Fréchet Regression on the Bures-Wasserstein Manifold

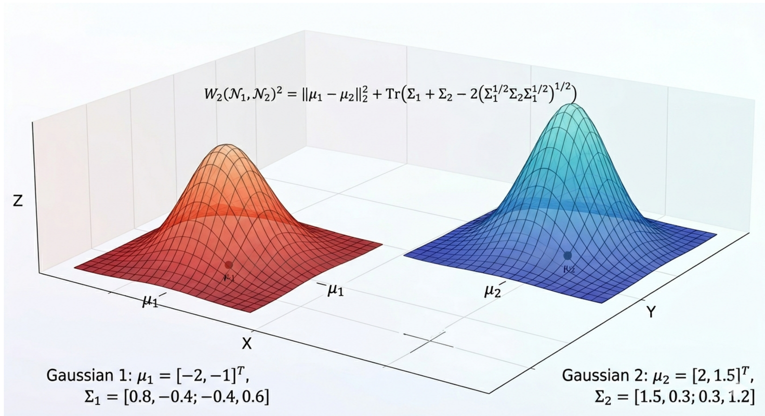
Duc Toan Nguyen, César A. Uribe
Department of Electrical and Computer Engineering, Rice University

RICE KEN KENNEDY INSTITUTE

NetSci Boston 2026

Bures-Wasserstein Manifold

The **Bures-Wasserstein manifold** $\mathbb{S}^d_{++}$ is the space of symmetric positive definite matrices.



Why BW?

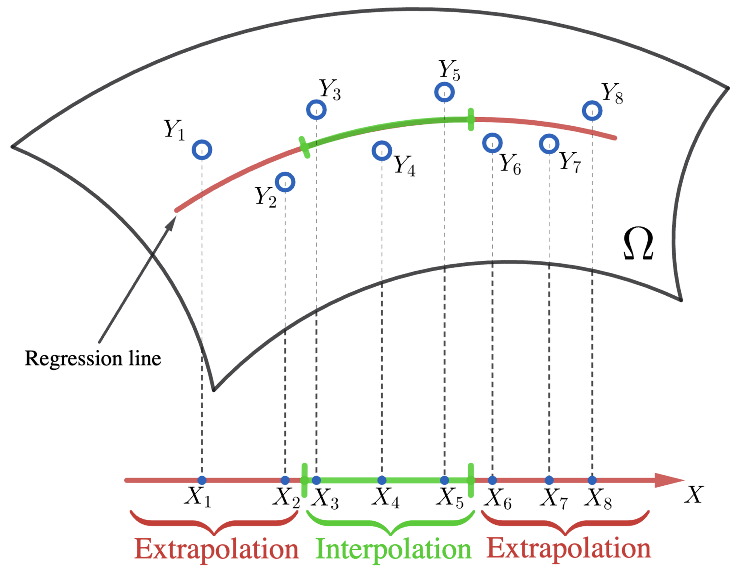
- BW reduces Frobenius "swelling effect",
- BW does **NOT** require matrix logarithms, unlike affine-invariant (Fisher-Rao) and log-Euclidean metrics.

Fréchet Regression

Global Fréchet Regression: Given n independent samples $(X_k, Y_k) \sim \mathcal{F}$,

$$\hat{m}_G(x) = \arg\min_{\omega \in \Omega} \frac{1}{n} \sum_{k=1}^{n} s_{G,k}(x) d^2(Y_k, \omega), \quad (1)$$

where $s_{G,k}(x) = 1 + (X_k - \bar{X})^\top \hat{\Sigma}^{-1}(x - \bar{X})$.



Problem statement

Problem: Given n SPD matrices Σ_k and their weights $\lambda_k \in \mathbb{R}$, for $k \in \{1, ..., n\}$, such that $\sum_{k=1}^n \lambda_k = 1$, we want to solve

$$\min_{S \in \mathbb{S}^d_{++}} F(S) := \sum_{k=1}^{n} \lambda_k W_2^2(S, \Sigma_k) \quad (2)$$
$$= \sum_{i \in \mathcal{I}} \lambda_i^+ W_2^2(S, \Sigma_i) - \sum_{j \in \mathcal{J}} \lambda_j^- W_2^2(S, \Sigma_j),$$

for $\lambda_i^+, \lambda_j^- > 0, \mathcal{I} = \{k : \lambda_k > 0\}, \mathcal{J} = \{k : \lambda_k < 0\}$.

