Exponentiated Symmetric Matrix Distributions with Applications to Linear Inverse Problems

Polymath Jr. Program

Introduction: SPD Matrices

- SPD Matrices satisfy
  - $\Sigma = \Sigma^T$
  - $\lambda_i(\Sigma) > 0, \ \forall i$
  - The matrix can be decomposed in several useful ways

- Covariance Matrices
  - Covariance matrices are necessarily SPD
  - Population values often unknown

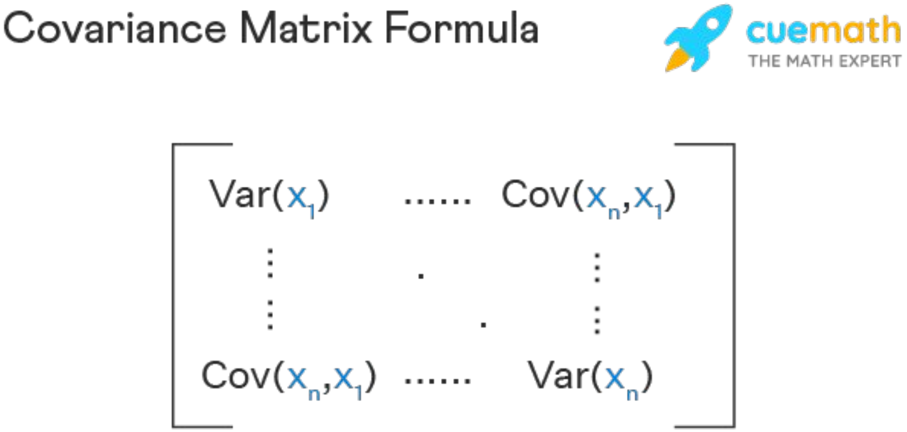


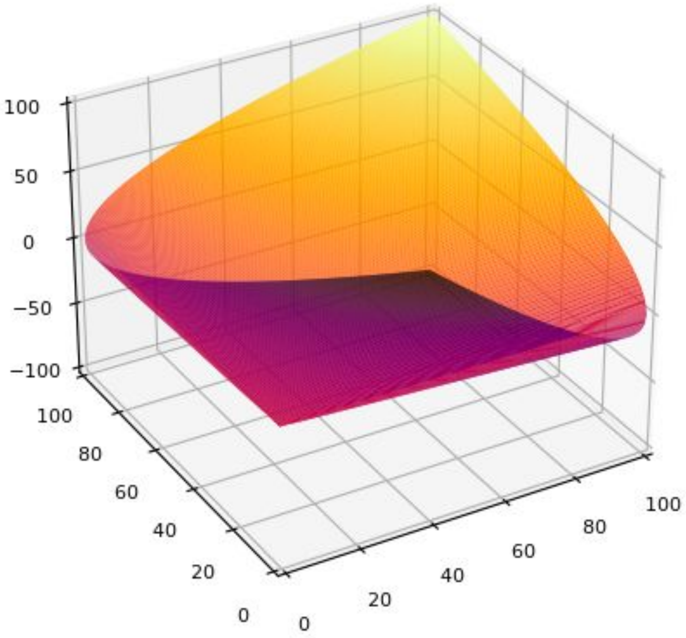
Fig. courtesy of CueMath

Introduction: SPD Manifold and Random Matrices

- Manifold of SPD Matrices
  - The set of d x d SPD matrices forms a Riemannian Manifold, $\mathbb{P}_d$, with dimension d(d+1)/2

$$\mathbb{P}_d \subseteq \mathbb{H}_d \subseteq \mathbb{M}_d$$

- Random Matrix Ensembles
  - Random matrices with elements drawn from a Normal distribution with zero-mean and non-identity covariance Φ are drawn from the "CGSE"

