Exponentiated Symmetric Matrix Distributions with Application to Linear Inverse Problems

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Symmetric Positive Definite Matrices

$A \in \mathbb{R}^{d \times d}$ is *symmetric positive definite* (SPD) if

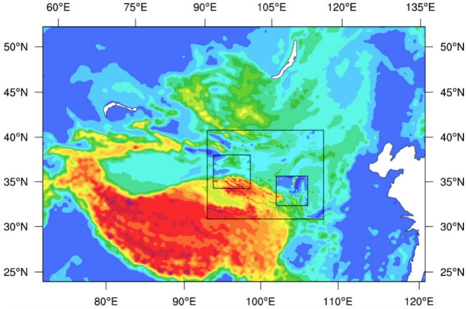
- $A = A^T$
- $\boldsymbol{y}^\top A \boldsymbol{y} > 0 \; \forall \boldsymbol{y} \neq 0 \Leftrightarrow \lambda_\mathrm{i}(\mathrm{A}) > 0, \; \mathrm{i} \in \{1, \ldots, \mathrm{d}\}$

For a random vector $\mathrm{X} \in \mathbb{R}^d$, the *covariance matrix* of X is defined as

- $\mathrm{cov}(\mathrm{X}, \mathrm{X}) = \mathbb{E}\left[(\mathrm{X} - \mathbb{E}[\mathrm{X}])(\mathrm{X} - \mathbb{E}[\mathrm{X}])^\top\right]$
- Always **positive semidefinite**.

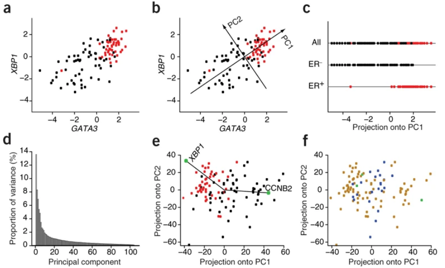
Why are Symmetric Positive Definite Matrices Useful?

Inverse problems. Source: TSA

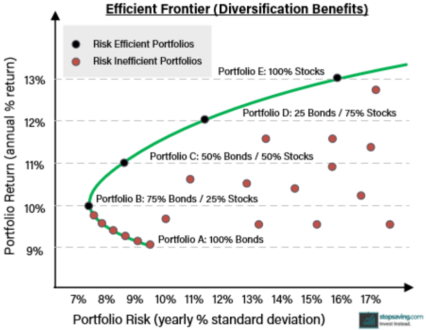


Sequential inference. Source: NCAR ensemble wind forecast

Why are Symmetric Positive Definite Matrices Useful?



Dimension reduction/PCA. Source: Ringnér 2008



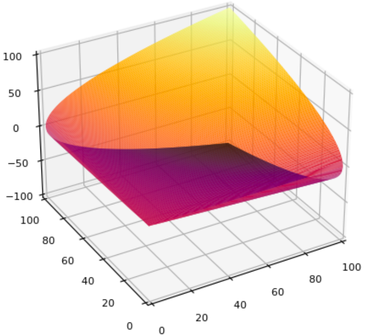
Finance, e.g., portfolio theory. Source: StopSaving.com

The Manifold of SPD Matrices

The set

$$\mathbb{P}_d = \{S \in \mathbb{R}^{d\times d} : S = S^\top,\ \lambda_i(S) > 0,\ i = 1, \ldots, d\}$$

is a **Riemannian manifold** with non-Euclidean geometry.



Exponentiation can be used to map symmetric matrices onto the manifold: given $\Sigma \in \mathbb{P}_d$, define

$$\exp_\Sigma(B) = \Sigma^{\frac{1}{2}} \exp(\Sigma^{-\frac{1}{2}} B \Sigma^{-\frac{1}{2}}) \Sigma^{\frac{1}{2}},$$

for $B \in \mathbb{H}_d = \{A \in \mathbb{R}^{d\times d} : A = A^\top\}$.