Minimizer Existence

Example (Negative weights): Let $\lambda_1 = 2$, $\lambda_2 = -1$, $\Sigma_1 = I$, $\Sigma_2 = 9I$, and $f(S) := \lambda_1 W_2^2(S, \Sigma_1) + \lambda_2 W_2^2(S, \Sigma_2)$. Then, the gradient $\nabla f(S) \succ 0$.

Theorem: Let $\Sigma_1, \ldots, \Sigma_n \in \mathbb{S}^d_{++}$ and $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$ with $\sum_{k=1}^n \lambda_k = 1$. If the **Spectral Dominance of Positive Weights** condition holds, i.e.,

$$\sum_{i \in \mathcal{I}} \lambda_i^+ \sqrt{\lambda_{\min}(\Sigma_i)} > \sum_{j \in \mathcal{J}} \lambda_j^- \sqrt{\lambda_{\max}(\Sigma_j)}, \quad (3)$$

then Problem (2) admits a solution.

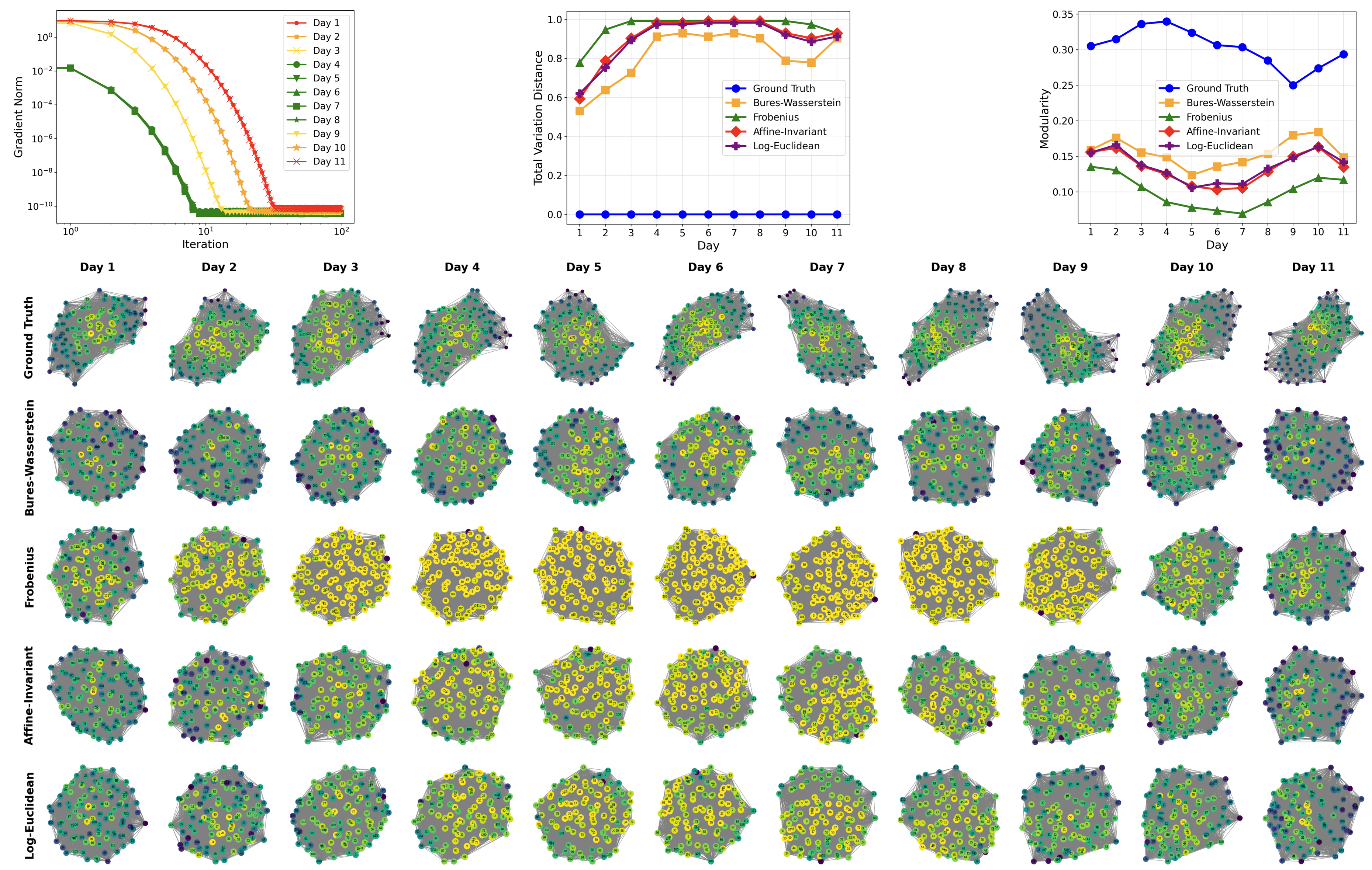
Minimizer Unique Existence