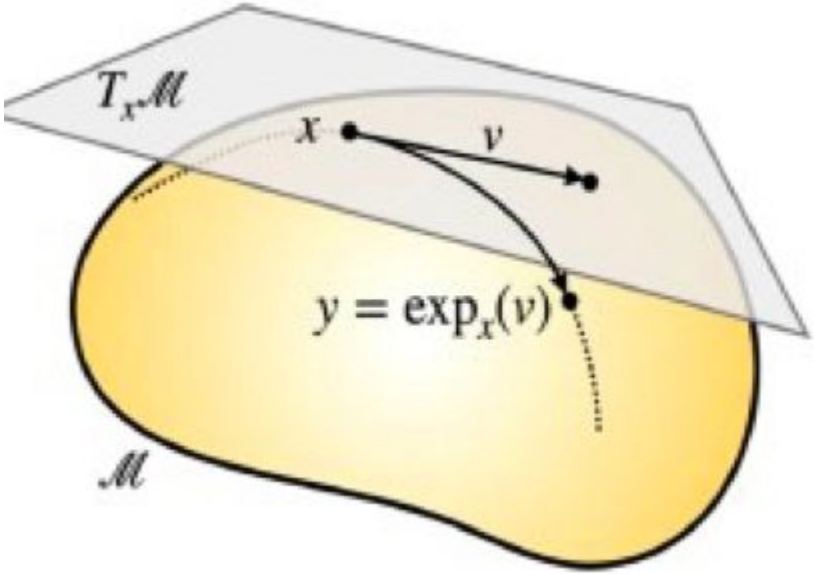


Introduction: Matrix Exponentiation and Applications

- Exponentiated Matrix Distributions
  - Sample random symmetric matrices from the CGSE and other ensembles
  - Map these matrices onto the SPD manifold via matrix exponentiation

- Applications to Linear Inverse Problems
  - Given observed data and known forward model, we wish to recover unknown parameters
    - $\mathbf{d} = A\mathbf{s} + \boldsymbol{\varepsilon}$
  - Bayesian solutions to linear-Gaussian inverse problems are parametrized by SPD matrices

Fig. courtesy of NeuroImage, 2021



Outline

1. **Characterizing** symmetric matrix distributions
2. **Exponentiating** symmetric matrix distributions
3. **Applying** SPD matrix distributions in Linear Inverse Problems

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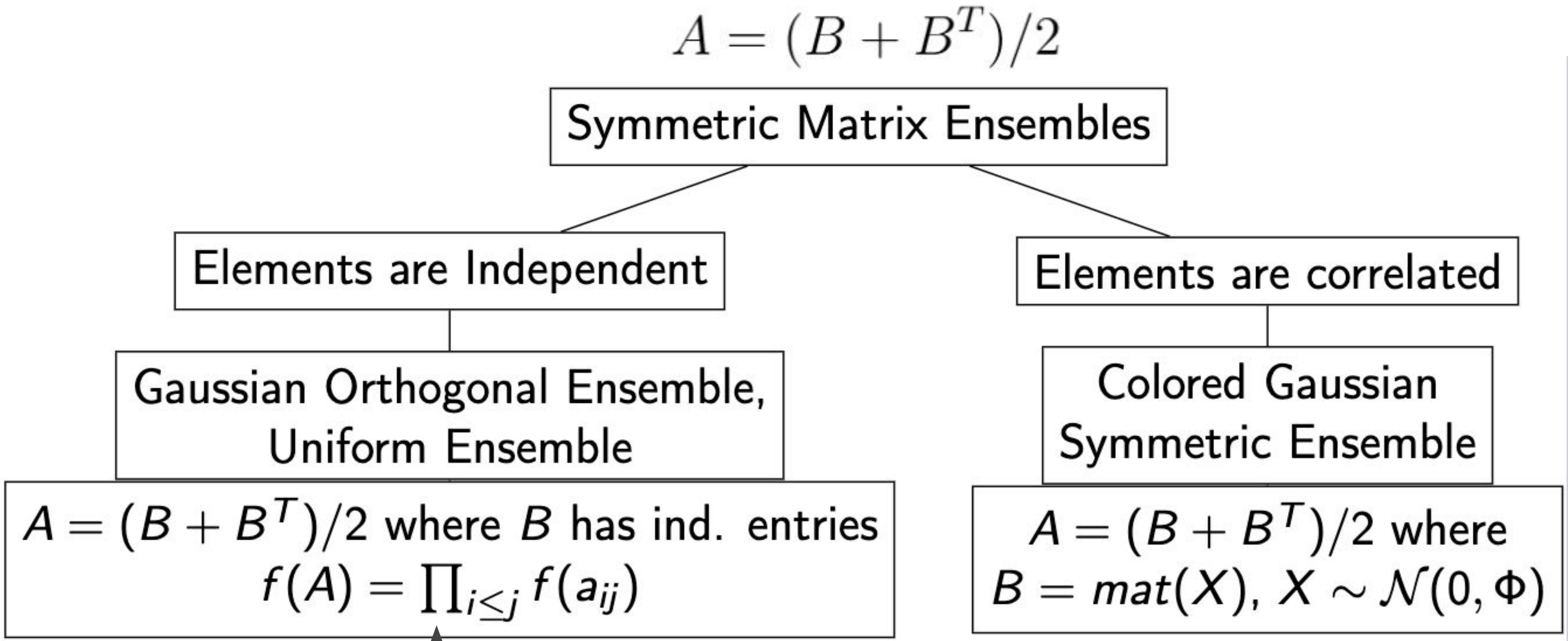
Characterizing Symmetric Matrix Distributions



