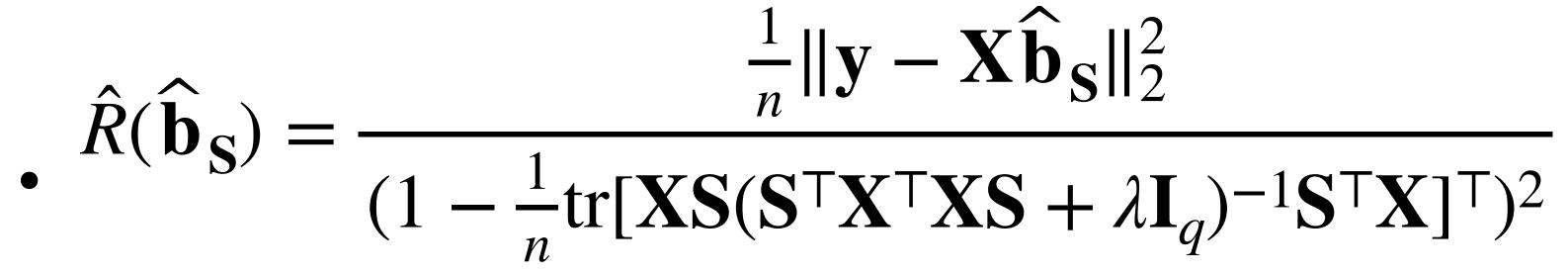
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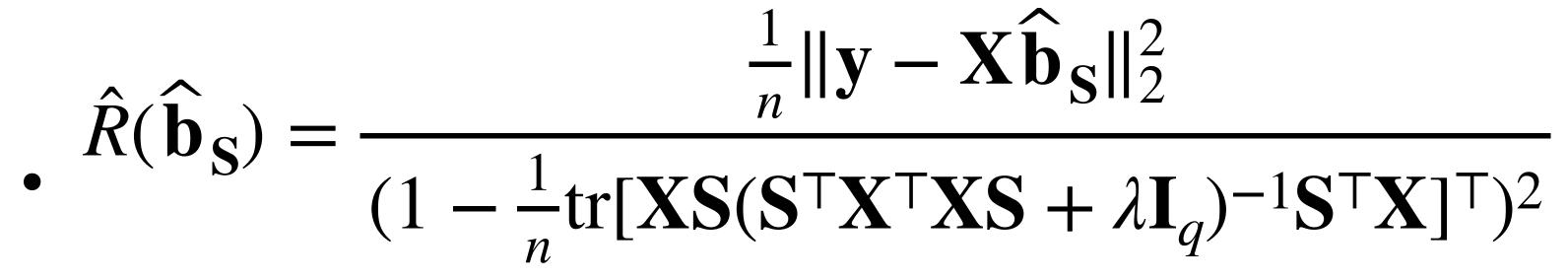
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Generalized cross-validation (GCV)

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- Costs the same as \widehat{b}_{S} to compute

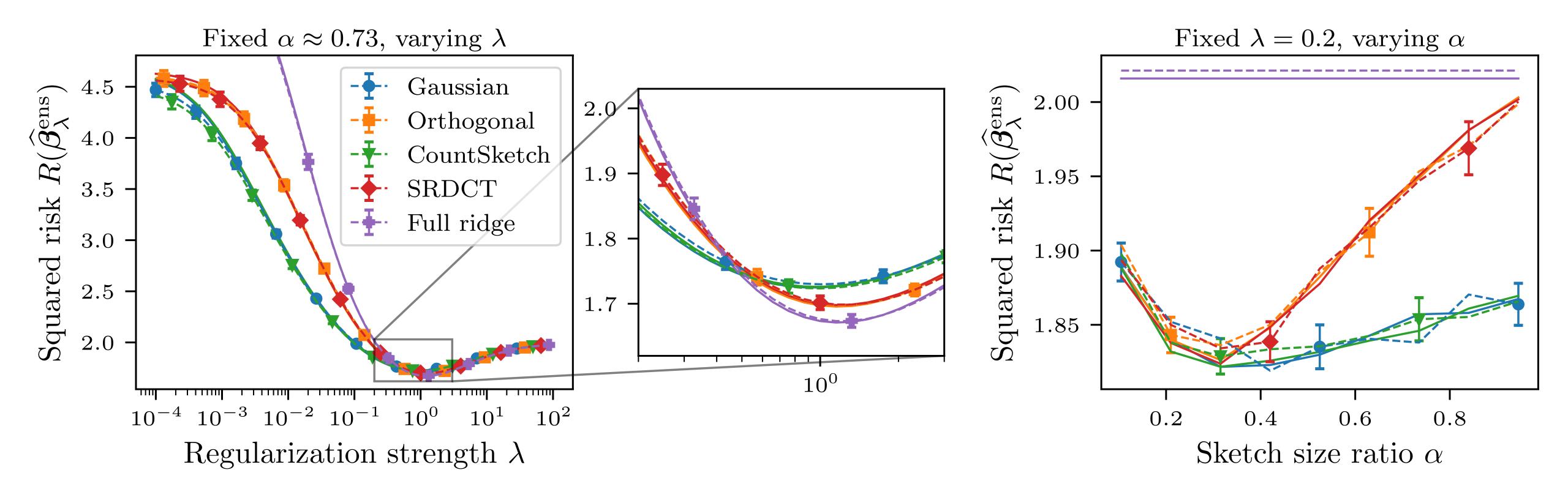
Generalized cross-validation (GCV)

