Lecture 12 - Dimensionality Reduction of Gaussian Random Fields

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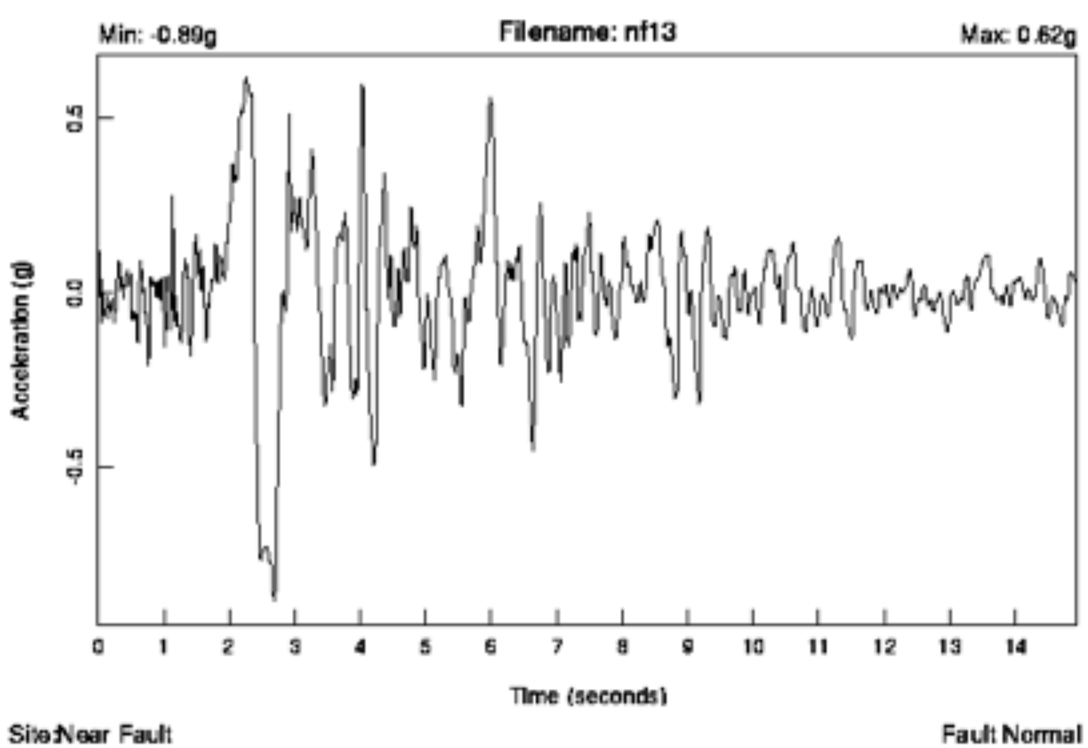
Objectives

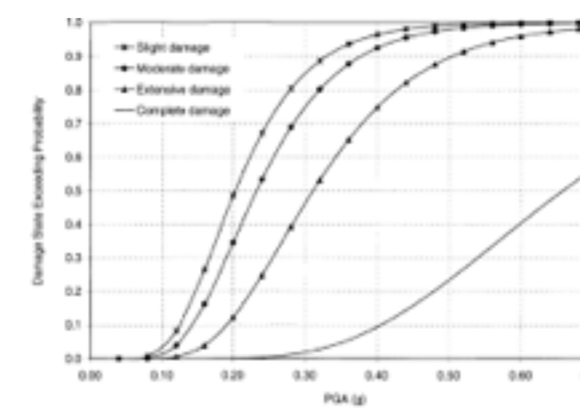
- Describe a Gaussian process with a finite number of uncorrelated random variables
- Use the reduced description to propagate uncertainties in functions through a model

Why do we need probability measures on functions?



Uncertainty in external forcing

Simulation



Fragility Curve

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Why do we need probability measures on functions?

Portfolio Risk

Uncertainty in external forcing

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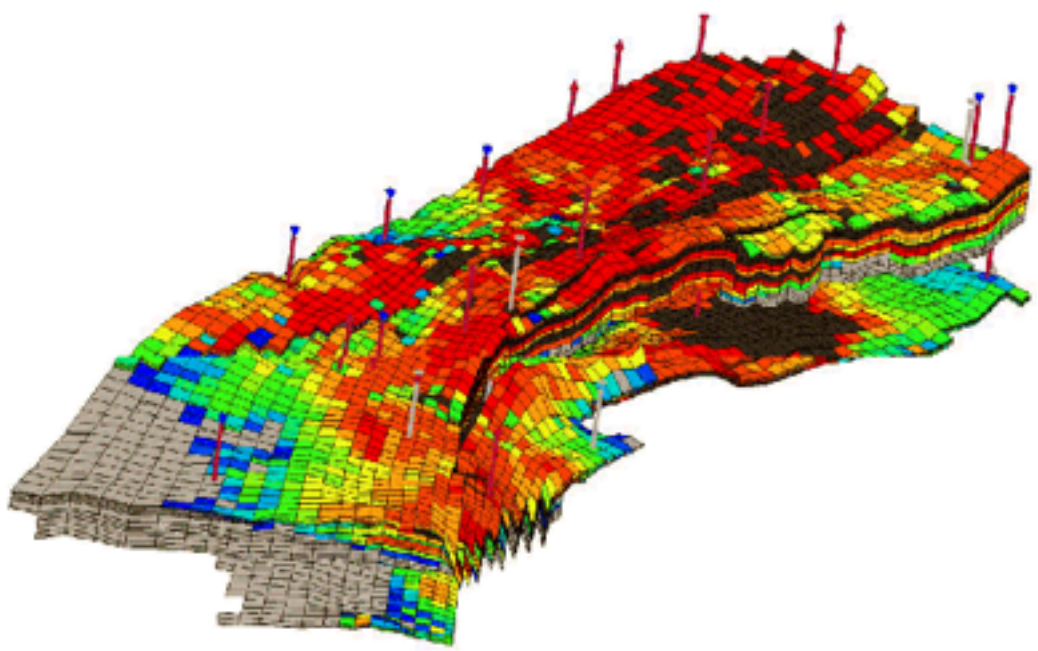
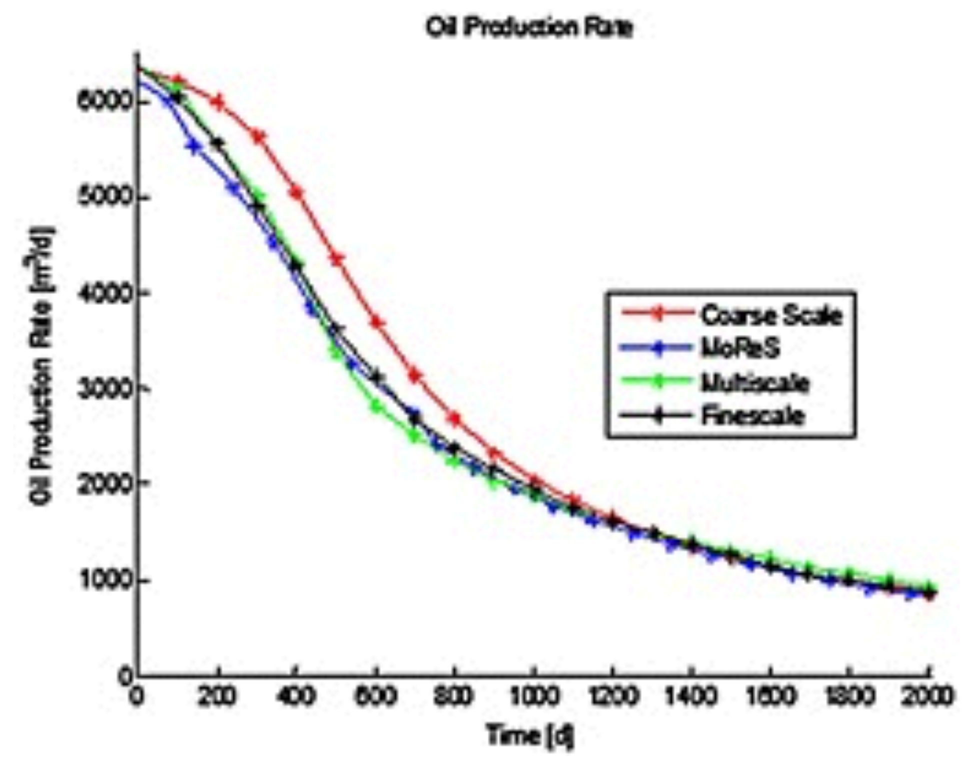
Why do we need probability measures on functions?