Joint Element Density

Isometric | Along x_1 | Along (x_2+x_3)/2 | Along x_4

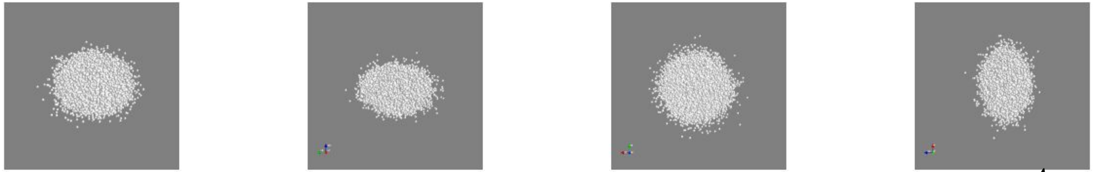


Figure 1: Gaussian Orthogonal Ensemble

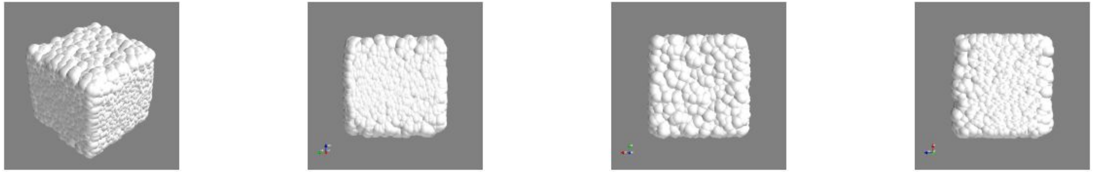


Figure 2: Uniform Ensemble

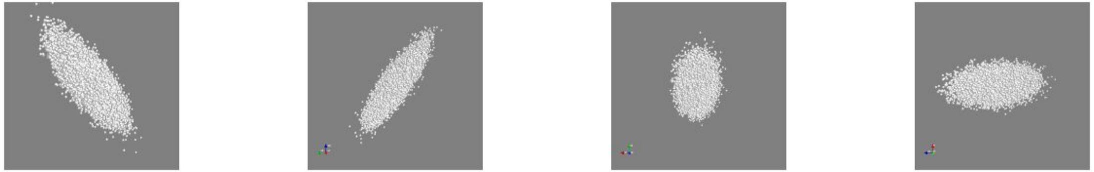


Figure 3: Colored Gaussian Symmetric Ensembles

$$B = \begin{bmatrix} x_1 & x_3 \\ x_2 & x_4 \end{bmatrix}$$

$$A = (B + B^T)/2 = \begin{bmatrix} x_1 & (x_2 + x_3)/2 \\ (x_2 + x_3)/2 & x_4 \end{bmatrix}$$

1) $x_i \sim \mathcal{N}(0, 1)$ i.i.d.