Theorem: Let $\Sigma_k \in \mathbb{S}^d_{++}$, for $k \in \{1, ..., n\}$, $\lambda := \min \lambda_{\min}(\Sigma_k)$ and $\mathcal{S}_\lambda = \{\Sigma \in \mathbb{S}^d_{++} : \lambda_{\min}(\Sigma) \geq \lambda\}$. Denote $\mu_+ = \sum_i \lambda_i^+, \mu_- = \sum_j \lambda_j^-$. Assume that there exist $\rho > 0$, $r > 0$ and $\Sigma_0 \in \mathcal{S}_\lambda$ such that

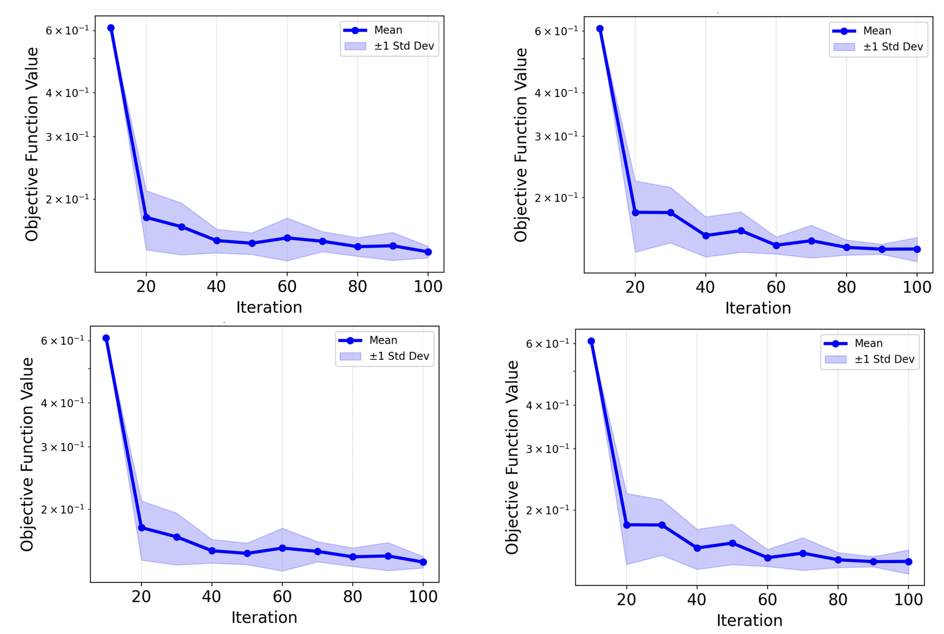
- $\Sigma_k \in B_r(\Sigma_0)$ for all $k \in \{1, ..., n\}$, where $B_r(\Sigma_0)$ is the geodesic ball centered at Σ_0 with radius r,
- $r < \rho/(\mu_+ + \mu_-)$,
- $\rho < \sqrt{\lambda}/2$,
- $B_\rho(\Sigma_0) \subset \mathcal{S}_\lambda$, and
- $\mu_+/\mu_- > (2\rho\sqrt{\Lambda^+})/(\tanh(2\rho\sqrt{\Lambda^+}))$.

Then, there is a **unique minimizer** in $B_\rho(\Sigma_0)$.