Uncertainty in field parameters

Simulation



Oil produced over time

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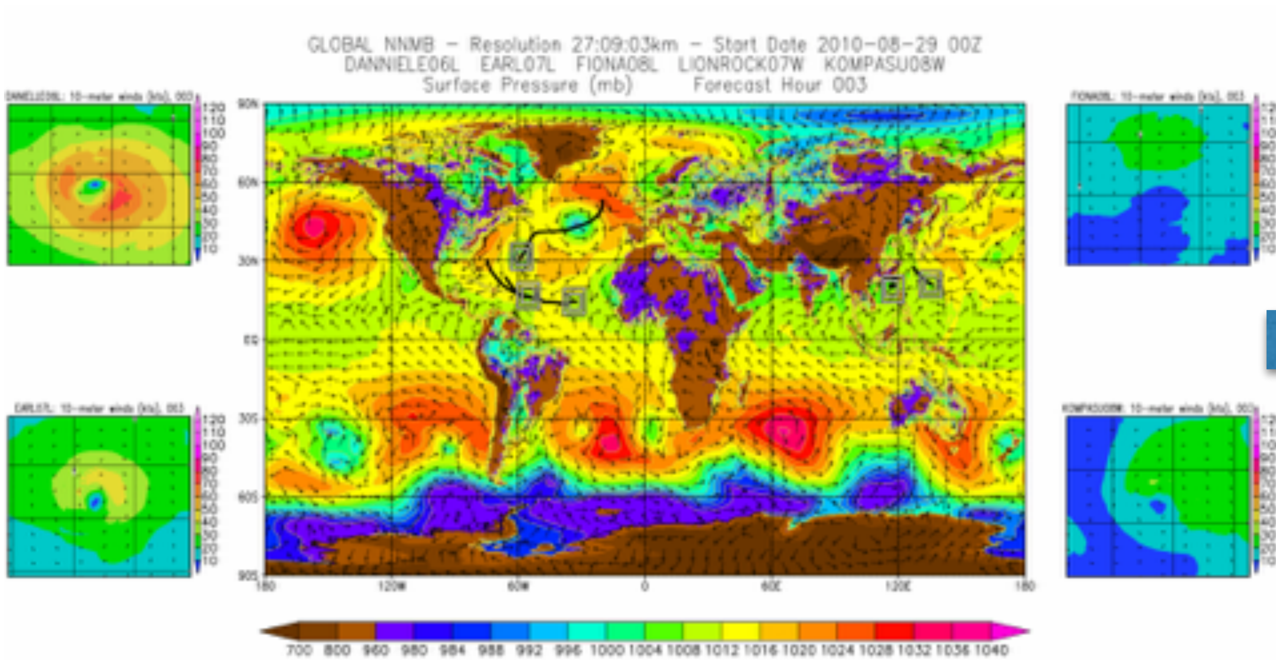
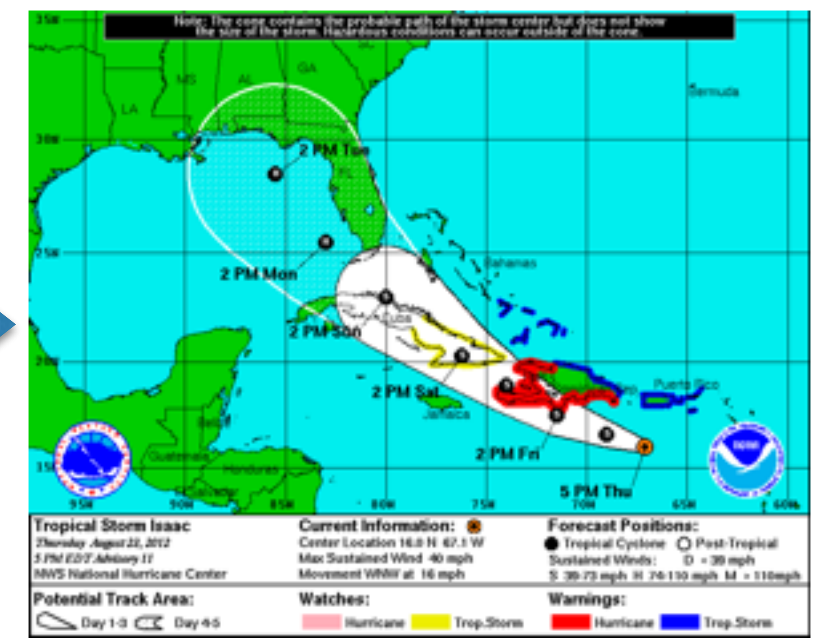
Why do we need probability measures on functions?





Hurricane path

Uncertainty in initial conditions

http://hwrf.aoml.noaa.gov/

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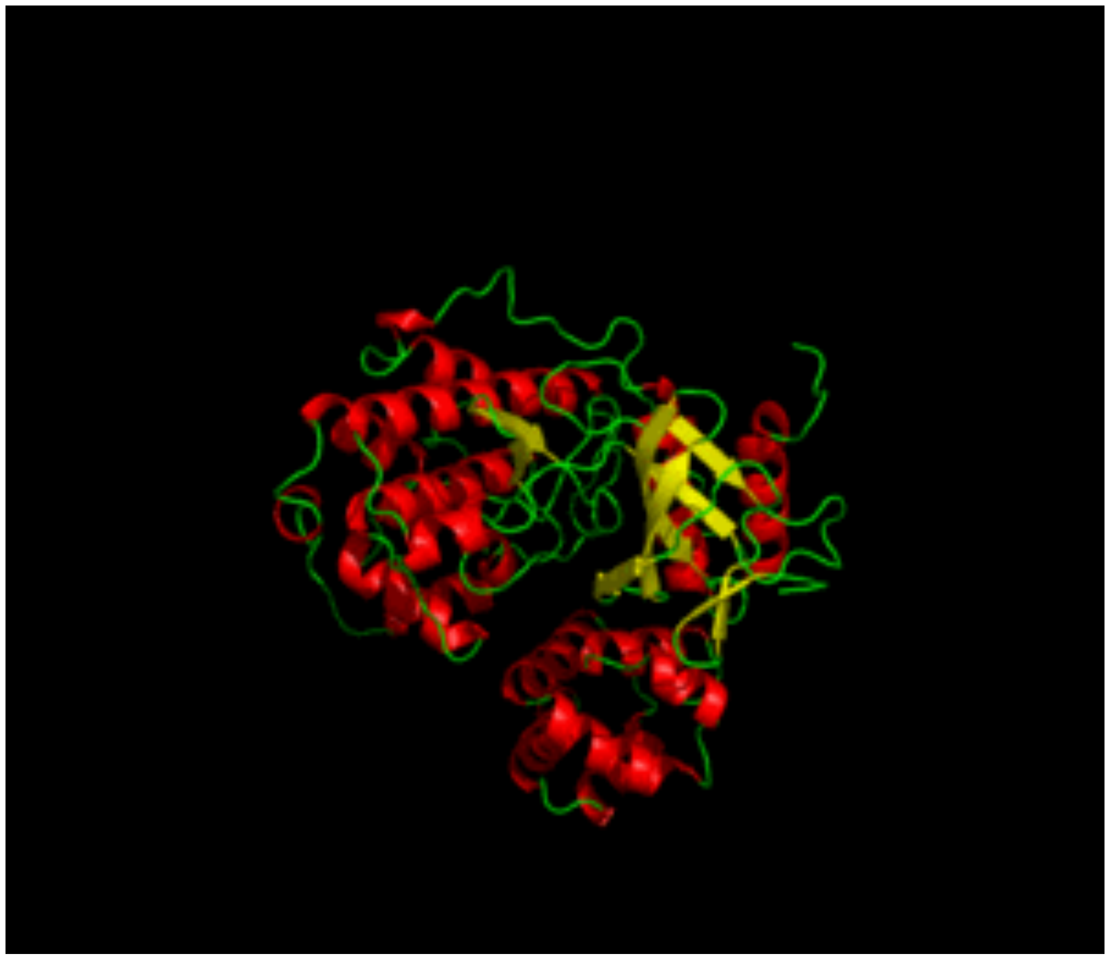
Why do we need probability measures on functions?



Simulation of the interaction of two biomolecules

Statistical mechanics:

$$p(\mathbf{q}) \propto \exp\left\{-\frac{V(\mathbf{q})}{k_B T}\right\}$$

Positions of all atoms

Boltzmann constant

Temperature

Empirical potential. We are not exactly sure about its form…

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For quantifying uncertainties in:

- External forcing
- Field parameters
- Initial conditions in PDEs
- Boundary conditions in PDEs
- Physical laws (e.g., constitutive relations, empirical force fields, etc.)
- …

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Model Stochastic PDE Problem

Consider the elliptic partial differential equation:

$$\nabla \left(\alpha(\mathbf{x}) \nabla u(\mathbf{x}) \right) = \rho(\mathbf{x})$$

with boundary conditions:

$$u(\mathbf{x}) = g_D(\mathbf{x}), \text{ on } \mathbf{x} \in \Gamma_D$$

$$\mathbf{n} \cdot \nabla u(\mathbf{x}) = q_N(\mathbf{x}), \text{ on } \mathbf{x} \in \Gamma_N$$

Any of these could be uncertain…

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$$\mathbf{n} \cdot \nabla u(\mathbf{x}) = g_N(\mathbf{x}),\ \text{on}\ \mathbf{x} \in \Gamma_N$$

Physical examples?