2) $x_i \sim \mathcal{U}(0, 1)$ i.i.d

3) $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \sim \mathcal{N}(\mathbf{0}, \Phi)$

Joint Element Density of the CGSE

$$A \sim CGSE(d, \Gamma)$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1d} \\ & a_{22} & \cdots & a_{2d} \\ & & \cdots & \vdots \\ & & \cdots & a_{dd} \end{bmatrix} \quad V = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{d(d+1)/2} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{22} \\ \vdots \\ a_{dd} \end{bmatrix}$$

$$a_{ij} = v_{f(i,j)}$$

$$f(i,j) = i + j(j-1)/2$$

$$1 \leq i \leq j \leq d,$$

$$f^{-1}(p) = \left(p - j(j-1)/2, j = \lceil \sqrt{(2p + 1/4)} + 1/2 \rceil - 1\right)$$

$$f^{-1}(p) = (i_p, j_p) \text{ and } f^{-1}(q) = (i_q, j_q)$$

$$\Psi = [\psi_{pq}] \qquad \psi_{pq} = \Gamma_{i_q j_q}^{i_p j_p} = \Gamma_{i_p j_p}^{i_q j_q}$$

$$V \sim \mathcal{N}(\mathbf{0}, \Psi)$$

$$f_{CGSE(d,\Gamma)} = f(V) = \frac{1}{\sqrt{(2\pi)^{d(d+1)/2}|\Psi|}} \exp\left(-\frac{1}{2} V^T \Psi^{-1} V\right)$$

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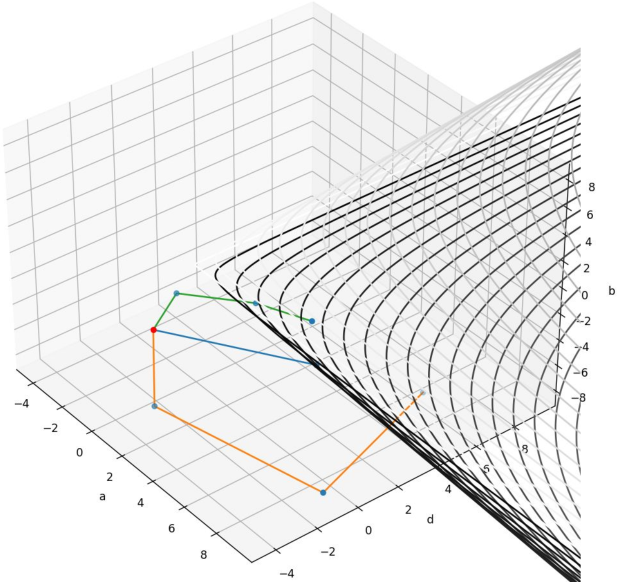
Exponentiating Symmetric Matrix Distributions

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

Matrix Exponential:

