VŠB TECHNICKÁ UNIVERZITA OSTRAVA | FAKULTA ELEKTROTECHNIKY A INFORMATIKY | KATEDRA APLIKOVANÉ MATEMATIKY

Approximation of Karhunen-Loève Decomposition of Isotropic Gaussian Random Fields Using Orthogonal Polynomials and Gaussian Quadratures

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Goal of the thesis

- Review of the theory of orthogonal polynomials:
  - Three-term recurrence
  - Golub-Welsch algorithm
  - Generalization of Legendre polynomials and quadrature to any interval
  - Numerical experiments of quadrature rule convergence
- Karhunen-Loève decomposition of isotropic Gaussian random fields
  - Introduction to Karhunen-Loève decomposition
  - Galerkin method for approximating eigenpairs of autocovariance function
  - Numerical experiments of Galerkin matrix assembly and convergence of residuum of calculated eigenpairs

Goal: approximating KL decomposition and sampling GRF

- Random fields can be considered as a map $\Omega \to L^2(D)$.
- samples of random fields are then functions on spatial domains.
- Karhunen-Loève decomposition separates randomness and spatial behavior. It can be used for fast and efficient sampling.
- Autocovariance function of isotropic Gaussian random fields is used for decomposition.

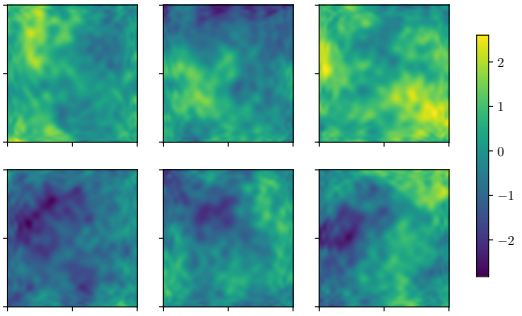

Figure 1: Sample realizations of a 2D random field with an exponential covariance function $(c(x, y) = \exp(-\|x - y\|))$

Legendre polynomials and Quadrature rules

Construction of orthogonal polynomials

Can be constructed using the three-term recurrence:

$$\pi_{k+1}(x) = (x - \alpha_k)\,\pi_k(x) - \beta_k \pi_{k-1}(x), \quad k = 0, 1, 2, \ldots,$$

$$\pi_{-1}(x) = 0, \pi_0(x) = 1.$$

Can be modified for the construction of normalized polynomials.

Visualization of Legendre polynomials

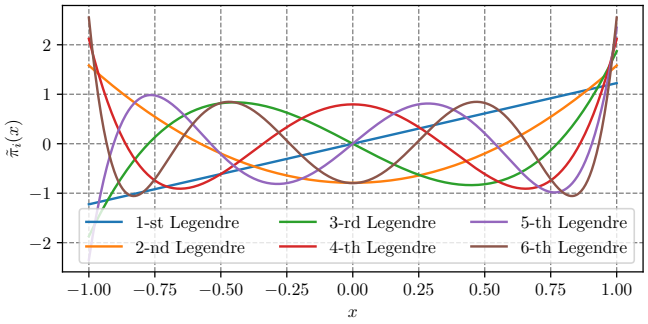

Figure 2: Normalized Legendre polynomials

Golub-Welsch algorithm

- Coefficients of the three-term recurrence define the Jacobi matrix:

$$J_n := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_n} \\ 0 & & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}$$

- eigenvalues of the Jacobi matrix are quadrature nodes τ_j and the quadrature weights $\lambda_i = \beta_0 \boldsymbol{v}_{i,1}^2$, where $\boldsymbol{v}_i$ is corresponding eigenvector.

$$\int_I f(x) w(x)\, dx \approx \sum_{j=1}^{n} \lambda_j f(\tau_j).$$

Generalization of Legendre polynomials

- Integral over $I =< a, b >$
- Legendre polynomial transformation:

$$\pi_i(x) = \pi_i^L \left(\frac{a+b}{a-b} + \frac{2}{b-a} x \right) \sqrt{\frac{2}{b-a}}.$$