- Electrostatics
- Steady state heat
- Subsurface flow
- …

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$$\mathbf{n}\cdot\nabla u(\mathbf{x}) = g_N(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_N$$

Since it is positive:

$$\alpha(\mathbf{x}) = \exp\left\{f(\mathbf{x})\right\}$$

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

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Gaussian process

We are uncertain about a function:

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

Anything we know (potentially observed input/output data)

Could be prior or posterior mean/covariance

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Sampling from a GP

Pick a bunch of test points:

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$$

Look at the function values at these points:

$$\mathbf{f}_{1:n} = \{f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)\}$$

By definition, we have:

$$p\left(\mathbf{f}_{1:n}|\mathbf{x}_{1:n}, I\right) = \mathcal{N}\left(\mathbf{f}_{1:n}|\mathbf{m}_{1:n}, \mathbf{K}_n\right)$$

You need n random variables to sample from this…

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Model Stochastic PDE Problem

Where do you need to sample in order to solve this?

$$\nabla\left(\alpha(\mathbf{x})\nabla u(\mathbf{x})\right) = \rho(\mathbf{x})$$
$$u(\mathbf{x}) = g_D(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_D$$
$$\mathbf{n}\cdot\nabla u(\mathbf{x}) = g_N(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_N$$

Depends on the numerical method you employ…

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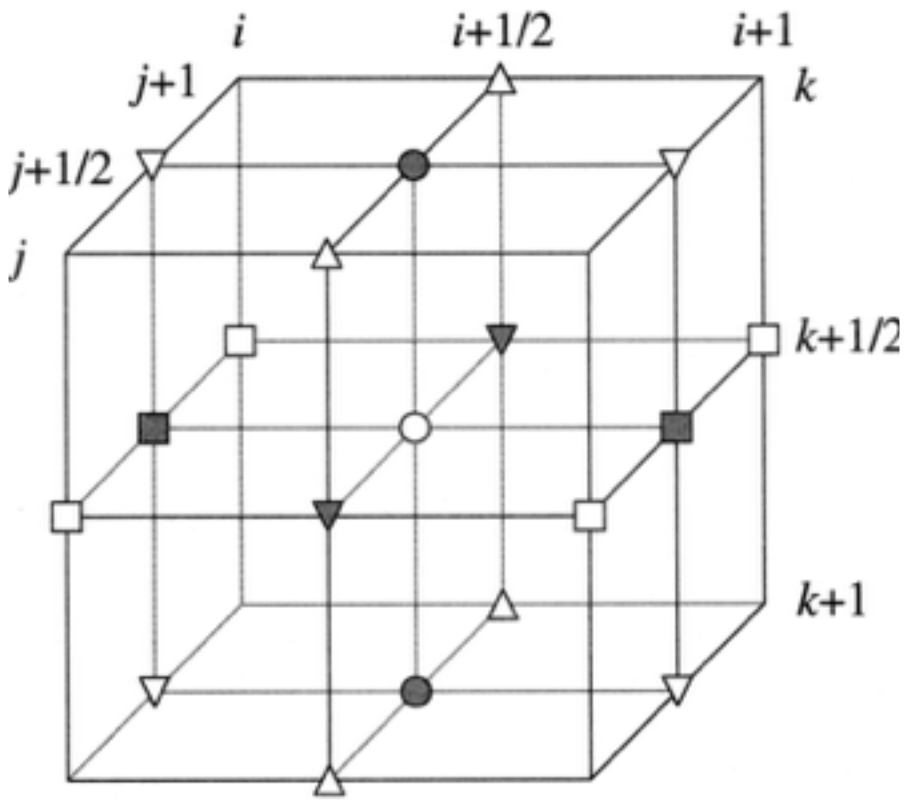
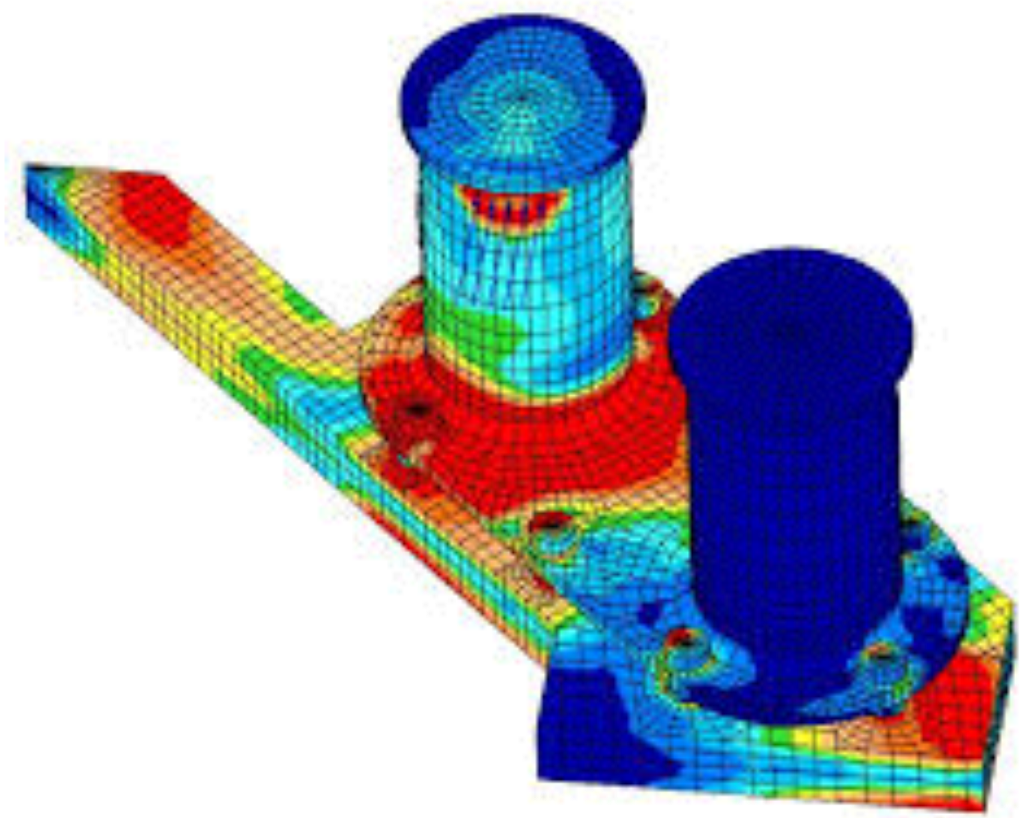
Discretization of PDEs





You need to sample at:

- cell centers/faces
- quadrature points of each element
- …

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The Curse of Dimensionality

Where do you need to sample in order to solve this?

$$\nabla\left(\alpha(\mathbf{x})\nabla u(\mathbf{x})\right) = \rho(\mathbf{x})$$
$$u(\mathbf{x}) = g_D(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_D$$
$$\mathbf{n}\cdot\nabla u(\mathbf{x}) = g_N(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_N$$

Suppose the domain is a box and that you discretize using a 100x100x100 regular grid.

n=1,000,000 random numbers to propagate through…

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Dimensionality Reduction

Can you describe this:

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

using just a few random variables?

Yes!

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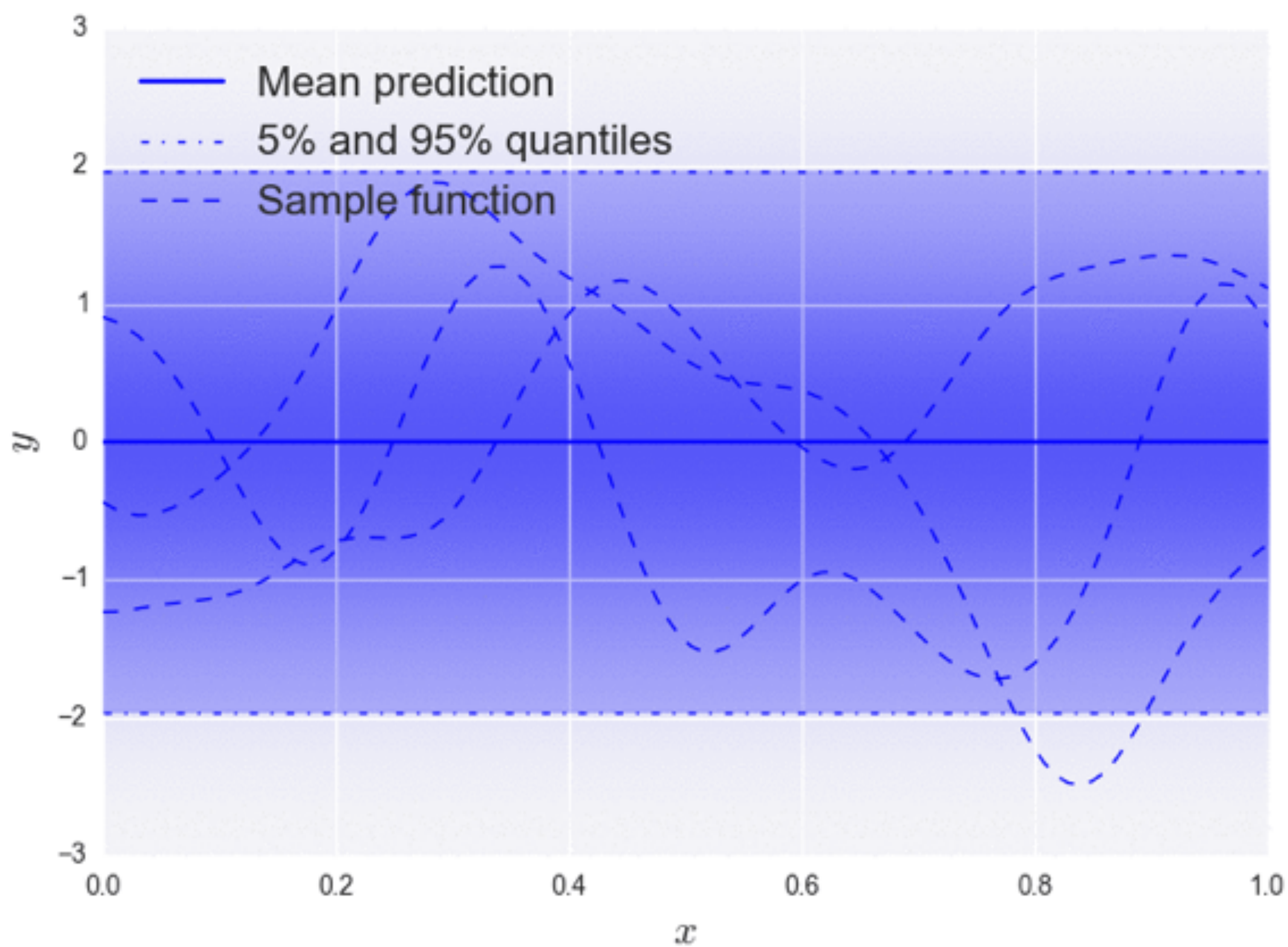
If things are smooth, then yes…

