University of Pennsylvania
STAT 991: Random Matrix Theory Class Presentation

Asymptotic Risk of

High-Dimensional Regression

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Linear Regression

High-Dimensional Linear Regression

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$$\hat{\beta}_\lambda = \arg\min_{b \in \mathbb{R}^d} \left[\frac{1}{n} \sum_{i=1}^n \left(y_i - b^\top x_i \right)^2 + \lambda ||b||_2^2 \right] \tag{2}$$

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- **Random design assumption**: β is random with

$$\mathbb{E}[\beta] = 0 \quad \text{and} \quad \mathrm{Cov}(\beta) = \frac{\alpha^2}{d} I_{d\times d} \tag{3}$$

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- Ridge regression has a closed-form solution

$$\hat{\beta}_\lambda = (X^\top X + n\lambda I)^{-1} X^\top Y$$

Risk of the estimator

- **Question:** What is the risk of $\hat{\beta}_\lambda$?

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r_\lambda(X) &= \mathbb{E}\left[\left(x^\top \hat{\beta}_\lambda - x^\top \beta - \varepsilon\right)^2 \middle| X\right] \\
&= 1 + \mathbb{E}\left[\left\{x^\top\left(\hat{\beta}_\lambda - \beta\right)\right\}^2 \middle| X\right] \\
&= 1 + \mathbb{E}\left[\left(\hat{\beta}_\lambda - \beta\right)^\top \Sigma \left(\hat{\beta}_\lambda - \beta\right) \middle| X\right]
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- We can also write

$$
\begin{aligned}
\hat{\beta}_\lambda - \beta &= \left(X^\top X + \lambda n I\right)^{-1} X^\top (X\beta + \varepsilon) - \beta \\
&= -\lambda n \left(X^\top X + \lambda n I\right)^{-1} \beta + \left(X^\top X + \lambda n I\right)^{-1} X^\top \varepsilon
\end{aligned}
$$

Risk of the estimator

- If we plug this back to the risk, we get

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r_\lambda(X) = 1 &+ (\lambda n)^2 \, \mathbb{E}\left[\beta^\top \left(X^\top X + \lambda n I\right)^{-1} \Sigma \left(X^\top X + \lambda n I\right)^{-1} \beta \,\middle|\, X\right] \\
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- Set $\hat{\Sigma} = n^{-1} X^\top X$ and $\gamma_d = d/n$:

$$r_\lambda(X) = 1 + \frac{\gamma_d}{d} \operatorname{Tr}\left(\Sigma \left(\widehat{\Sigma} + \lambda I\right)^{-1}\right) + \left(\lambda \alpha^2 - \gamma_d\right) \frac{\lambda}{d} \operatorname{Tr}\left(\Sigma \left(\widehat{\Sigma} + \lambda I\right)^{-2}\right)$$

Risk of the estimator

So, to analyze the asymptotic risk, we should look at the following two traces:

- **Trace 1**:
$$\frac{\gamma_d}{d} \operatorname{Tr}\left(\Sigma\left(\widehat{\Sigma}+\lambda I\right)^{-1}\right)$$
- **Trace 2**:
$$\left(\lambda\alpha^2-\gamma_d\right)\frac{\lambda}{d} \operatorname{Tr}\left(\Sigma\left(\widehat{\Sigma}+\lambda I\right)^{-2}\right)$$

Notation and Assumptions

- For a matrix A, define

$$F_A(x) = p^{-1} \sum_{i=1}^{p} \mathrm{I}\left(\lambda_i(A) \leq x\right).$$

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- Assume that the spectral distribution F_Σ of Σ converges to a limit H supported on $[0, \infty)$.

Notation and Assumptions

- We defined the Stieltjes transform of a measure G as

$$m_G(z) = \int_{l=0}^{\infty} \frac{dG(l)}{l - z}, \quad z \in \mathbb{C} \backslash \mathbb{R}^+.$$

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- Stieltjes transform of the spectral measure of $\hat{\Sigma}$

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- The companion Stieltjes transform is defined as

$$\gamma(m(z) + 1/z) = v(z) + 1/z \text{ for all } z \in \mathbb{C}\backslash\mathbb{R}^+$$

A result of Ledoit and Péché (2011)

The main step to derive the limiting risk, is proving the following theorem:

Theorem (Ledoit and Péché (2011))

Assume that $m_{\widehat{\Sigma}}(z) \to m(z)$ *and let* $v(z)$ *be the companion transform for* $m(z)$*. We have*

$$\frac{1}{d}\operatorname{tr}\left(\Sigma\left(\widehat{\Sigma}+\lambda I_{d\times d}\right)^{-1}\right) \to_{a.s.} \frac{1}{\gamma}\left(\frac{1}{\lambda v(-\lambda)}-1\right) \quad \textit{as } n, d \to \infty$$

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Before we prove it, lets use it to derive the asymptotic risk.