- Quadrature transformations
  - nodes:

$$\tau_i = \frac{a+b}{2} + \frac{b-a}{2} \tau_i^L$$

  - weights:

$$\lambda_i = \frac{b-a}{2} \lambda_i^L$$

Quadrature examples

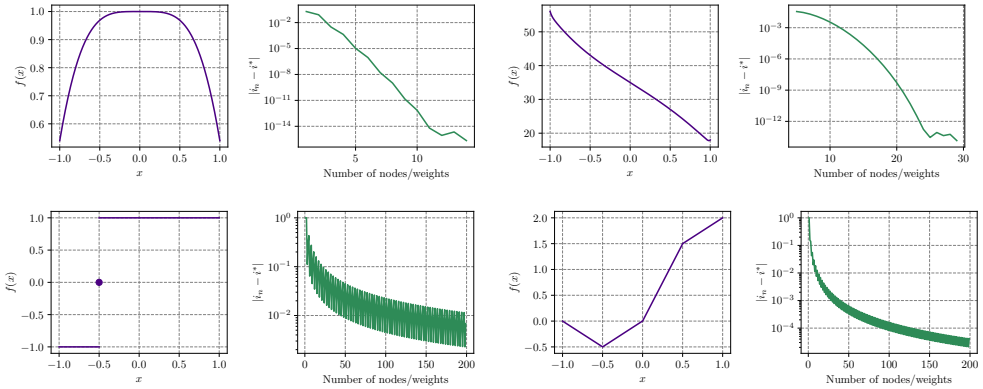

Figure 3: Examples of Integrated function (purple) and the convergence of numerical integration (green)

Computation time

Eigenpairs are obtained using a specialized algorithm for Hermite three-diagonal matrices

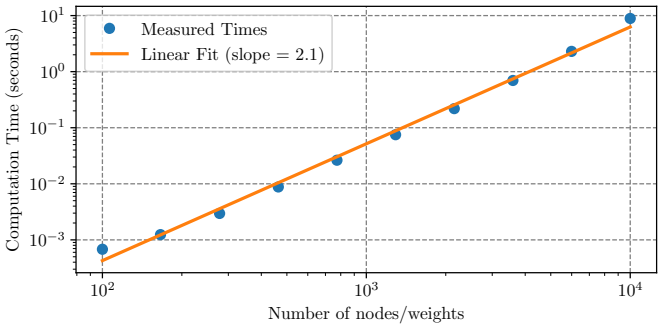

Figure 4: Log-Log Plot of Computation Time vs. Jacobi Size n

Karhunen-Loève expansion

Karhunen-Loève expansion

$X : \mathcal{T} \times \Omega \to \mathbb{R}$ is a random field (isotropic, Gaussian with zero mean).

$$X(t, \omega) = \sum_{j=1}^{\infty} \gamma_j(\omega) \sqrt{\lambda_j} u_j(t),$$

(λ_j, u_j) are eigenpairs of the autocovariance operator C:

$$(Cu)(x) \coloneqq \int_{\mathcal{T}} c(x, y)\, u(y)\, dy,$$

$$\gamma_j(\omega) \coloneqq \langle X(t, \omega), u_j(t) \rangle_{L^2(\mathcal{T})}.$$

for Gaussian random field $\gamma_j(\omega)$ are i.i.d. $N(0, 1)$.

