Approximating Random Gaussian Fields

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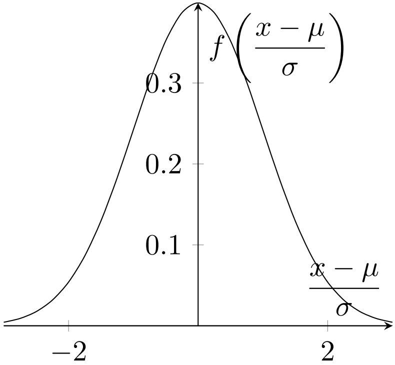
Review of Gaussian Variables (Finite Dimensions)

- Gaussian random variable: $x \sim \mathcal{N}(\mu, \sigma^2)$
  - mean $\mu = \mathbb{E}[x]$, variance $\sigma^2 = \mathrm{Var}(x)$



- Multivariate gaussian $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$, where $\boldsymbol{x} = [x_1, ..., x_n]^T$
  - mean $\boldsymbol{\mu} = [\mu_1, ..., \mu_n]^T$
  - Covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$
  - where

$$\Sigma_{jj} = \mathrm{Var}(x_j), \quad \Sigma_{ij} = \mathbb{E}\left[(x_i - \mu_i)(x_j - \mu_j)\right]$$

Gaussian Process (Infinite Dimensions)

- $X(x) \sim \mathcal{N}(\mu(x), \mathcal{C})$, where $x \in [0,1]$
- $\mu(x) \in C^2\,[0,1]$ is the mean function
- $\mathcal{C}$ is the *Covariance Operator*, defined via a covariance *kernel* $c(x,y)$:

$$f : [0,1] \to \mathbb{R}, \quad \mathcal{C}f := \int_0^1 c(x,y) f(y)\,dy$$

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$$c(x,y) := \mathbb{E}\left[(X(x) - \mu(x))(X(y) - \mu(y))\right] \quad \text{pointwise expectation}$$

- $\mathcal{C} : C^2\,[0,1] \to C^2\,[0,1]$
- Problem: $C^2\,[0,1]$ is infinite dimensional! We cannot sample this space feasibly!
- Solution: Karhunen-Loéve Series Expansion

Karhunen-Loéve Series Expansion (KLSE)

- Let $\{\lambda_k, \phi_k\}_{k=1}^{\infty}$ be the orthonormal eigenexpansion of $\mathcal{C}$:

$$\mathcal{C}\phi_k = \lambda_k \phi_k$$

- Let $\xi_k \sim \mathcal{N}(0, \lambda_k)$ be independently distributed random gaussian variables (act as Fourier Modes)
- Then

$$\left[X(x) = \mu(x) + \sum_{k=1}^{\infty} \xi_k \phi_k(x) \right] \sim \mathcal{N}(\mu(x), \mathcal{C})$$

- We can approximate this via a finite dimensional variable:

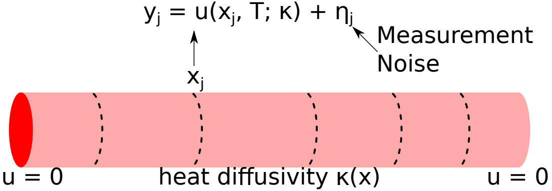
$$\tilde{X}_N(x) = \mu(x) + \sum_{k=1}^{N} \xi_k \phi_k(x) \approx X(x)$$

- This builds a finite dimensional approximation to the infinite dimensional target space

$$\mathbb{R}^N \to C^2\left[0, 1\right] \quad \boldsymbol{\xi} \mapsto X(x) \sim \mathcal{N}(\mu(x), \mathcal{C})$$

Model Problem

- Inverse problem for thermal properties of a system
- Goal: determine $\kappa(x)$ given noisy measurments y_j of temperature at time T



- Model PDE

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u}{\partial x}\right) \quad x \in (0,1) \quad 0 \leq t \leq T$$
$$u(x, t=0) = u_0(x) \quad u(0,t) = u(1,t) = 0 \tag{1}$$

- Assume κ is a log normal random variable

$$\hat{\kappa}(x) = e^{\mathbb{E}[X(x)]}, \quad X \sim \mathcal{N}(\mu, \mathcal{C}) \tag{2}$$

Bayesian Approach

- Guess a distribution, called a *prior*: $X^{(0)} \sim \mathcal{N}(m_0, \mathcal{C}_0)$
- Generate a sample X from the prior, can deduce the probability of observing samples $\boldsymbol{y}$ from solving the PDE
- $[\mathcal{G}(\kappa)]_j = u(x_j, T; \kappa)$ is solution at measured locations from $\kappa(x)$
- Bayes' formula (*Posterior* approximating true distribution):

$$\mathbb{P}^{\boldsymbol{u}}(X = \chi) = \sum_{\mathcal{G}(e^X)} \mathbb{P}(\mathcal{G}\left(e^X\right) = \boldsymbol{u} \mid X = \chi)\mathbb{P}_0(X = \chi)$$