 $\hat{R}(\hat{\mathbf{b}}_{\mathbf{S}}) = \frac{\frac{1}{n} \|\mathbf{y} - \mathbf{X}\hat{\mathbf{b}}_{\mathbf{S}}\|_{2}^{2}}{(1 - \frac{1}{n} \operatorname{tr}[\mathbf{X}\mathbf{S}(\mathbf{S}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{S} + \lambda\mathbf{I}_{q})^{-1}\mathbf{S}^{\mathsf{T}}\mathbf{X}]^{\mathsf{T}})^{2}}$

- Costs the same as $\hat{\mathbf{b}}_{\mathbf{S}}$ to compute
- Theorem (PP & LeJeune, 2024). For any asymptotically free sketch S, under random data assumptions on X,

 $R(\mathbf{b}_{\mathbf{S}}) \simeq R(\mathbf{b}_{\mathbf{S}})$

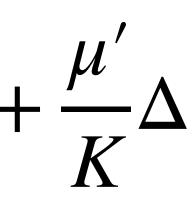
$$\hat{\mathbf{b}}_{\mathbf{S}}) \simeq R(\hat{\mathbf{b}}_{\mu}) + \mu' \Delta.$$



• Let $\widehat{\mathbf{b}}_{K} = \frac{1}{K} \sum_{k=1}^{K} \mathbf{S}_{k} (\mathbf{S}_{k}^{\top} \mathbf{X}^{\top} \mathbf{X} \mathbf{S}_{k} + \lambda \mathbf{I}_{q})^{-1} \mathbf{X}^{\top} \mathbf{y}$

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• Then $\hat{R}(\hat{\mathbf{b}}_{K}) \simeq R(\hat{\mathbf{b}}_{K}) \simeq R(\hat{\mathbf{b}}_{\mu}) + \frac{\mu'}{K}\Delta$

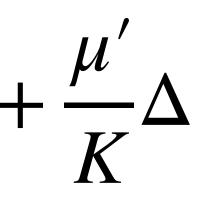


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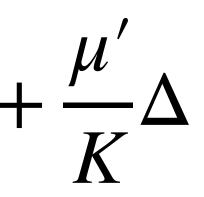
$$R(\hat{\mathbf{b}}_{\mu}) \simeq 2\hat{R}(\hat{\mathbf{b}}_{K=2}) - \hat{R}(\hat{\mathbf{b}}_{K=1})$$



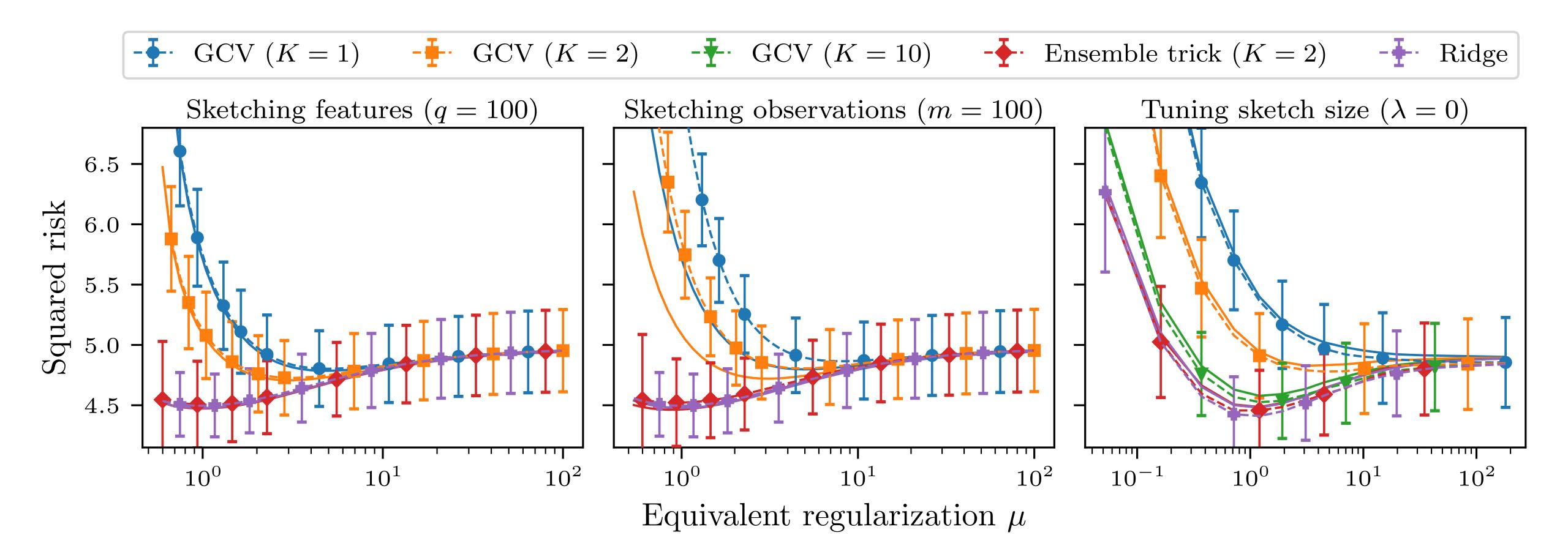
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- Given the mapping $\lambda \mapsto \mu$, this admits a consistent estimator $R(\hat{\mathbf{b}}_{\mu}) \simeq 2\hat{R}($
- Cost (for iterative solver) is $\mathcal{O}(4nq)$ versus $\mathcal{O}(2np)$, efficient if $q \ll p$



$$(\hat{\mathbf{b}}_{K=2}) - \hat{R}(\hat{\mathbf{b}}_{K=1})$$



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- Hilbert space.
- subsampled randomized Hadamard transform.
- scale regression.
- Dobriban, E., and Sheng, Y. (2021). Distributed linear regression by averaging. lacksquare
- the sketched pseudoinverse.
- \bullet validation, and tuning.

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