Limiting Risk of Ridge Regression

- **First Trace**: Ledoit and Péché (2011) proves that

$$\frac{1}{d}\operatorname{tr}\left(\Sigma\left(\widehat{\Sigma}+\lambda I_{d\times d}\right)^{-1}\right)\to_{a.s.}\frac{1}{\gamma}\left(\frac{1}{\lambda v(-\lambda)}-1\right):=\kappa(\lambda)$$

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- After simplification, the limiting risk converges almost surely

$$r_\lambda(X)\to_{a.s.}\frac{1}{\lambda v(-\lambda)}\left\{1+\left(\frac{\lambda\alpha^2}{\gamma}-1\right)\left(1-\frac{\lambda v^\top(-\lambda)}{v(-\lambda)}\right)\right\}.$$

Properties of the Solution

- From the formula, the optimal ridge parameter λ is

$$\lambda^\star = \gamma\alpha^{-2},$$

and we have

$$r_{\lambda^\star}(X) \to_{a.s.} \frac{1}{\lambda^\star v(-\lambda^\star)}.$$

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- With $\Sigma = I_{d\times d}$, by the Marchenko-Pastur theorem we have

$$r_\lambda(X) \to 1 + \gamma m_I(-\lambda;\gamma) + \lambda\left(\lambda\alpha^2 - \gamma\right) m_I^\top(-\lambda;\gamma)$$

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  where $m_I(\cdot;\gamma)$ is the Stieltjes transform of the Marchenko Pastur law.
- In this case, the optimal risk can be written in a closed form.

Computing in the General Case

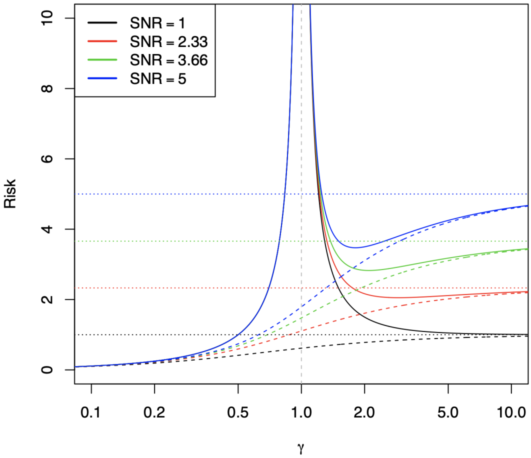
Silverstein and Choi (1995) show that $v(z)$ is the unique solution with positive imaginary part of the Silverstein equation:

$$-\frac{1}{v(z)} = z - \gamma \int \frac{t dH(t)}{1 + t v(z)}, z \in \mathbb{C}^+.$$

This equation can be solved by a fixed-point algorithm to compute $v(z)$ for all $z \in \mathbb{C}^+$.

Plots!

Assume $\Sigma = I$. This is the risk plot as a function of γ for ridgeless $\lambda \to 0$ (dashed) and optimal ridge (solid), for different SNRs.



Proof of Ledoit and Péché (2011)

[We will use bold symbols for matrices from now on]

- Remember that $\mathbf{X} \in \mathbb{R}^{n \times d}$ and define $\hat{\mathbf{\Sigma}} = \frac{1}{n}\mathbf{X}^\top\mathbf{X}$. Let $\mathbf{G} = (\lambda\mathbf{I} + \hat{\mathbf{\Sigma}})^{-1}$ be the resolvent.

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- We are interested in computing traces of the form

$$\frac{1}{d}\mathrm{Tr}(\mathbf{G}\mathbf{\Sigma}) \quad \text{and} \quad \frac{1}{d}\mathrm{Tr}(\mathbf{G})$$

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- There are many ways to do it; e.g., leave-one-out analysis, free probability, etc. Here, we use a method based on Stein's formula.

Proof of Ledoit and Péché (2011)

Let's first remind the Stein's formula. Hong Hu talked about it briefly last time:

Lemma (Stein's Formula)

Let $X \sim \mathcal{N}(0, \boldsymbol{\Sigma})$ and $f : \mathbb{R}^d \to \mathbb{R}$ have gradient with at most polynomial growth at infinity. Then for all $i_0 = 1, \ldots, d$:

$$\mathbb{E} X_{i_0} f\left(X_1, \ldots, X_d\right) = \sum_{k=1}^{d} \Sigma_{i_0 k}\, \mathbb{E}\left(\partial_k f\right)\left(X_1, \ldots, X_d\right)$$

Matrix version of Stein's formula

Theorem

For $\mathbf{F} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ *a good behaving matrix-valued function, we have*

$$\mathbb{E}\left[X^\top \mathbf{F}(X)X\right] = \mathbb{E}\left[\mathrm{Tr}\,\boldsymbol{\Sigma}\mathbf{F}(X)\right] + \mathbb{E}\sum_{k=1}^{d}\left(\boldsymbol{\Sigma}\left(\partial_k \mathbf{F}\right)(X)X\right)_k$$