Random Matrix Theory

Random SPD matrix ensembles can be generated by exponentiating random symmetric matrices,

$$S = \exp_{\Sigma} \mathcal{E}, \quad \mathcal{E} \in \mathbb{H}_d,\ \mathbb{E}[\mathcal{E}] = 0$$

Our goal is to characterize these SPD matrix ensembles

- Joint element densities
- Spectral properties

Three Subprojects

Motivating Question

Given a parametric model for $\mathcal{E} \in \mathbb{H}_d$ with $\mathbb{E}[\mathcal{E}] = 0$, what can we say about the <u>transformed</u> random matrix $S = \exp_\Sigma \mathcal{E} \in \mathbb{P}_d$?

I. Characterizing symmetric matrix ensembles

II. Exponentiating symmetric matrix ensembles, $S = \exp_\Sigma \mathcal{E}$

III. Application: SPD Matrix Ensembles in Linear Inverse Problems

Characterizing Symmetric Matrix Ensembles

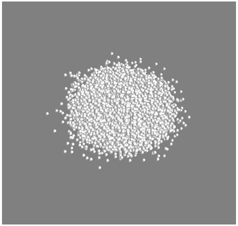
- Symmetric Matrix Ensembles
  - Elements are Independent
    - Gaussian Orthogonal, Uniform Ensemble
      - $A = (B + B^T)/2$ where B has ind. entries
        - $f(A) = \prod_{i \leq j} f(a_{ij})$
  - Elements are correlated
    - Colored Gaussian Symmetric Ensemble
      - $A = (B + B^T)/2$ where $B = \text{mat}(X)$, $X \sim \mathcal{N}(0, \Phi)$
        - $f(A)$ lacks product structure

Gaussian Orthogonal Ensemble

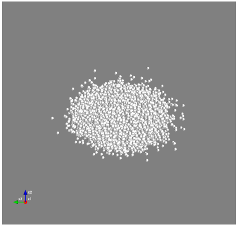
Let $B = [b_{ij}]$ where $b_{ij} \sim \mathcal{N}(0,1)$ and $A = \dfrac{B + B^T}{2}$

Then we have $A = [a_{ij}]$ with $a_{ij} \sim \mathcal{N}\left(0, \frac{1}{2}\right)$ for $i \neq j$ and $\mathcal{N}(0,1)$ for $i = j$

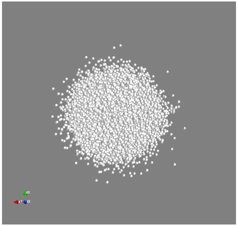
For $d = 2$, Let $A = \begin{bmatrix} a_1 & a_2 \\ a_2 & a_3 \end{bmatrix}$. We generate 10^4 realizations of A and plot in a_1-a_2-a_3 space



(a) Isometric view



(b) a_3-a_2 plane



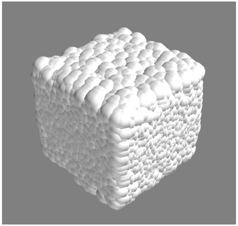
(c) a_1-a_3 plane

Uniform Ensemble

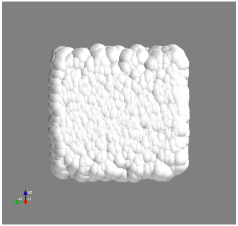
Let $B = [b_{ij}]$ where $b_{ij} \sim U(0,1)$ and $A = \dfrac{B + B^T}{2}$

Then we have $A = [a_{ij}]$ with $a_{ij} \sim Tri\left(0, 1, \frac{1}{2}\right)$ for $i \neq j$ & $U(0,1)$ for $i = j$

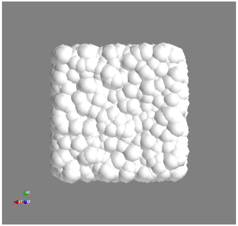
Visualizing A as previously,



(a) Isometric View



(b) a_3-a_2 plane



(c) a_1-a_3 plane

Colored Gaussian Symmetric Ensemble

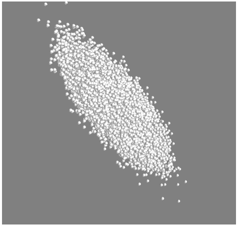
Illustration for $d = 2$

Let Φ be a 4×4 covariance matrix and $X = [x_1 \; x_2 \; x_3 \; x_4]^\top \sim \mathcal{N}(0, \Phi)$.