Infinitely smooth SE covariance



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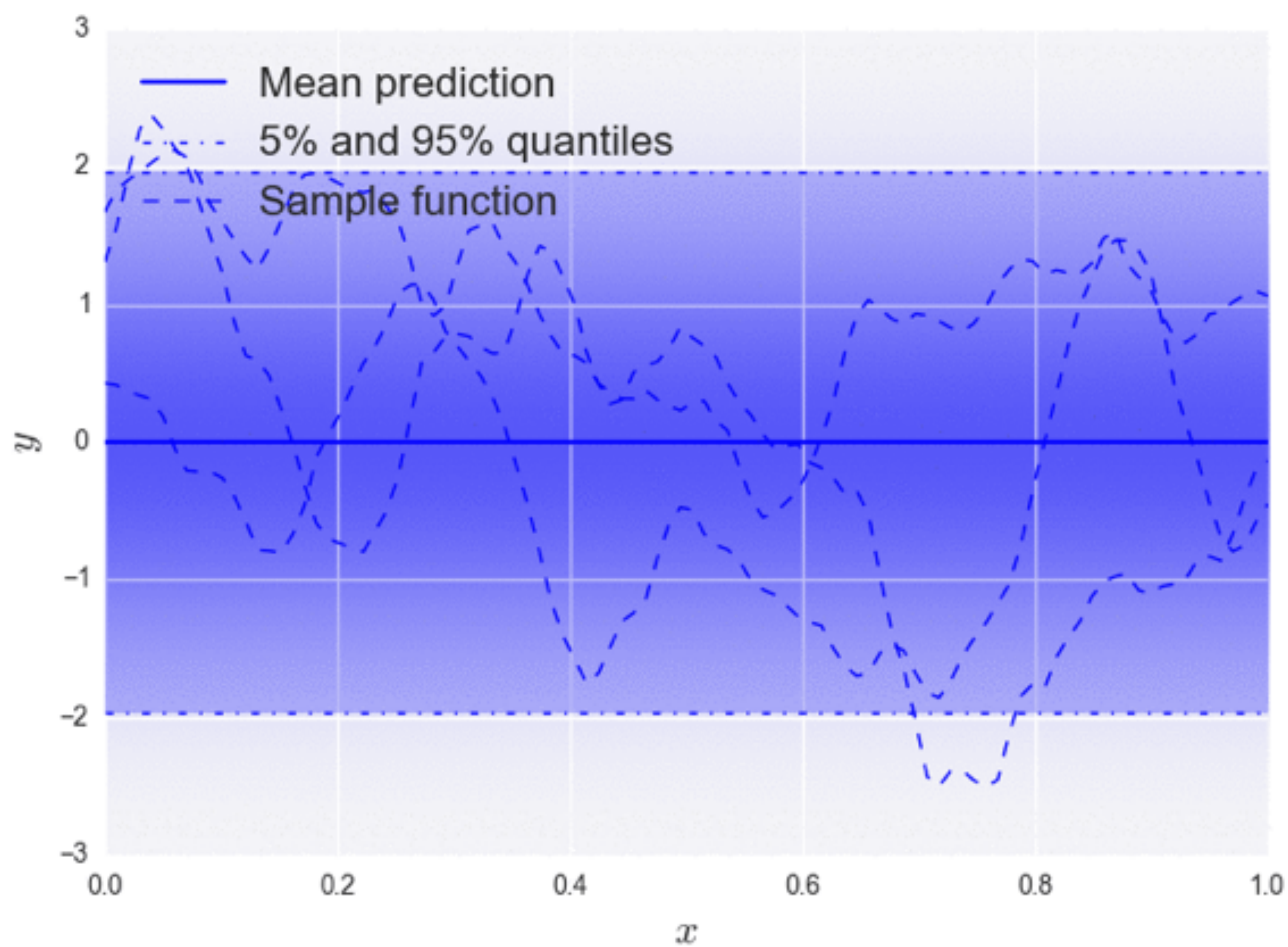
As smoothness decreases, we probably need more

Matern 2-3, 2 times differentiable



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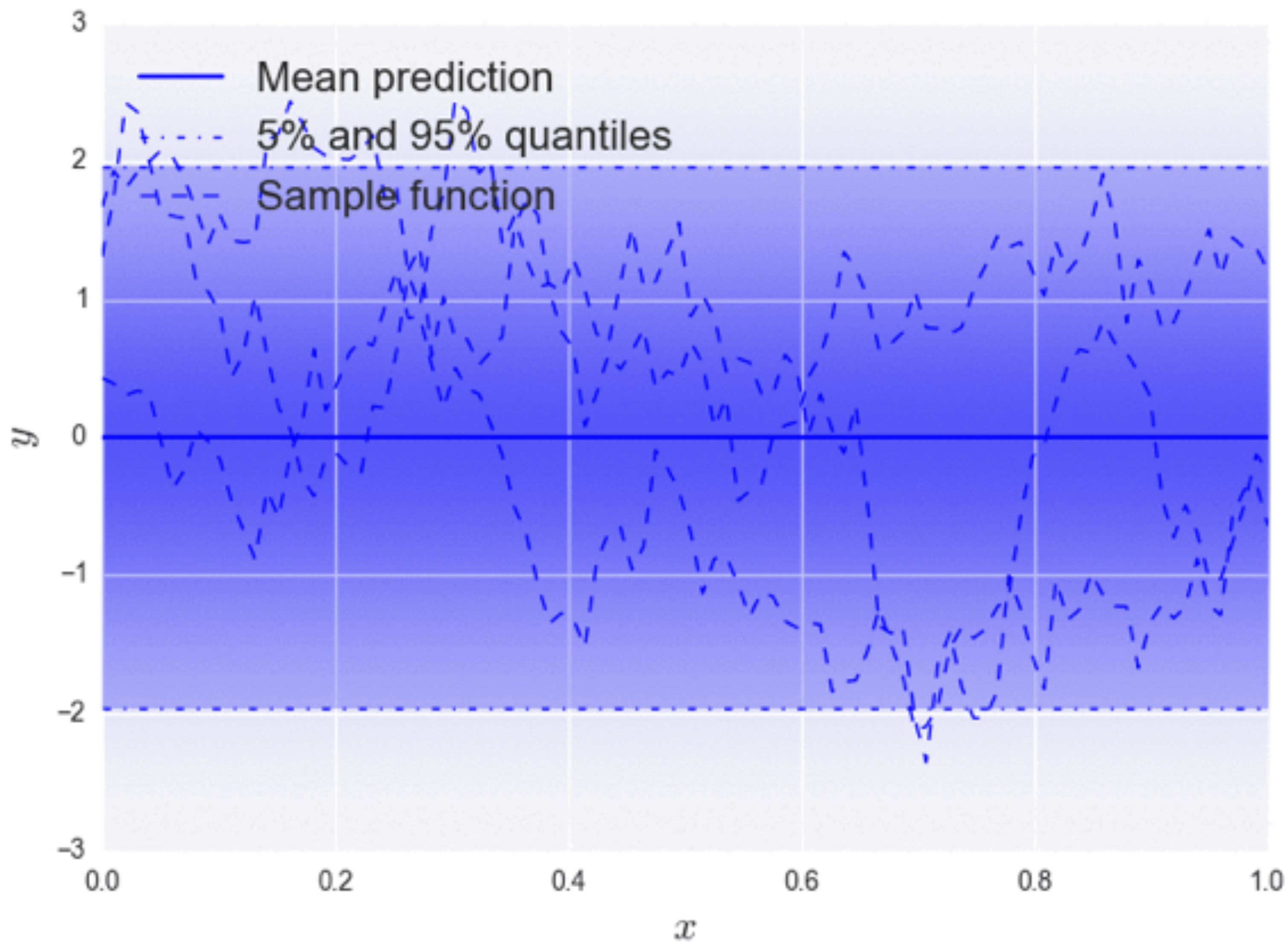
and more…

Exponential, continuous, nowhere differentiable



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Karhunen-Loeve Expansion (KLE)

Consider a GP:

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot, \cdot)\right)$$

Then, you can actually express any sample from this as:

$$f(\mathbf{x}; \boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty} \xi_i \sqrt{\lambda_i} \phi_i(\mathbf{x})$$

$$\boldsymbol{\xi} = \{\xi_1, \xi_2, \dots\}$$

Standard normal

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Karhunen-Loeve Expansion (KLE)

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$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

Then, you can actually express any sample from this as:

$$f(\mathbf{x};\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

with

$$\xi_i \sim \mathcal{N}(0,1)$$

$$\int k(\mathbf{x},\mathbf{x}')\phi_i(\mathbf{x}')d\mathbf{x}' = \lambda_i\phi_i(\mathbf{x})$$

Eigenvalues/functions of covariance function

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Proof of KLE

It suffices to show that:

$$f(\mathbf{x};\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

has the same mean and covariance as the GP.