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

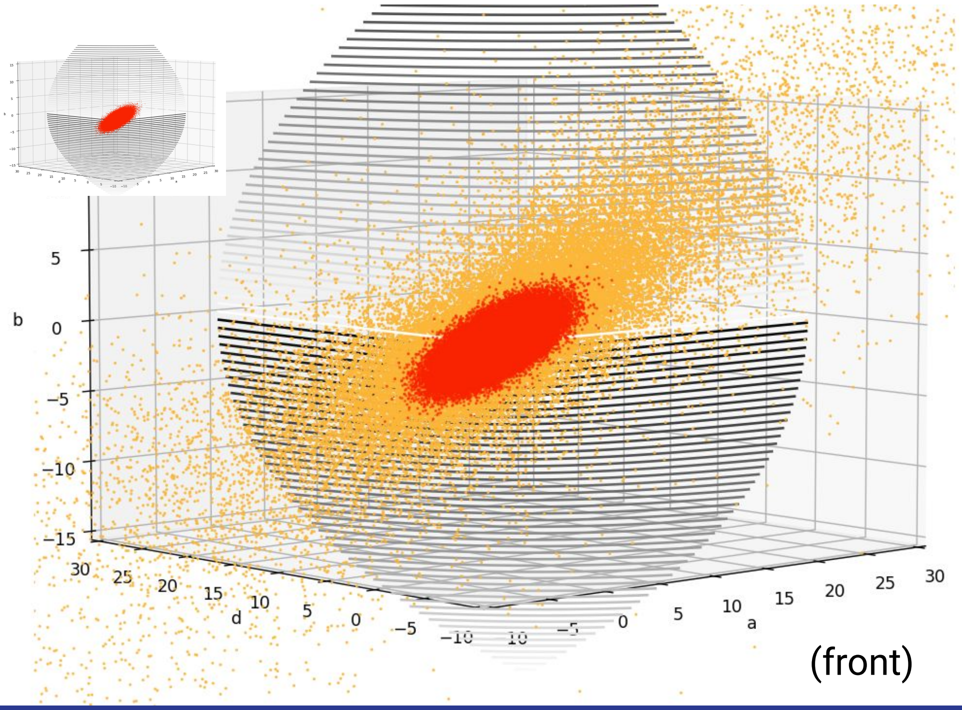


Matrix Exponential Base Σ:

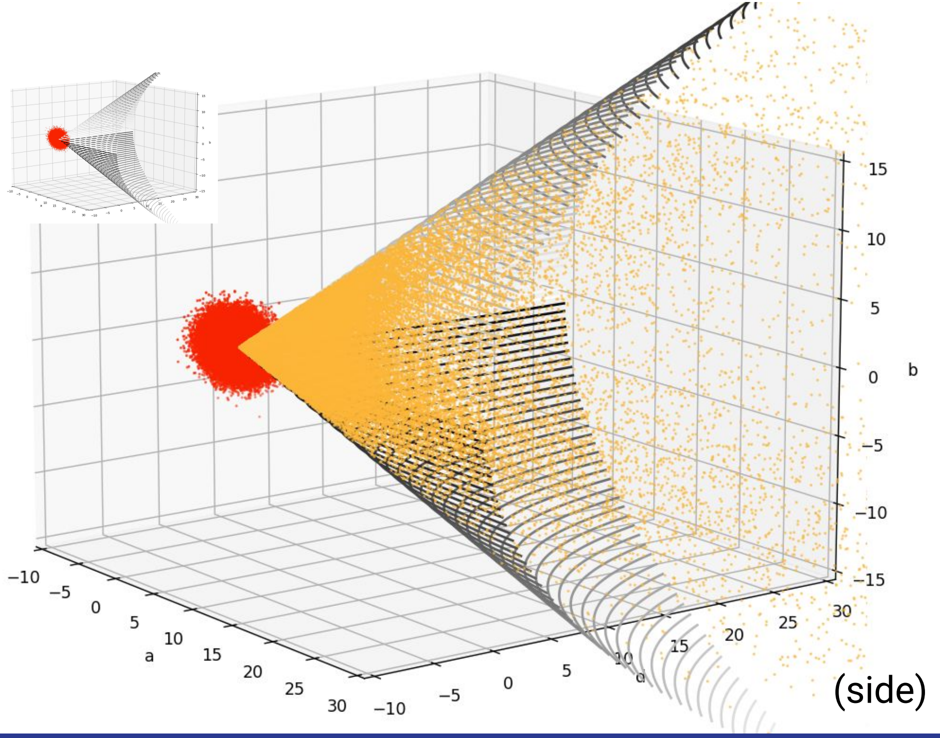
$$S = \exp_\Sigma \mathcal{E} \equiv \Sigma^{1/2} \exp(\Sigma^{-1/2} \mathcal{E} \Sigma^{-1/2}) \Sigma^{1/2}$$