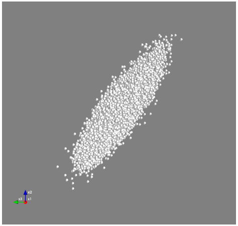
Set $B = \mathrm{mat}(X) = \begin{bmatrix} x_1 & x_3 \\ x_2 & x_4 \end{bmatrix}$ and $A = \begin{bmatrix} x_1 & (x_2 + x_3)/2 \\ (x_2 + x_3)/2 & x_4 \end{bmatrix}$.

We say $A \sim \mathrm{CGSE}(2, \Phi)$.

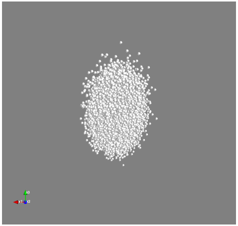
Visualizing A as previously,



(a) Isometric view



(b) a_3-a_2 plane



(c) a_1-a_3 plane

Eigenvalue Densities

Joint eigenvalue density for the Gaussian orthogonal ensemble:

$$f(\lambda_1, \ldots, \lambda_d) \propto \prod_{i<j} |\lambda_i - \lambda_j| \exp\left(-\sum_{i=1}^{d} \frac{\lambda_i^2}{2}\right)$$

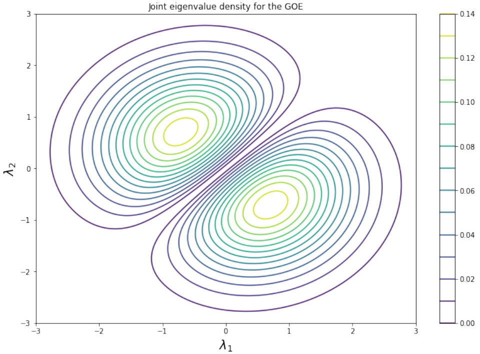
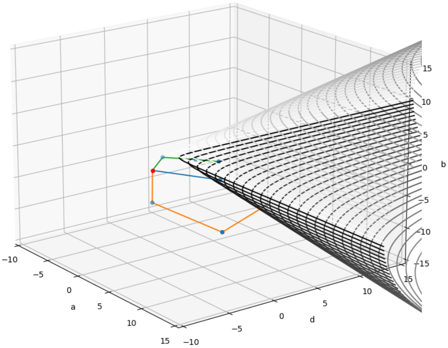


Figure 6: Contour plot of $f(\lambda_1, \lambda_2)$ in $d = 2$

Exponentiating Symmetric Matrix Ensembles



$$\mathcal{E} \in \mathbb{H}_d,\ \Sigma \in \mathbb{P}_d$$

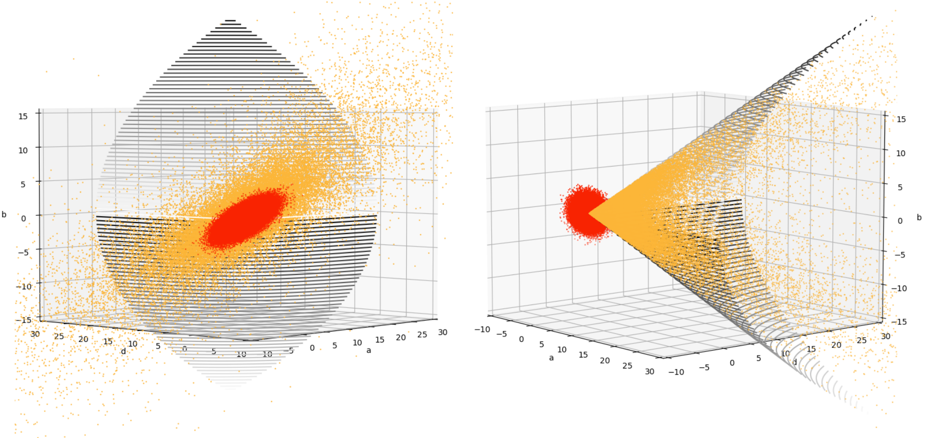
Matrix Exponential:

$$\begin{aligned}\exp(\mathcal{E}) &= \exp(Q^\top \Lambda Q) \\ &= Q^\top \exp(\Lambda) Q \\ &= Q^\top \mathrm{diag}\{e^{\lambda_1}, \cdots, e^{\lambda_n}\} Q\end{aligned}$$