Here we go:

$$\mathbb{E}_{\boldsymbol{\xi}}[f(\mathbf{x};\boldsymbol{\xi})] = m(\mathbf{x}) + \sum_{i=1}^{\infty}\overset{0}{\mathbb{E}_{\xi_i}[\xi_i]}\sqrt{\lambda_i}\phi_i(\mathbf{x}) = m(\mathbf{x})$$

$$\mathbb{C}[f(\mathbf{x};\boldsymbol{\xi}), f(\mathbf{x}';\boldsymbol{\xi})] = \mathbb{E}\left[\left(f(\mathbf{x};\boldsymbol{\xi}) - m(\mathbf{x})\right)\left(f(\mathbf{x}';\boldsymbol{\xi}) - m(\mathbf{x}')\right)\right]$$

$$= \sum_{i=1}^{\infty}\lambda_i\phi_i(\mathbf{x})\phi_i(\mathbf{x}') = k(\mathbf{x},\mathbf{x}')$$

Mercer's Theorem

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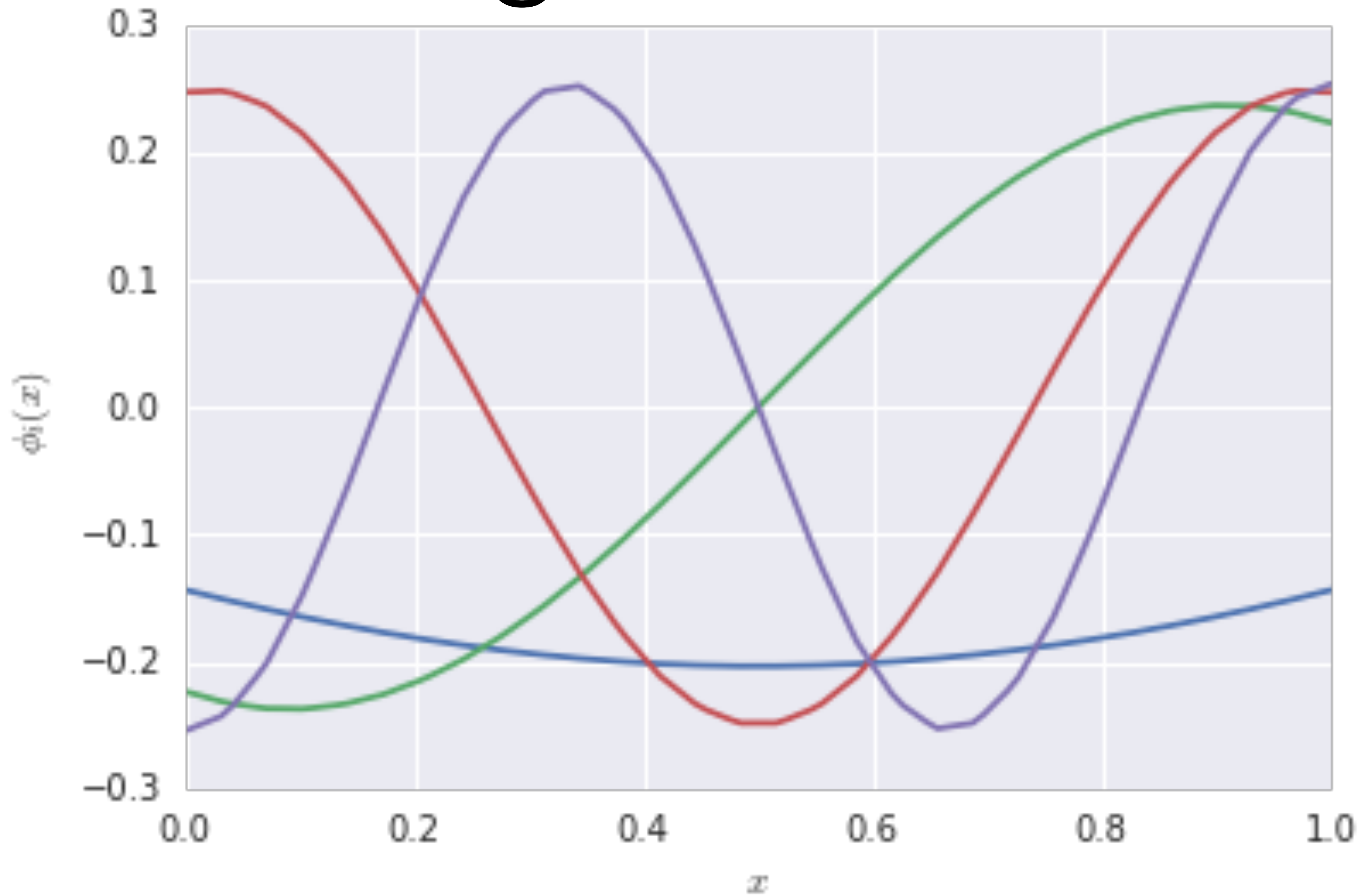
Example: SE Covariance, the eigenfunctions



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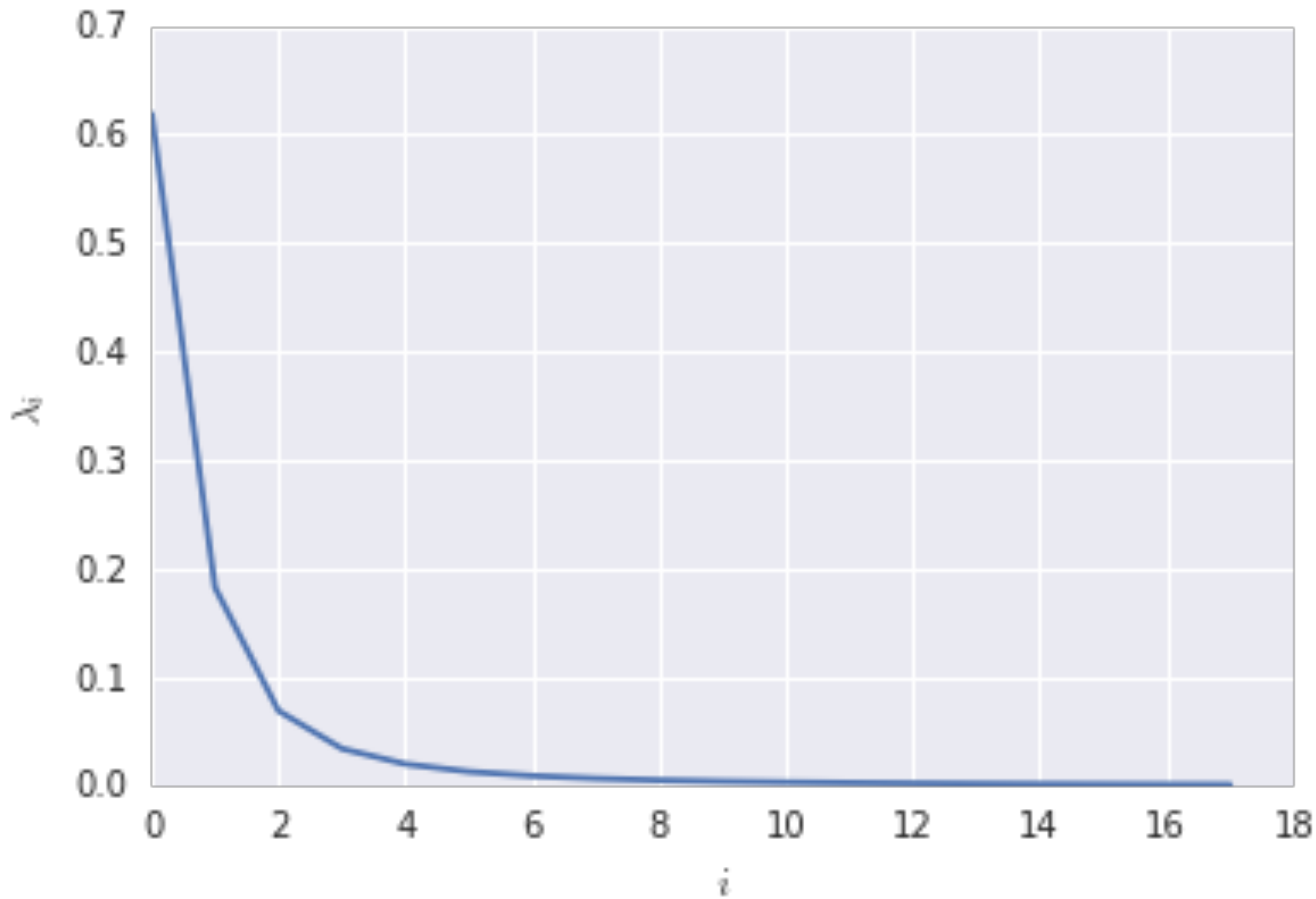
Example: SE Covariance, the eigenvalues