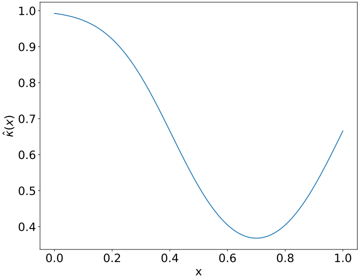
- Where

$$\mathcal{G}\left(e^X\right) \sim \sum_{X \sim \mathcal{N}(m_0, \mathcal{C}_0)} \mathbb{P}(\mathcal{G}\left(e^X\right) = \boldsymbol{u} \mid X = \chi)\mathbb{P}_0(X = \chi)$$

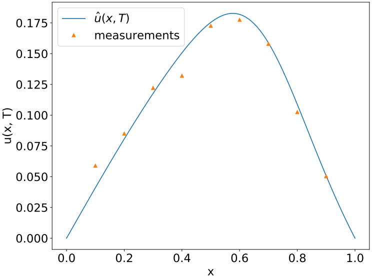
- This is a two stage process
  1. Sample the prior and build a distribution for $\mathcal{G}\left(e^X\right)$
  2. Apply Bayes' formula over the generated distribution to build the posterior for X

An Example

- Let $\hat{\kappa}(x) = \exp\left(e^{-10(x-0.7)^2}\right)$ for $x \in [0,1]$
- Exact solution is $\hat{u}(x,T)$ at final time T
- Measurements $y_j = \hat{u}(x_j, T) + \eta_j$, noise level $\gamma = 0.01$
- $x_j = 0.1, 0.2, ..., 0.9$



(a) $\hat{\kappa}(x)$



(b) $\hat{u}(x,T)$ and measurements y_j

Prior (on $\log \kappa$)

- Let $m_0(x) \equiv 0$
- $(\mathcal{C}_0 f)(x) = \displaystyle\int_0^1 c(x,y) f(y)\, dy$

$$c(x,y) = \begin{cases} -x(1-y) & 0 \le x \le y \le 1 \\ -y(1-x) & 0 \le y < x \le 1 \end{cases}$$

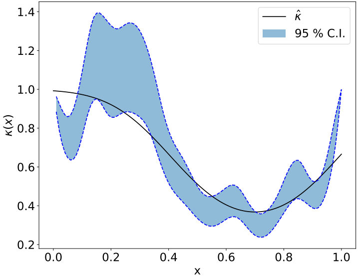
- Eigenexpansion of $\mathcal{C}_0$:

$$\phi_k(x) = \sqrt{2}\sin(k\pi x), \quad \lambda_k = \frac{1}{k^2\pi^2}$$

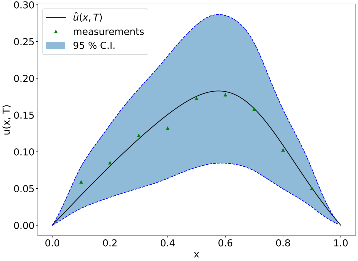
- Measurement points have $\Delta x = 0.1$, so any ϕ_k for $k > 20$ is unresolved
  - This gives a cutoff $K_{\max} = 20$
  - $X(x) \approx \displaystyle\sum_{k=1}^{K_{\max}} \xi_k \sqrt{2}\sin(k\pi x)$
  - $\xi_k \sim \mathcal{N}\left(0, \dfrac{1}{k^2\pi^2}\right)$

Results

- 100,000 iterations through MCMC Metropolis Algorithm
- Pointwise 95% confidence intervals

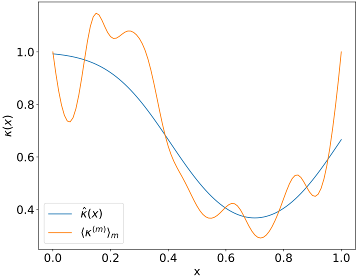


(a) Confidence interval for fitting $\hat{\kappa}(x)$

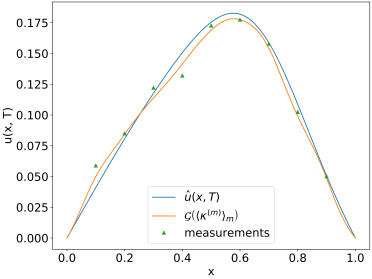


(b) Confidence interval for $\hat{u}(x, T)$

Computed Averages



(a) Comparison of $\hat{\kappa}(x)$ with computed pointwise average



(b) Comparison of $\hat{u}(x, T)$ with resulting solution from computed $\kappa(x)$

- Very little deviation in $u(x, T)$ despite larger deviations in $\kappa(x)$
- General trend of $\hat{\kappa}$ is resolved

Conclusions

- KLSE Provides a framework to approximate random fields $X \sim \mathcal{N}(\mu, \mathcal{C})$
- Bayesian approach can be used to approximate a distribution using a guess for the distribution (prior) and a model for the conditional probability (Bayes formula)
- This approach is commonly used to solve inverse problems
- Major drawback is the number of trials needed (100,000)
- Extension to project: Can we learn a better prior as we go?

$$\mathcal{N}(m_0, \mathcal{C}_0) \to \mathcal{N}(m_0(x; \boldsymbol{\theta}), \mathcal{C}_0(\boldsymbol{\theta}))$$

References

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