Matrix Exponential With Base Σ:

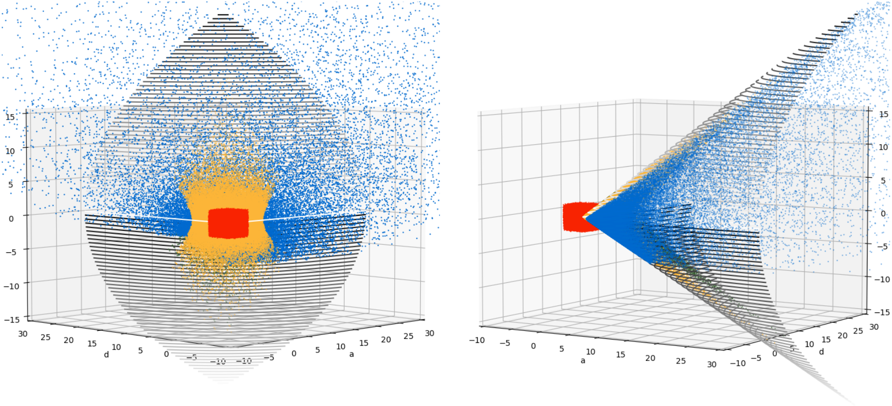
$$\begin{aligned}S &= \exp_\Sigma \mathcal{E} \\ &\equiv \Sigma^{1/2} \exp\left(\Sigma^{-1/2}\mathcal{E}\Sigma^{-1/2}\right)\Sigma^{1/2}\end{aligned}$$

Exponentiating Symmetric Matrix Ensembles



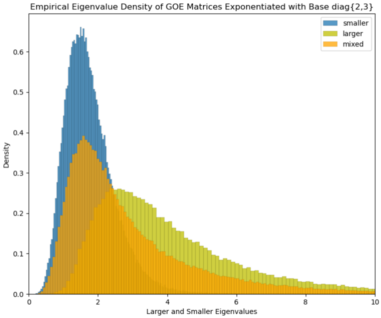
CGSE with $\Phi = \begin{bmatrix} 2 & 1 & 1 & -1 \\ 1 & 2 & 1 & -1 \\ 1 & 1 & 2 & -1 \\ -1 & -1 & -1 & 2 \end{bmatrix}$ exponentiated with base $\Sigma = I$.

Exponentiating Symmetric Matrix Ensembles

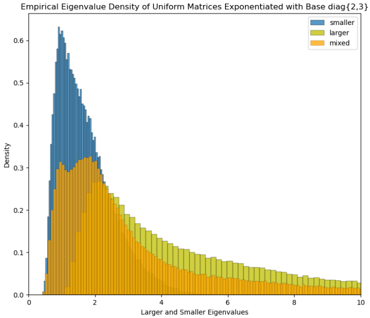


Uniform symmetric ensemble exponentiated with bases $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$ (yellow) and $\begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}$ (blue).

Empirical Eigenvalue Density



(a) Exponentiated GOE eigenvalue density



(b) Exponentiated uniform symmetric ensemble ($d = 2, r = 2$) eigenvalue density

Can we obtain the analytic expression for the eigenvalue density of exponentiated matrices?

Special Case: Diagonal Base in $d = 2$

What about the eigenvalue density of $\exp_\Sigma \mathcal{E}$ where $\mathcal{E} \sim \mathrm{GOE}(2)$ and $\Sigma \in \mathbb{P}_2$ diagonal?