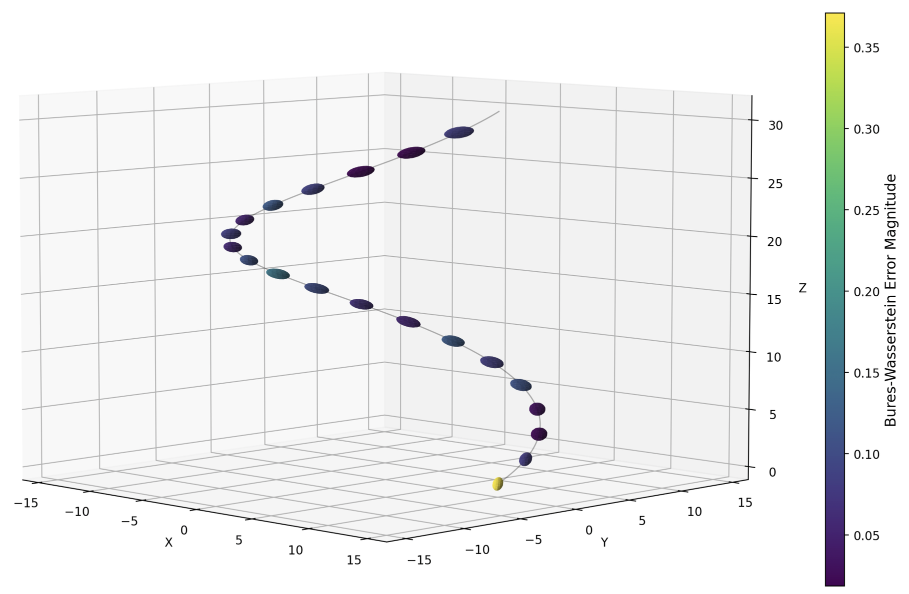
Network Regression with Ant Social Networks



Large-scale Diffusion Tensor Imaging (DTI)



Objective Values over 100 iterations of RSGD



Visualization of tensors

Additional Properties

Bounded Region: If the condition (3) holds, then:

$$\left(\sum_{i \in \mathcal{I}} \lambda_i^+ \sqrt{\lambda_{\min}(\Sigma_i)} - \sum_{j \in \mathcal{J}} \lambda_j^- \sqrt{\lambda_{\max}(\Sigma_j)}\right)^2 I \prec S_*,$$

$$\left(\sum_{i \in \mathcal{I}} \lambda_i^+ \sqrt{\lambda_{\max}(\Sigma_i)} - \sum_{j \in \mathcal{J}} \lambda_j^- \sqrt{\lambda_{\min}(\Sigma_j)}\right)^2 I \succ S_*.$$

No local maximum: S_* is not a local maximum.

Algorithm

Algorithm 1 General BWGD

1: **Input**: SPD matrices Σ_k, weights λ_k, initial S_0, step-size η, epochs T.
2: **for** $t = 1, 2, \ldots, T$ **do**
3: $\tilde{S}_t = (1 - \eta)I + \eta \sum_{k=1}^n \lambda_k \, \mathrm{GM}(S_{t-1}^{-1}, \Sigma_k)$
4: // $-\eta \nabla_{\mathrm{bw}} F(S_{t-1})$
5: $S_t = \tilde{S}_t S_{t-1} \tilde{S}_t$
6: // $\exp_{S_{t-1}}(-\eta \nabla_{\mathrm{bw}} F(S_{t-1}))$
7: **end for**
8: **Return** $\bar{\Sigma} = S_T$

NOTE: Convergence rate $\mathcal{O}(1/T)$ with $\eta \leq 1/L$. With condition (3), Algorithm 1 is **projection-free**

Large-scale Reformulation

$$F(S) = \sum_{i \in \mathcal{I}} \lambda_i^+ W_2^2(S, \Sigma_i) - \sum_{j \in \mathcal{J}} \lambda_j^- W_2^2(S, \Sigma_j)$$
$$= \sum_{i \in \mathcal{I}, j \in \mathcal{J}} \frac{\lambda_i^+}{\mu_+} \frac{\lambda_j^-}{\mu_-} \left(\mu_+ W_2^2(S, \Sigma_i) - \mu_- W_2^2(S, \Sigma_j)\right)$$
$$= \sum_{i \in \mathcal{I}, j \in \mathcal{J}} \frac{\lambda_i^+}{\mu_+} \frac{\lambda_j^-}{\mu_-} f_{ij}(S),$$

for $\lambda_i^+, \lambda_j^- > 0, \mu_+ := \sum_i \lambda_i^+, \mu_- := \sum_j \lambda_j^-, S \in \mathbb{S}^d_{++}$.

Stochastic Gradient:

$$\nabla f_{ij}(S) = I - \left(\mu_+ \mathrm{GM}(S^{-1}, \Sigma_i) - \mu_- \mathrm{GM}(S^{-1}, \Sigma_j)\right).$$

Conditions for Pairwise Formulation:

$$(\mu_+) \min_{i \in \mathcal{I}} \sqrt{\lambda_{\min}(\Sigma_i)} > (\mu_-) \max_{j \in \mathcal{J}} \sqrt{\lambda_{\max}(\Sigma_j)}$$