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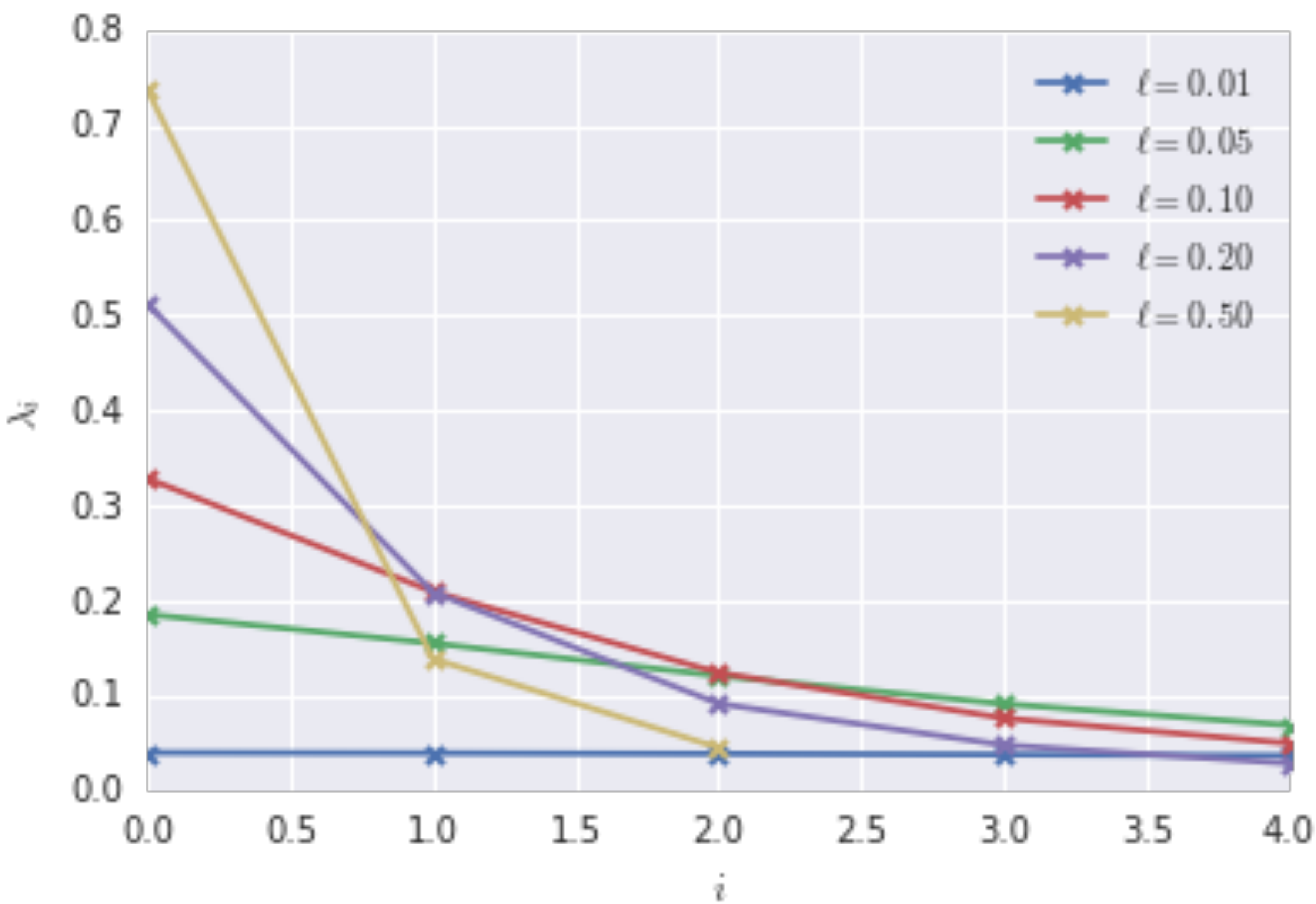
Example: SE Covariance, increasing the length scale



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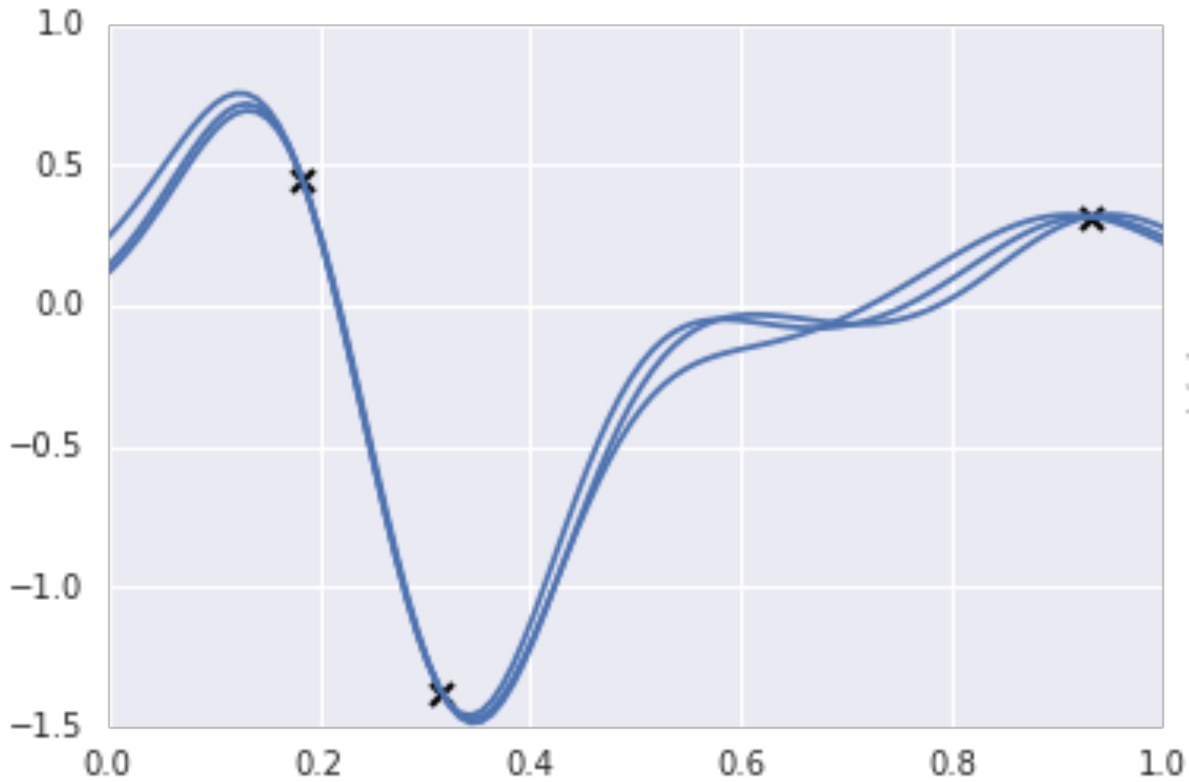
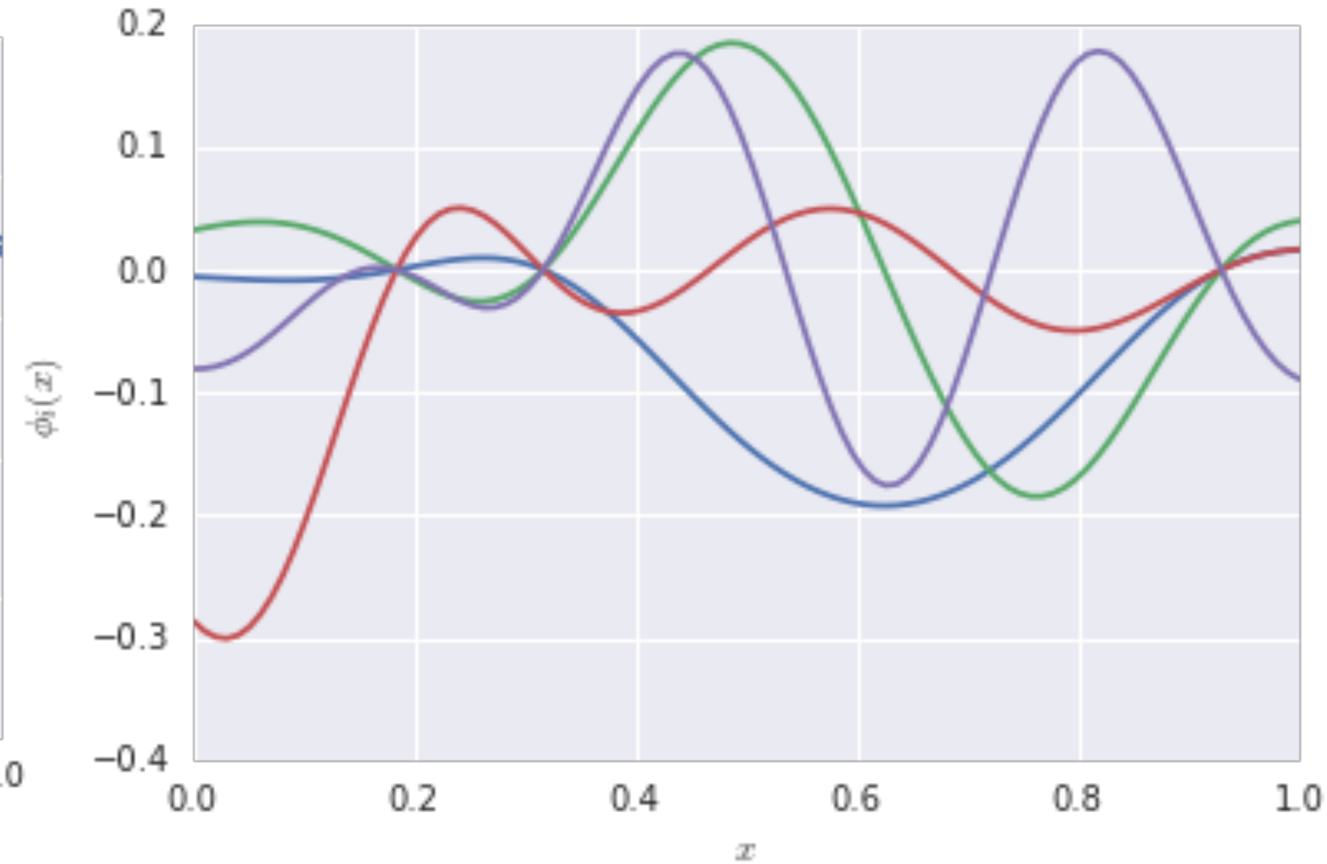
Posterior Covariance

$$f(\mathbf{x};\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty} \xi_i \sqrt{\lambda_i} \phi_i(\mathbf{x})$$





The eigenfunctions are zero at the points where we have observations!

