Butterfly-Accelerated Gaussian Random Fields on Manifolds

Paul G. Beckman [1] Samuel F. Potter [2] Michael O'Neil [1]

[1]Courant Institute of Mathematical Sciences, New York University [2]Coreform LLC

Fast algorithms for covariances on surfaces

The fast Fourier transform (FFT) allows efficient sampling of stationary Gaussian random fields (GRFs) on closed curves. How can we generalize these stochastic processes and the corresponding numerical methods to develop fast sampling algorithms on general manifolds?

GRFs on closed curves

Z is a mean zero GRF on a closed curve Γ if for any locations $s, s' \in \Gamma$ the corresponding observations $Z(s), Z(s') \in \mathbb{C}$ are Gaussian

$$\mathbb{E}Z(s) = 0$$
$$\mathrm{Cov}\left(Z(s), Z(s')\right) = \mathbb{E}\left(Z(s)\overline{Z(s')}\right) = k(s, s')$$

for some positive definite function $k : \Gamma \times \Gamma \to \mathbb{C}$.

If $k(s, s') = k(s - s')$, then Z has the Karhunen-Loève (KL) expansion

$$Z(s) = \sum_{\ell=0}^{\infty} \sqrt{\gamma(\ell^2)} e^{i\ell s} W_\ell, \quad W_\ell \overset{\text{i.i.d.}}{\sim} N(0,1)$$

where γ is the *spectral density* of the process.

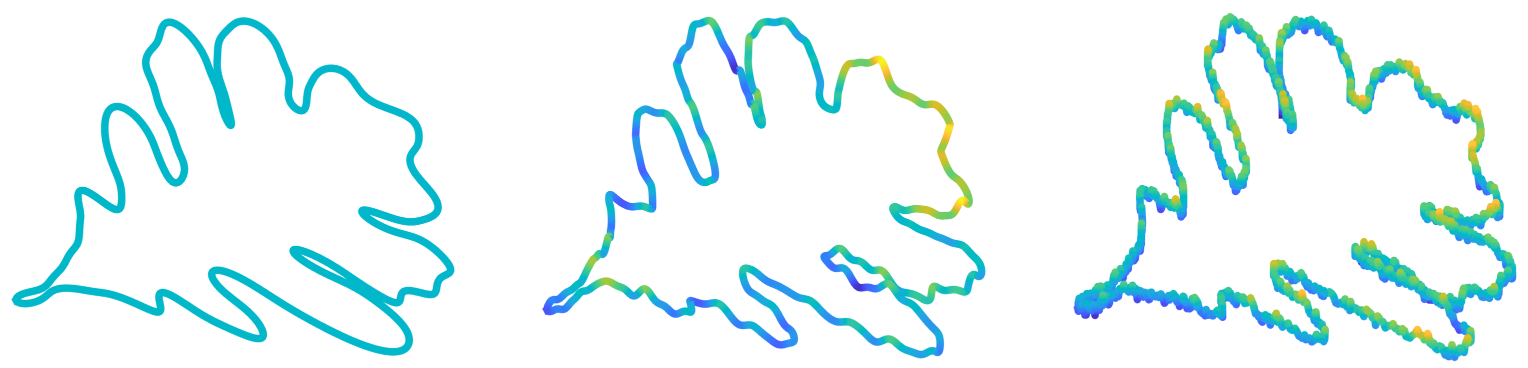


Figure 1. KL expansion with $\ell = 2, 256,$ and 8192 terms on an oak leaf contour with $\gamma(\lambda) = (1+\lambda)^{-\frac{1}{2}}$

FFT-accelerated GRFs on closed curves

Evaluating the truncated KL expansion

$$Z(s) = \sum_{\ell=0}^{n-1} \sqrt{\gamma(\ell^2)} e^{i\ell s} W_\ell, \quad W_\ell \overset{\text{i.i.d.}}{\sim} N(0,1)$$

at n equispaced points in arclength

$$Z\left(\frac{2\pi j}{n}\right) = \sum_{\ell=0}^{n-1} \sqrt{\gamma(\ell^2)} e^{2\pi i j \ell / n} W_\ell \quad \text{for } j = 0, \ldots, N-1$$

is precisely a discrete Fourier transform

$$\boldsymbol{z} = \boldsymbol{\Phi}\sqrt{\boldsymbol{D}}\boldsymbol{w}$$

where $\boldsymbol{D} = \mathrm{diag}\left(\gamma(0), \ldots, \gamma\left((n-1)^2\right)\right)$, $\boldsymbol{w} \sim N(\boldsymbol{0}, \boldsymbol{I})$. The FFT provides $\mathcal{O}(n \log n)$ sampling.