We let

$$\Sigma = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \in \mathbb{P}_2,\ \mathcal{E} = \begin{bmatrix} x & y \\ y & z \end{bmatrix} \in \mathbb{H}_2$$

and consider the eigenvalues of

$$S = \exp_\Sigma \mathcal{E} = \Sigma^{\frac{1}{2}} \exp\left(\Sigma^{-\frac{1}{2}} \mathcal{E} \Sigma^{-\frac{1}{2}}\right) \Sigma^{\frac{1}{2}}$$

Special Case: Diagonal Base in $d = 2$

Set

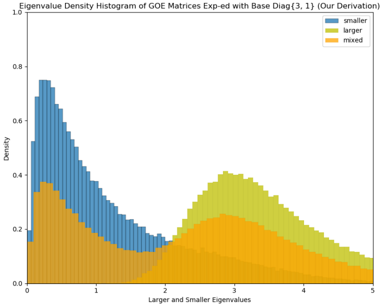
$$\Delta = a^2z^2 - 2abxz + b^2x^2 + 4aby^2, \quad u_1 = \frac{\sqrt{\Delta} + az - bx}{2\sqrt{\Delta}}, \quad u_2 = \frac{\sqrt{\Delta} - az + bx}{2\sqrt{\Delta}}$$

$$\lambda_1 = \frac{-\sqrt{\Delta} + az + bx}{2ab}, \quad \lambda_2 = \frac{\sqrt{\Delta} + az + bx}{2ab}$$

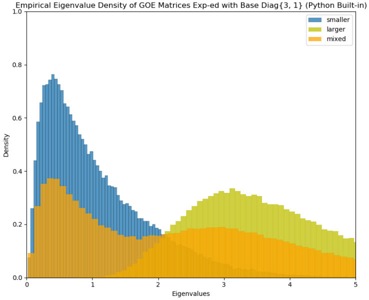
After much ~~weeping and gnashing of teeth~~ algebra, we have

$$\mu_{1,2} = \frac{1}{2}\left[\pm\sqrt{\begin{aligned}&\left(a(u_1e^{\lambda_1} + u_2e^{\lambda_2}) + b(u_2e^{\lambda_1} + u_1e^{\lambda_2})\right)^2 \\ &+ 4abe^{\lambda_1}e^{\lambda_2}(u_1 - u_2)^2\end{aligned}} \right. \\ \left. + a\left(u_1e^{\lambda_1} + u_2e^{\lambda_2}\right) + b\left(u_2e^{\lambda_1} + u_1e^{\lambda_2}\right)\right]$$

Special Case: Diagonal Base in $d = 2$



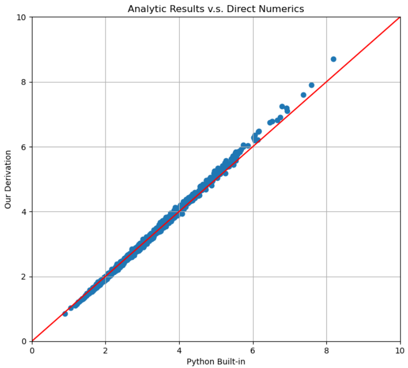
(a) Density rendered by our formula for eigenvalues



(b) Empirical density rendered by Python built-in functions (iterative method)

Special Case: Diagonal Base in $d = 2$

Reliability of The Derivation



Eigenvalue results computed from analytic formula compared with Python built-in functions for eigenvalue computation:

$$\mathcal{E} \sim \mathrm{GOE}(2)$$

$$\Sigma = \begin{bmatrix} 30 & 0 \\ 0 & 3 \end{bmatrix}$$

Linear Inverse Problems

$$\boldsymbol{d} = \boldsymbol{A}\boldsymbol{s} + \boldsymbol{\epsilon}$$

where

- $\boldsymbol{d} \in \mathbb{R}^m$ is observed data
- $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the known forward operator
- $\boldsymbol{s} \in \mathbb{R}^n$ is unknown information we want to recover
- $\boldsymbol{\epsilon} \in \mathbb{R}^m$ is measurement error

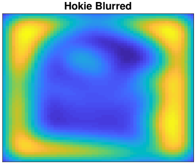
One may try to use least squares to solve for $\boldsymbol{s}$.