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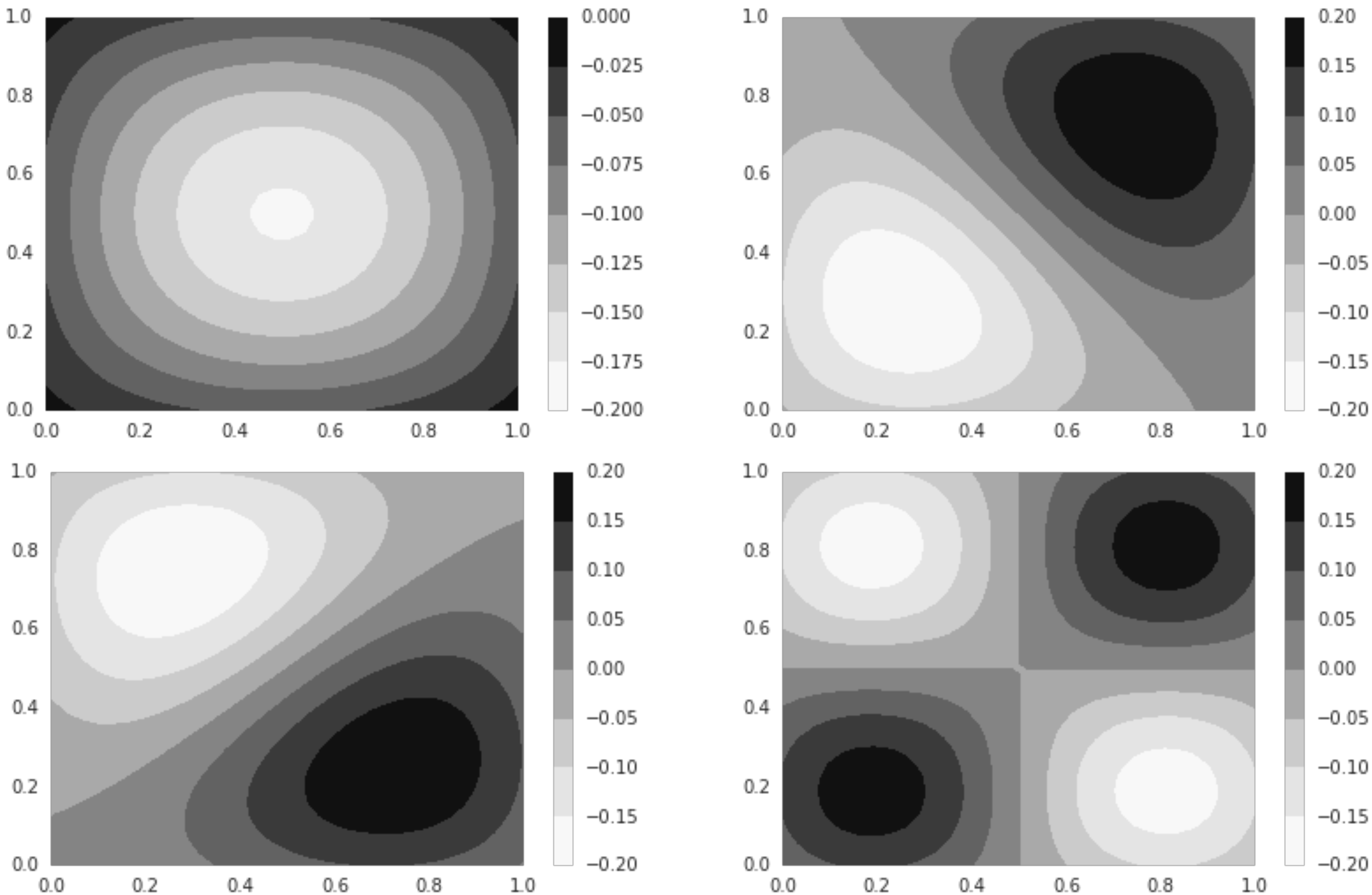
SE, in two-dimensions



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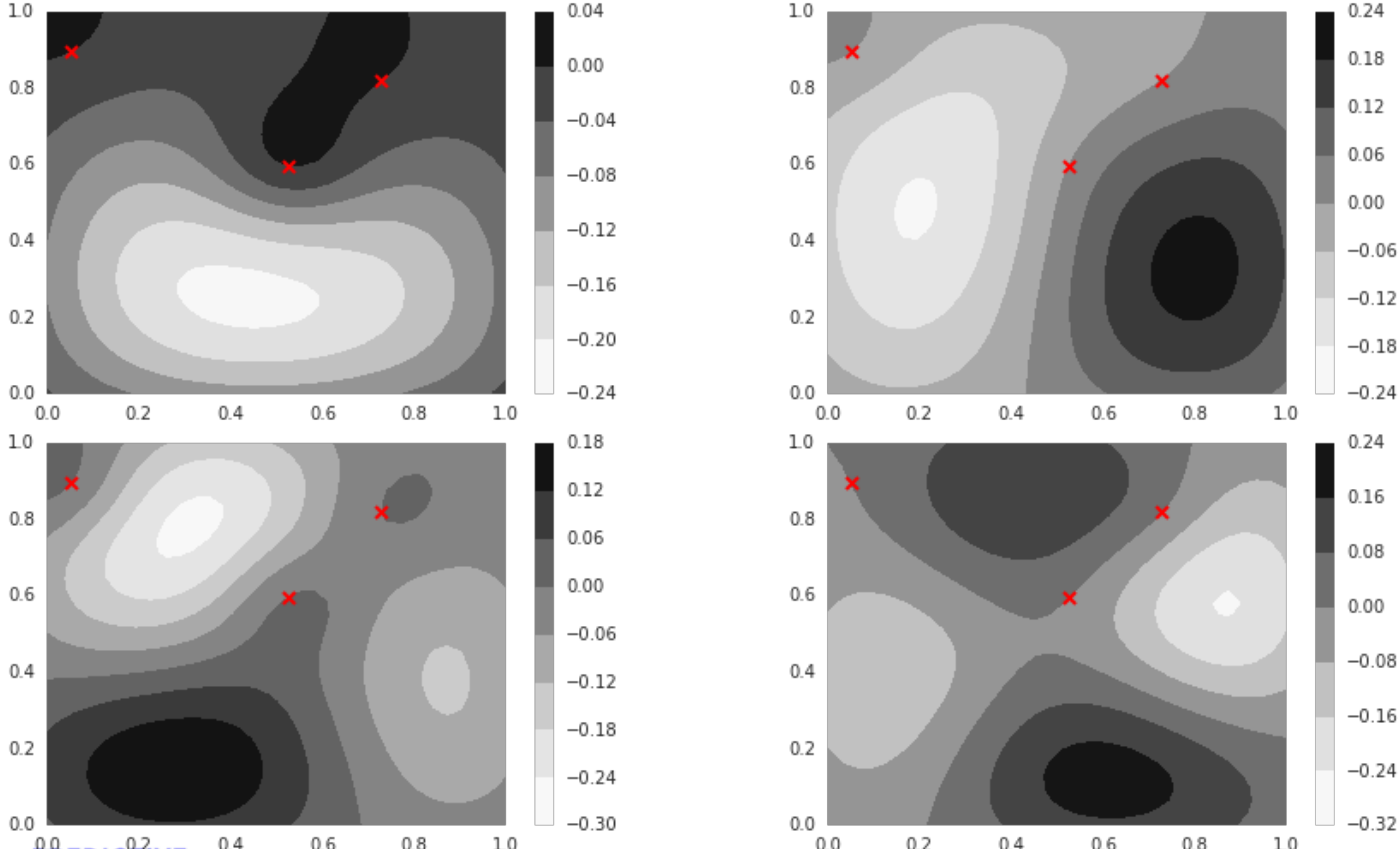
SE, in two-dimensions with observations



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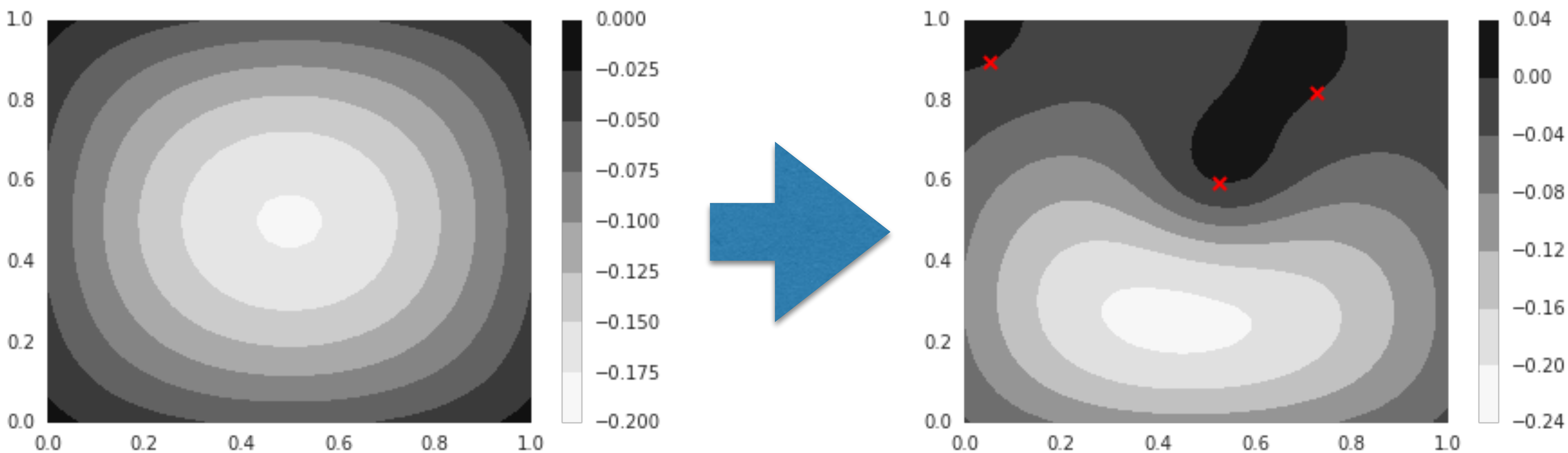
How did the eigenfunctions change?