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Proof.

$$\begin{aligned}
\mathbb{E} X^\top \mathbf{F}(X) X &= \mathbb{E} \sum_{ij} X_i X_j F(X)_{ij} \\
&= \mathbb{E} \sum_{ijk} \Sigma_{ik} \frac{\partial}{\partial X_k} X_j F(X)_{ij} \\
&= \mathbb{E} \sum_{ijk} \Sigma_{ik} \left[\delta_{j=k} F(X)_{ij} + X_j \left(\partial_k \mathbf{F}\right)(X)_{ij}\right] \\
&= \mathbb{E}\left[\operatorname{Tr} \boldsymbol{\Sigma} \mathbf{F}(X)\right] + \mathbb{E} \sum_{ijk} \Sigma_{ik} X_j \left(\partial_k \mathbf{F}\right)(X)_{ij} \\
&= \mathbb{E}\left[\operatorname{Tr} \boldsymbol{\Sigma} \mathbf{F}(X)\right] + \mathbb{E} \sum_{k} \left[\boldsymbol{\Sigma}\left(\partial_k \mathbf{F}\right)(X) X\right]_k
\end{aligned}$$

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- We want to write $\frac{1}{n}\mathrm{Tr}(\mathbf{G}\boldsymbol{\Sigma})$ in terms of $\frac{1}{n}\mathrm{Tr}(\mathbf{G})$.

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- Note that we have

$$\frac{1}{n}\mathrm{Tr}(\mathbf{G}\hat{\boldsymbol{\Sigma}}) = \frac{1}{n}\mathrm{Tr}\left(\mathbf{G}(\hat{\boldsymbol{\Sigma}} + \lambda I - \lambda I)\right) = \gamma - \frac{\lambda}{n}\mathrm{Tr}(\mathbf{G}).$$

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- We will start with $\frac{1}{n}\mathrm{Tr}(\mathbf{G}\hat{\boldsymbol{\Sigma}})$.

Proof of Ledoit and Péché (2011)

$$\mathbb{E}\left[X^\top \mathbf{F}(X)X\right] = \mathbb{E}\left[\operatorname{Tr} \mathbf{\Sigma}\mathbf{F}(X)\right] + \mathbb{E}\sum_{k=1}^{d} \left(\mathbf{\Sigma}\left(\partial_k \mathbf{F}\right)(X)X\right)_k$$

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$$\begin{aligned}
\mathbb{E}\operatorname{Tr}\mathbf{G}\hat{\boldsymbol{\Sigma}} &= \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\operatorname{Tr}\mathbf{G}X(i)X(i)^\top\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[X(i)^\top \mathbf{G}X(i)\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[\operatorname{Tr}\mathbf{G}\boldsymbol{\Sigma}\right] + \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{d}\mathbb{E}\left[e_k^\top \boldsymbol{\Sigma}\left(\frac{\partial}{\partial X(i)_k}\mathbf{G}\right)X(i)\right]
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\end{aligned}$$

What is $\frac{\partial \mathbf{G}}{\partial X(i)_k} = \frac{\partial}{\partial X(i)_k}\left[(\lambda \mathbf{I} + \hat{\boldsymbol{\Sigma}})^{-1}\right]$?

$$\frac{\partial\,\mathbf{G}}{\partial X(i)_k} = \frac{1}{n}\left[\mathbf{G}\left(e_k X(i)^\top + X(i)e_k^\top\right)\mathbf{G}\right]$$