When Least Squares Fails

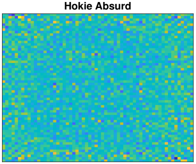
Least squares solution:

$$\boldsymbol{s}_{ls} = \underset{\boldsymbol{s}\in\mathbb{R}^n}{\arg\min}(||\boldsymbol{d} - \boldsymbol{A}\boldsymbol{s}||^2) \iff \boldsymbol{A}^T\boldsymbol{A}\boldsymbol{s}_{ls} = \boldsymbol{A}^T\boldsymbol{d}$$

(a) Original Image



(b) Given Image($\boldsymbol{d}$)



(c) due Lst. squares ($\boldsymbol{s}_{ls}$)

We need **regularization** in order to obtain reasonable solutions[1]

[1] Example couresty of Mark Embree (Virginia Tech)

Bayesian Formulation

One way to regularize the solution is to adopt a *Bayesian* framework. Assume

$$\boldsymbol{s} \sim \mathcal{N}(\mu, \alpha^2 \Gamma_{\text{prior}}) \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 \Gamma_{\text{noise}})$$

We use these assumptions and Bayes' Theorem to obtain a posterior probability distribution for $\boldsymbol{s}$ given $\boldsymbol{d}$, $\pi_{\text{post}}(\boldsymbol{s}|\boldsymbol{d})$

Bayesian Formulation

Bayes' Theorem: $\pi_{\text{post}}(\boldsymbol{s}|\boldsymbol{d}) \propto \pi_{\text{prior}}(\boldsymbol{s})\pi(\boldsymbol{d}|\boldsymbol{s})$.

Gaussian assumptions:

$$\pi_{\text{prior}}(\boldsymbol{s}) \propto \exp\left(-\frac{1}{2\alpha^2}\left((\boldsymbol{s}-\mu)^T\Gamma_{\text{prior}}^{-1}(\boldsymbol{s}-\mu)\right)\right)$$

$$\pi(\boldsymbol{d}|\boldsymbol{s}) \propto \exp\left(-\frac{1}{2\sigma^2}\left((\boldsymbol{d}-A\boldsymbol{s})^T\Gamma_{\text{noise}}^{-1}(\boldsymbol{d}-A\boldsymbol{s})\right)\right)$$

With $\Gamma_{\text{prior}}^{-1} = L^TL$ and $\Gamma_{\text{noise}}^{-1} = W^TW$ and setting $\lambda = \frac{\sigma}{\alpha}$ we have:

$$\pi_{\text{post}}(\boldsymbol{s}|\boldsymbol{d}) \propto \exp\left(-\frac{1}{2\sigma^2}\left(||W(\boldsymbol{d}-\boldsymbol{A}\boldsymbol{s})||^2 + \lambda^2||L(\boldsymbol{s}-\boldsymbol{\mu})||^2\right)\right)$$

Bayesian Formulation

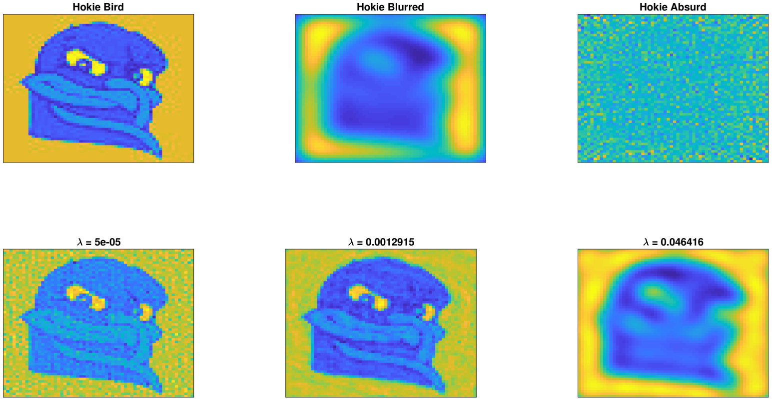
By maximizing $\pi_{\text{post}}(\boldsymbol{s}|\boldsymbol{d})$, we get the *maximum a posteriori* estimate $\boldsymbol{s}_{\text{map}}$ for $\boldsymbol{s}$,

$$\boldsymbol{s}_{\text{map}} = \arg\min_{\boldsymbol{s}}(||W(\boldsymbol{d} - \boldsymbol{A}\boldsymbol{s})||^2 + \lambda^2||L(\boldsymbol{s} - \boldsymbol{\mu})||^2)$$

$$\Updownarrow$$

$$\boldsymbol{s}_{\text{map}} = (\boldsymbol{A}^T\Gamma_{\text{noise}}^{-1}\boldsymbol{A} + \lambda^2\Gamma_{\text{prior}}^{-1})^{-1}(\boldsymbol{A}^T\Gamma_{\text{noise}}^{-1}\boldsymbol{d} + \lambda^2\Gamma_{\text{prior}}^{-1}\boldsymbol{\mu})$$