References

[LP23] Annika Lang and Mike Pereira, *Galerkin–Chebyshev approximation of Gaussian random fields on compact Riemannian manifolds*, BIT Numerical Mathematics **63** (2023), no. 4, 51.

[LYM+15] Yingzhou Li, Haizhao Yang, Eileen R Martin, Kenneth L Ho, and Lexing Ying, *Butterfly factorization*, Multiscale Modeling & Simulation **13** (2015), no. 2, 714–732.

GRFs on manifolds

Note that $\lambda_\ell = \ell^2, \phi_\ell = e^{i\ell s}$ are eigenvalues and eigenfunctions of the Laplacian on Γ

$$-\Delta_\Gamma \phi_\ell = \lambda_\ell \phi_\ell.$$

This suggests an analogous method of constructing GRFs on manifolds

$$Z(\boldsymbol{s}) = \sum_{\ell=0}^{\infty} \sqrt{\gamma(\lambda_\ell)} \phi_\ell(\boldsymbol{s}) W_\ell, \quad W_\ell \overset{\text{i.i.d.}}{\sim} N(0,1)$$

where λ_ℓ and ϕ_ℓ are eigvalues and eigenfunctions of the Laplace-Beltrami operator on $\mathcal{M}$

$$-\Delta_{\mathcal{M}} \phi_\ell = -\sum_{i=1}^{d}\sum_{j=1}^{d} \frac{1}{\sqrt{|g|}} \frac{\partial}{\partial x_i} \left(\sqrt{|g|} (g^{-1})_{ij} \frac{\partial \phi_\ell}{\partial x_j}\right) = \lambda_\ell \phi_\ell.$$

In practice we use an n-point discretization of $\mathcal{M}$ with corresponding discrete eigenproblem

$$\boldsymbol{L}\boldsymbol{\phi}_\ell = \lambda_\ell \boldsymbol{M}\boldsymbol{\phi}_\ell.$$

The manifold harmonic transform

The *manifold harmonic transform* $\boldsymbol{\Phi}$ has similar structure to the DFT matrix

Figure 2. Eigenvectors $\boldsymbol{\phi}_\ell$ for $\ell = 1, 2, 3, 4, 5, 12, 30, 500, 1000, 2000$ on armadillo mesh with $n = 5407$ vertices

Truncation error and Weyl's law

The true covariance of the process is

$$\boldsymbol{\Sigma} := \mathrm{Cov}(\boldsymbol{z}) = \mathbb{E}(\boldsymbol{z}\boldsymbol{z}^*) = \boldsymbol{\Phi}\boldsymbol{D}\boldsymbol{\Phi}^*.$$

Let $\boldsymbol{\Phi}_\ell := \boldsymbol{\Phi}(:, 1:\ell)$ and $\boldsymbol{D}_\ell = \boldsymbol{D}(1:\ell, 1:\ell) = \mathrm{diag}\left(\gamma(\lambda_0), \ldots, \gamma(\lambda_\ell)\right)$.

The operator norm error between $\boldsymbol{\Sigma}$ and its low-rank approximation is

$$\left\|\boldsymbol{\Sigma} - \boldsymbol{\Phi}_\ell \boldsymbol{D}_\ell \boldsymbol{\Phi}_\ell^*\right\| = \left\| \sum_{m=\ell+1}^{n} \gamma(\lambda_m) \boldsymbol{\phi}_m \boldsymbol{\phi}_m^* \right\| = \left(\sum_{m=\ell+1}^{n} \gamma^2(\lambda_m) \right)^{\frac{1}{2}}. \qquad (\star)$$

This requires $\lambda_{\ell+1}, \ldots, \lambda_n$ but we've only computed $\lambda_1, \ldots, \lambda_\ell$.

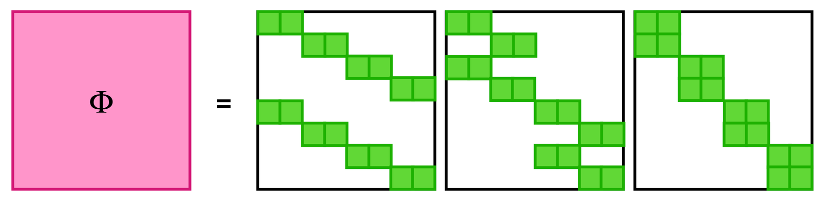
For $d = 2$, Weyl's law says that the growth in the eigenvalues of $-\Delta_{\mathcal{M}}$ is asymptotically linear

$$\lambda_m \sim \alpha m + \beta \quad \text{as} \quad m \to \infty.$$

We use least squares to fit $\hat{\lambda}_m = \hat{\alpha} m + \hat{\beta}$ and estimate $(\star)$ using $\hat{\lambda}_{\ell+1}, \ldots, \hat{\lambda}_n$.