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\begin{aligned}
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&= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{d}\mathbb{E}\left[e_k^\top \mathbf{\Sigma}\left(\mathbf{G}\left(e_k X(i)^\top + X(i)e_k^\top\right)\mathbf{G}\right)X(i)\right] \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{d}\mathbb{E}\left[e_k^\top \mathbf{\Sigma}\mathbf{G} e_k X(i)^\top \mathbf{G} X(i) + e_k^\top \mathbf{\Sigma}\mathbf{G} X(i) e_k^\top \mathbf{G} X(i)\right] \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{E}\left(\mathrm{Tr}(\mathbf{\Sigma}\mathbf{G})X(i)^\top \mathbf{G}X(i) + X(i)^\top \mathbf{G}\mathbf{\Sigma}\mathbf{G}X(i)\right) \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n}\mathbb{E}\left[\mathrm{Tr}(\mathbf{\Sigma}\mathbf{G})\,\mathrm{Tr}(\mathbf{G}\hat{\mathbf{\Sigma}})\right] + \frac{1}{n}\mathbb{E}\left[\mathrm{Tr}(\mathbf{G}\mathbf{\Sigma}\mathbf{G}\hat{\mathbf{\Sigma}})\right]
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\begin{aligned}
&\mathbb{E}\,\mathrm{Tr}\left[\mathbf{G}\hat{\mathbf{\Sigma}}\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{d}\mathbb{E}\left[e_k^\top \mathbf{\Sigma}\left(\mathbf{G}\left(e_k X(i)^\top + X(i)e_k^\top\right)\mathbf{G}\right)X(i)\right] \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{d}\mathbb{E}\left[e_k^\top \mathbf{\Sigma}\mathbf{G}e_k X(i)^\top \mathbf{G}X(i) + e_k^\top \mathbf{\Sigma}\mathbf{G}X(i)e_k^\top \mathbf{G}X(i)\right] \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{E}\left(\mathrm{Tr}(\mathbf{\Sigma}\mathbf{G})X(i)^\top \mathbf{G}X(i) + X(i)^\top \mathbf{G}\mathbf{\Sigma}\mathbf{G}X(i)\right) \\
&= \mathbb{E}\left[\mathrm{Tr}\,\mathbf{G}\mathbf{\Sigma}\right] + \frac{1}{n}\mathbb{E}\left[\mathrm{Tr}(\mathbf{\Sigma}\mathbf{G})\,\mathrm{Tr}(\mathbf{G}\hat{\mathbf{\Sigma}})\right] + \frac{1}{n}\mathbb{E}\left[\mathrm{Tr}(\mathbf{G}\mathbf{\Sigma}\mathbf{G}\hat{\mathbf{\Sigma}})\right]
\end{aligned}
$$

Dividing both sides by n and by Gaussian Lipschitz concentration inequality, we have

$$
\frac{1}{n}\,\mathrm{Tr}\left(\mathbf{G}\hat{\mathbf{\Sigma}}\right) = \frac{1}{n}\,\mathrm{Tr}(\mathbf{G}\mathbf{\Sigma}) + \frac{1}{n}\,\mathrm{Tr}(\mathbf{\Sigma}\mathbf{G})\cdot\frac{1}{n}\,\mathrm{Tr}(\mathbf{G}\hat{\mathbf{\Sigma}}) + o(1).
$$

Proof of Ledoit and Péché (2011)

We proved that

$$\frac{1}{n}\operatorname{Tr}\left(\mathbf{G}\hat{\mathbf{\Sigma}}\right) = \frac{1}{n}\operatorname{Tr}(\mathbf{G}\mathbf{\Sigma}) + \frac{1}{n}\operatorname{Tr}(\mathbf{\Sigma}\mathbf{G}) \cdot \frac{1}{n}\operatorname{Tr}(\mathbf{G}\hat{\mathbf{\Sigma}}) + o(1).$$

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This implies that

$$\frac{1}{n}\operatorname{Tr}(\mathbf{G}\mathbf{\Sigma}) \approx \frac{\frac{1}{n}\operatorname{Tr}\left(\mathbf{G}\hat{\mathbf{\Sigma}}\right)}{1 + \frac{1}{n}\operatorname{Tr}\left(\mathbf{G}\hat{\mathbf{\Sigma}}\right)} + o(1).$$

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We proved that

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In other words, we have

$$\begin{aligned}\frac{1}{n}\operatorname{Tr}\left((\lambda I + \hat{\mathbf{\Sigma}})^{-1}\mathbf{\Sigma}\right) &\approx \frac{\gamma - \frac{\lambda\gamma}{d}\operatorname{Tr}\left((\lambda I + \hat{\mathbf{\Sigma}})^{-1}\right)}{1 + \gamma - \frac{\lambda\gamma}{d}\operatorname{Tr}\left((\lambda I + \hat{\mathbf{\Sigma}})^{-1}\right)} + o(1) \\ &= \frac{1}{\gamma}\left(\frac{1}{\lambda v_{\hat{\mathbf{\Sigma}}}(-\lambda)} - 1\right) + o(1) \to \frac{1}{\gamma}\left(\frac{1}{\lambda v_{\mathbf{\Sigma}}(-\lambda)} - 1\right) \quad \square\end{aligned}$$

More General Results

Fixed β

- Eigenvalue Decomposition: $\Sigma \rightsquigarrow (s_1, v_1), \ldots, (s_d, v_d)$.
- Assume that

$$\widehat{H}_n(s) := \frac{1}{d} \sum_{i=1}^{d} 1_{\{s \geq s_i\}} \to H(s)$$

$$\widehat{G}_n(s) = \frac{1}{\|\beta\|_2^2} \sum_{i=1}^{d} \langle \beta, v_i \rangle^2 1_{\{s \geq s_i\}} \to G(s)$$

- Hastie, Montanari, Rosset, and Tibshirani (2020) derive the asumptotic risk in this case.

References

References

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  A short proof of Ledoit-Péché's RIE formula for covariance matrices
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Thank You!