Bayesian Linear Inverse Problems



Reconstruction quality is dependent on choice of **regularization parameter** λ

From Linear Inverse Problems to Random Matrices

For fixed data and forward operator, the solution to a linear inverse problem is *parametrized* by Γ_{prior} and Γ_{noise}

- Usually $\Gamma_{\text{noise}} = I$ for white noise
- Γ_{prior} is a modeling choice, and we want the final image to have high reconstruction accuracy

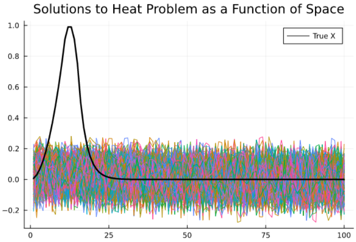
We model $\Gamma_{\text{prior}} = \exp_{\Sigma}(\mathcal{E})$ where $\mathcal{E}$ is a symmetric random matrix with $\mathbb{E}[\mathcal{E}] = 0$ and Σ is a chosen SPD matrix.

Given this distribution for Γ_{prior}, we are interested in the distribution of $\boldsymbol{s}_{\text{map}}$

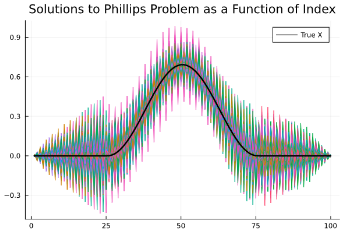
SPD Matrix Ensembles in Linear Inverse Problems

Matrix exponentiation tends to inflate condition number

- Well-studied phenomenon in differential equations (e.g., Loan 1977)
- When the prior covariance matrix is ill-conditioned, the optimal regularization parameter is $\approx 0 \Rightarrow$ **reversion to least squares**



(a) Heat Problem with $\lambda = 1$



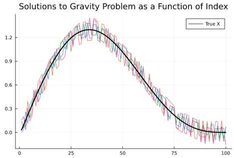
(b) Phillips Problem with $\lambda = 10^{-10}$

Controlling Conditioning

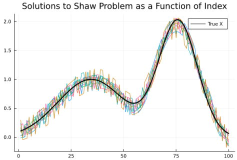
- Random Perturbation
  - For poorly conditioned A, the sum $M = A + N_n$ for random N_n is well-conditioned with high probability (Tao and Vu 2007)
  - If $A \in \mathbb{P}_d$, sample N_n from the Wishart Ensemble to ensure $M \in \mathbb{P}_d$
- Damping the Inversion
  - $M = A + cI$
  - Inflating the diagonal stabilizes eigenvalues
  - c is known as the Marquardt-Levenberg coefficient
  - Tradeoff between stabilizing matrix and retaining original information

Linear Inverse Problem Solutions

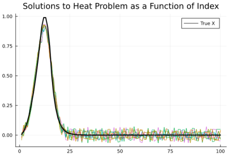
- Damping the inversion provides considerable improvement to input data reconstruction across a range of regularization parameters
  - $\mathcal{E} \sim \text{GOE}(100)$
  - $\Sigma \sim \text{Wishart Ensemble}$
- Inverse problems obtained via Matrix Depot package in Julia



(a) Gravity Surveying



(b) Image Restoration



(c) Heat Equation

In Summary

Contributions

- Intuitive visualization of random symmetric and SPD matrices in $d = 2$
- Generalization of exponentiated matrix eigenvalue distributions
- Application of exponentiated symmetric matrix ensembles to covariance modeling in linear inverse problems

Future Work

- More general eigenvalue densities
- Additional joint element densities
- Refined linear inverse problem results