Compression error and the butterfly factorization

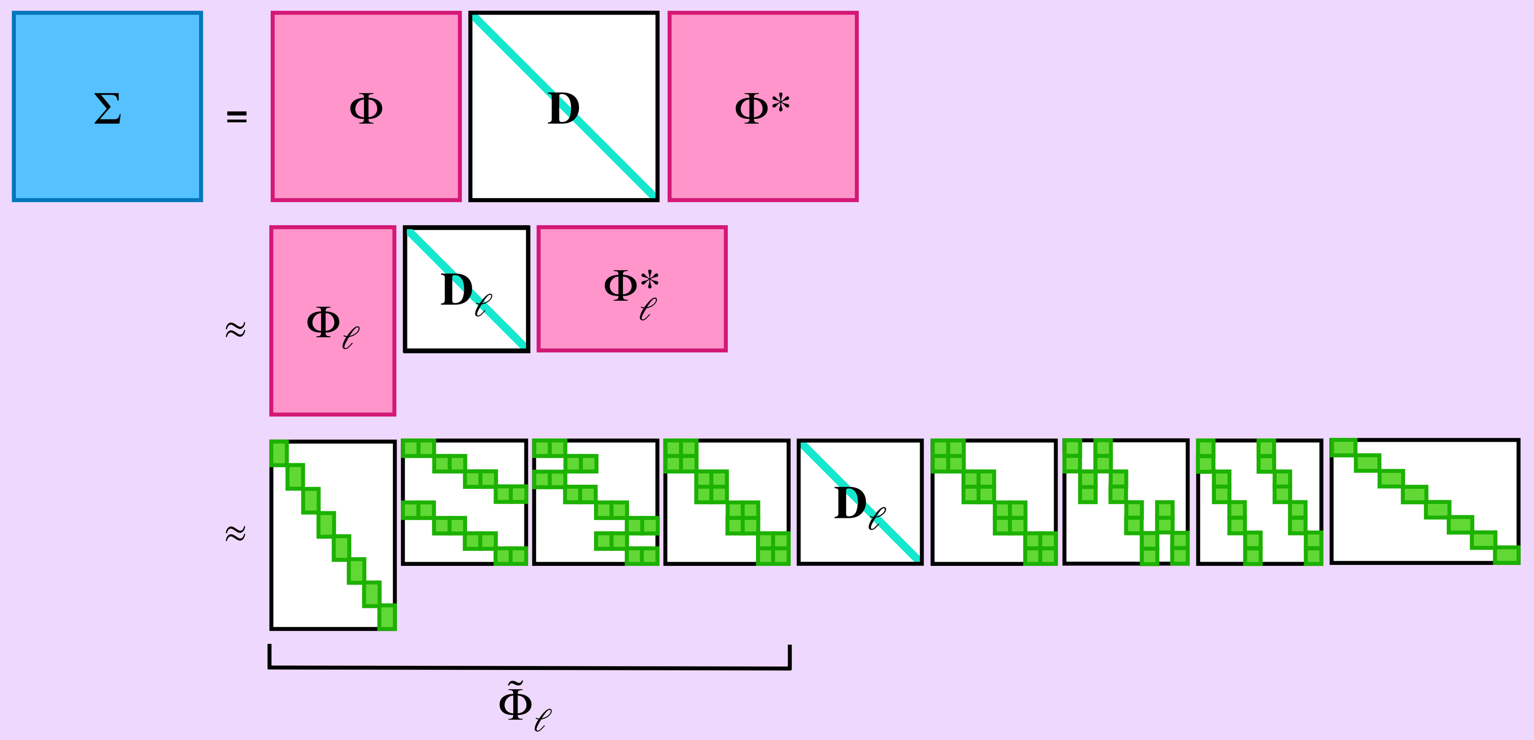
The FFT is a product of $\mathcal{O}(\log n)$ sparse matrices with recursive structure



The butterfly factorization [LYM+15] generalizes the FFT to include interactions of ε-rank $r > 1$.