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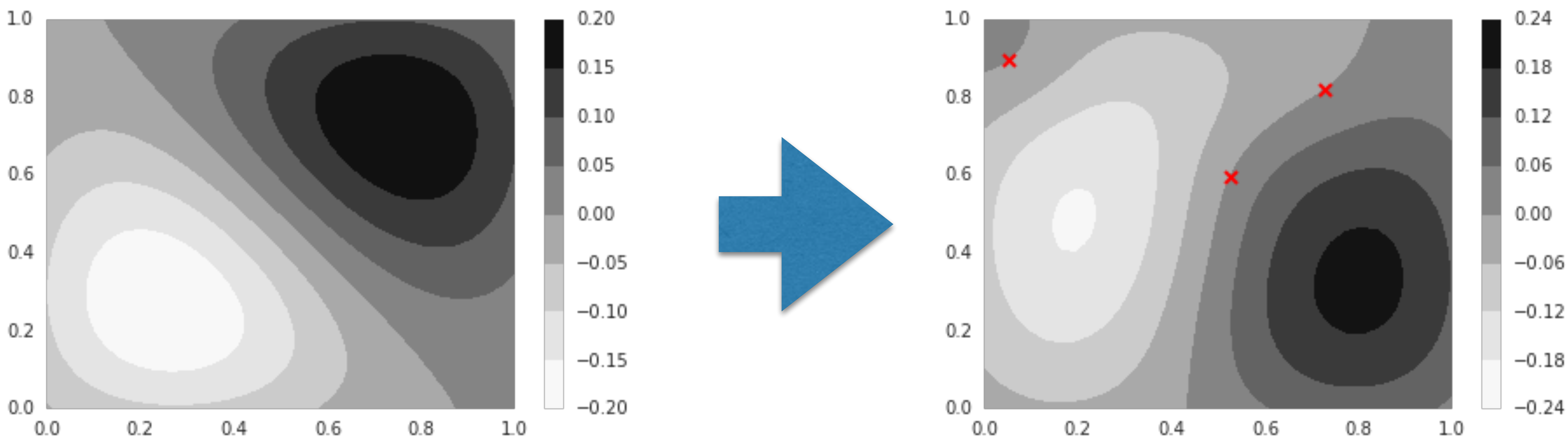
How did the eigenfunctions change?



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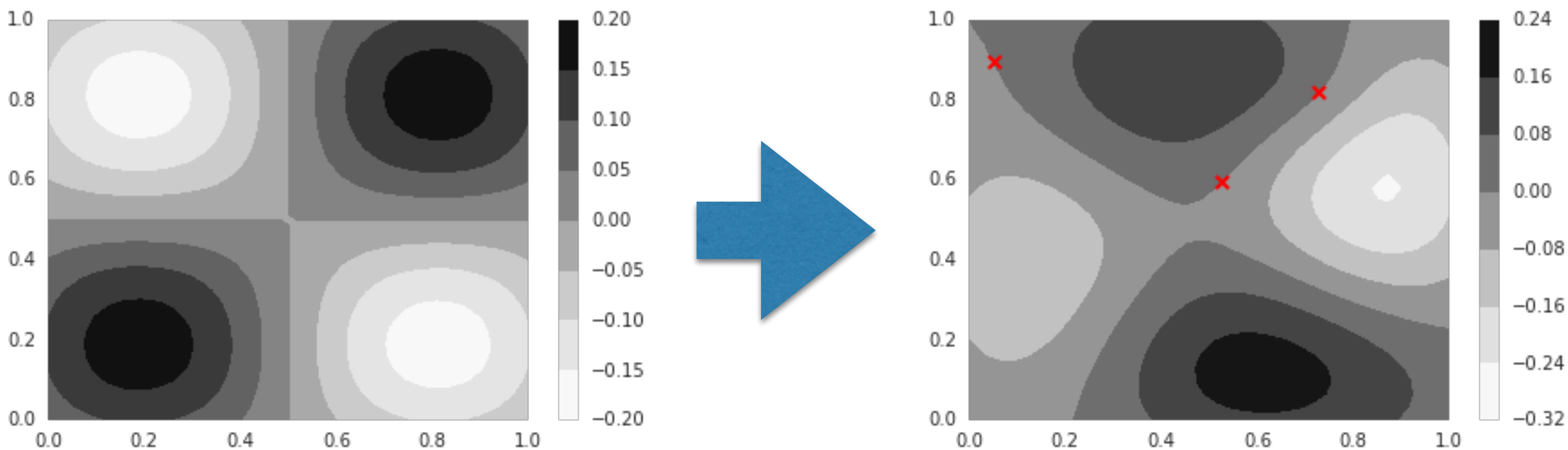

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Karhunen-Loeve Expansion (KLE)

Consider a GP:

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

Then, you can actually express any sample from this as:

$$f(\mathbf{x};\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

After some terms, these are zero!

with

$$\xi_i \sim \mathcal{N}(0,1) \qquad \int k(\mathbf{x},\mathbf{x}')\phi_i(\mathbf{x}')d\mathbf{x}' = \lambda_i\phi_i(\mathbf{x})$$

Where is the dimensionality reduction?

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Truncated Karhunen-Loeve Expansion (TKLE)

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

$$f(x;\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

$$\Downarrow$$

$$f(x;\xi) = m(\mathbf{x}) + \sum_{i=1}^{d}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

How do we select d?

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Truncated Karhunen-Loeve Expansion (TKLE)

$$p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot), k(\cdot,\cdot)\right)$$

$$f(x;\boldsymbol{\xi}) = m(\mathbf{x}) + \sum_{i=1}^{\infty} \xi_i \sqrt{\lambda_i}\phi_i(\mathbf{x})$$

$$f(x;\xi) = m(\mathbf{x}) + \sum_{i=1}^{d} \xi_i \sqrt{\lambda_i}\phi_i(\mathbf{x})$$

$$\sum_{i=1}^{d} \lambda_i = 0.95 \times \sum_{i=1}^{\infty} \lambda_i$$

Energy or Variance of the field

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“OK, I’m sold!
How can I compute the KLE?”

The Nystrom Approximation

We need to solve a Fredholm integral equation:

$$\int k(\mathbf{x}, \mathbf{x}')\phi_i(\mathbf{x}')d\mathbf{x}' = \lambda_i \phi_i(\mathbf{x})$$

Approximate the left hand side with a quadrature:

$$\sum_{j=1}^{n_q} w_j k(\mathbf{x}, \mathbf{x}_j)\phi_i(\mathbf{x}_j) \approx \lambda_i \phi(\mathbf{x})$$

Assume that the equation holds at the quadrature points:

$$\sum_{j=1}^{n_q} w_j k(\mathbf{x}_r, \mathbf{x}_j)\phi_i(\mathbf{x}_j) \approx \lambda_i \phi(\mathbf{x}_r)$$

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The Nystrom Approximation

We need to solve a Fredholm integral equation:

$$\int k(\mathbf{x},\mathbf{x}')\phi_i(\mathbf{x}')d\mathbf{x}' = \lambda_i\phi_i(\mathbf{x})$$

$$\sum_{j=1}^{n_q} w_j k(\mathbf{x}_r,\mathbf{x}_j)\phi_i(\mathbf{x}_j) \approx \lambda_i\phi(\mathbf{x}_r)$$

$$\mathbf{K}_q\mathrm{diag}(w_1,\dots,w_{n_q})\mathbf{v}_i = \lambda_i\mathbf{v}_i$$

Eigenvalue problem

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The Nystrom Approximation

We need to solve a Fredholm integral equation:

$$\int k(\mathbf{x},\mathbf{x}')\phi_i(\mathbf{x}')d\mathbf{x}' = \lambda_i\phi_i(\mathbf{x})$$

$$\mathbf{K}_q\mathrm{diag}(w_1,\dots,w_{n_q})\mathbf{v}_i = \lambda_i\mathbf{v}_i$$

Eigenvalue problem

$$\phi_i(\mathbf{x}) = \lambda_i^{-1}\sum_{j=1}^{n_q} w_j k(\mathbf{x},\mathbf{x}_j)\phi_i(\mathbf{x}_j) = \lambda_i^{-1}\sum_{j=1}^{n_q} w_j k(\mathbf{x},\mathbf{x}_j)v_{ij}$$

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Model Stochastic PDE Problem

Consider the elliptic partial differential equation:

$$\nabla\left(\alpha(\mathbf{x})\nabla u(\mathbf{x})\right) = \rho(\mathbf{x})$$

with boundary conditions:

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$$\mathbf{n}\cdot\nabla u(\mathbf{x}) = g_N(\mathbf{x}),\ \text{on } \mathbf{x}\in\Gamma_N$$

Since it is positive:

$$\alpha(\mathbf{x}) = \exp\left\{f(\mathbf{x})\right\}$$

$$\cancel{p(f(\cdot)|I) = \mathrm{GP}\left(f(\cdot)|m(\cdot),k(\cdot,\cdot)\right)}$$

$$f(x;\xi) = m(\mathbf{x}) + \sum_{i=1}^{d}\xi_i\sqrt{\lambda_i}\phi_i(\mathbf{x})$$

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