Exponentiating Symmetric Matrix Distributions

Distribution: CGSE (red) → Exponentiated CGSE (yellow)



(front)



(side)

Exponentiating Symmetric Matrix Distributions

Density of A ~ CGSE(d, Γ)

$$f_{CGSE(d,\Gamma)} = f(V) = \frac{1}{\sqrt{(2\pi)^{d(d+1)/2}|\Psi|}} \exp\left(-\frac{1}{2}V^T\Psi^{-1}V\right)$$

Jacobian of Inverse Transformation

$\mathbb{J} = (1/|S|)\prod_{i<j} g(\lambda_i, \lambda_j)$ where

$$g(\lambda_i, \lambda_j) = \begin{cases} (\log(\lambda_i) - \log(\lambda_j))/(\lambda_i - \lambda_j) & \text{if } \lambda_i > \lambda_j \\ 1/\lambda_i & \text{if } \lambda_i = \lambda_j \end{cases}$$

Transformed Density of S = exp(A)

$$\mathbb{J} \cdot 1/\sqrt{(2\pi)^{d(d+1)/2}|\Psi|} \cdot \exp\left(-\tfrac{1}{2}\mathrm{vecd}(\log(S))^T\,\Psi^{-1}\,\mathrm{vecd}(\log(S))\right)$$

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Applying SPD Matrix Distributions to Linear Inverse Problems

$Ax = B$ where $A \in \mathbb{R}^{mxn}$ is the forward model

where $x \in \mathbb{R}^{n}$ is the unknown or what we would like to infer

where $b \in \mathbb{R}^{m}$ is the known data

Least Squares Equation: $(A^T A)x = A^T b$

$$x_{map} = \arg\max_{x \in \mathbb{R}^n} (\Pi_{post}(x|b))$$

$$\Pi_{post}(x|b) = \frac{\Pi_{prior}(x)\Pi_{like}(b|x)}{\Pi_{marginal}(b)}$$

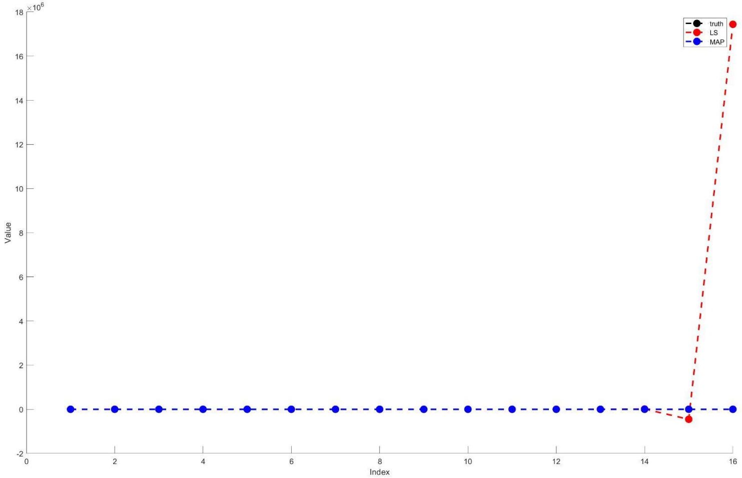
$$x_{map} = \left(A^T \Gamma_{noise}^{-1} A + \lambda^2 \Gamma_{prior}^{-1}\right)^{-1} \left(A^T \Gamma_{noise}^{-1} b + \lambda^2 \Gamma_{prior}^{-1} \mu\right)$$

Applying SPD Matrix Distributions to Linear Inverse Problems

Let A, d, μ, λ, and Γnoise – all parameters of our inverse problem except Γprior – be fixed.

Assume that Γprior comes from a projected symmetric matrix ensemble, Γprior = expΣ E where Σ ∈ Pn and E ∈ Hn is random with E[E] = 0n×n .

What is the resulting distribution of the solutions smap? Is there much variability? How faithful is smap to the original data s? How does varying Σ or the model for E change the solution distribution?



Thank you!