We can iteratively compute columns of $\boldsymbol{\Phi}$ and compress them into this form to tolerance ε.

Truncated and compressed covariance operator



Numerical example

Stanford bunny mesh ($n = 34{,}817$ vertices) discretized with linear finite elements

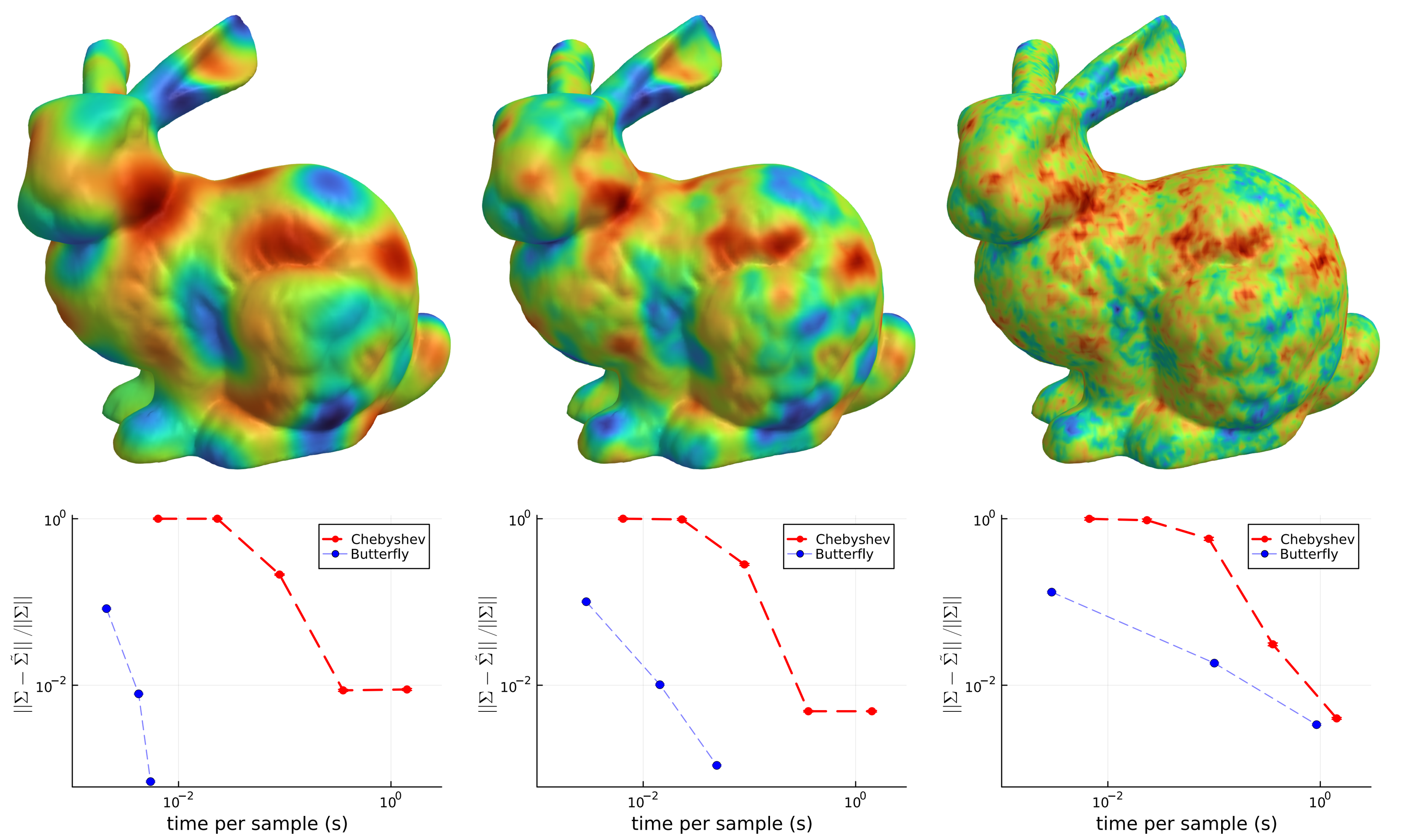


Figure 3. Relative operator norm error as a function of sampling time for Matérn processes $\gamma(\lambda) = (\alpha^2 + \lambda)^{-\frac{\nu}{4}-\frac{1}{2}}$ with $\nu = \infty, 4, \frac{1}{2}$. Timing comparison with the Chebyshev spectral approximation method of [LP23].

paul.beckman@cims.nyu.edu