$c(x, y) = c(\|x - y\|) = c(d)$. e.g. exp: $c(d) = e^{-d}$, squared exp:$c(d) = e^{-\frac{d^2}{2}}$, Matérn: $c(d) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{d}{\rho}\right)^{\nu} K_\nu \left(\sqrt{2\nu}\frac{d}{\rho}\right)$

Galerkin method

Galerkin method approximates eigenpairs of autocovariance operator with polynomial basis that is orthonormal on $\mathcal{T}$. We assume $\mathcal{T}$ is a multidimensional interval, then the basis is a tensor product of 1D Legendre polynomials.

$$A\overline{\boldsymbol{u}}_i = \lambda_{i,N} W \overline{\boldsymbol{u}}_i,$$

$$W_{k,j} = \int_{\mathcal{T}} \psi_k(\boldsymbol{x})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x}.$$

Matrix W is an identity matrix due to orthonormality of basis polynomials. We then have an eigenvalue problem with semi-definite matrix A.

$$A_{k,j} = \int_{\mathcal{T}} \int_{\mathcal{T}} \psi_k(\boldsymbol{y})\, c(\boldsymbol{x}, \boldsymbol{y})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x} d\boldsymbol{y}.$$

Entries of A are computed using multidimensional quadratures (tensor product of 1D quadratures)

$A_{i,j}$ calculation error of Matérn covariance

Calculated values are compared against matrix A^* with $N_r = 5000$ nodes. Matérn covariance $c(d) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{d}{\rho}\right)^{\nu} K_\nu \left(\sqrt{2\nu}\frac{d}{\rho}\right)$ has parameters $\nu = 0.5$ and $\rho = 1$.

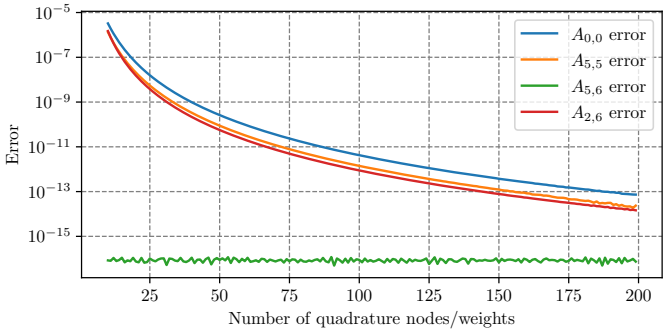

Figure 5: Error of entries $A_{k,l}$ obtained from Matérn covariance

Residuum

$$\|R_i\|_{L^2} = \left\| \int_{\mathcal{T}} c(x,y)\, \tilde{u}_i(y)\, dy - \tilde{\lambda}_i \tilde{u}_i(x) \right\|_{L^2} = \left(\int_{\mathcal{T}} \left(\int_{\mathcal{T}} c(x,y)\, \tilde{u}_i(y)\, dy - \tilde{\lambda}_i \tilde{u}_i(x) \right)^2 dx \right)^{1/2}.$$

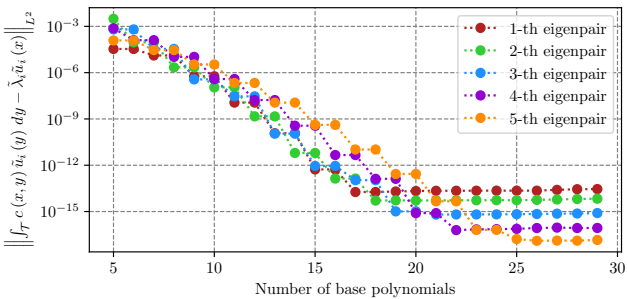

Figure 6: Residuum of eigenpairs obtained from Matérn covariance

Conclusion

What I have achieved:

- implemented Golub-Welsch algorithm for obtaining quadrature nodes and weights
- experimented with accuracy and computation time of Gaussian quadrature on different functions
- explained basics of random fields and Karhunen-Loève decomposition
- utilized Galerkin method for approximating eigenpairs (λ_j, u_j) for Karhunen-Loève decomposition
- shown computation error of elements of matrix A and a residuum of an approximation of eigenpairs (λ_j, u_j)

Thank you for your attention

Supervisor question

V grafu 4.1 sledujete pomalou konvergenci k přesné hodnotě integrálu při exponenciální kovarianci. Lze tento integrál efektivněji vyčíslit s ohledem na nespojitost derivace na přímce $y = x$? Jaký byste zvolil postup, aby bylo možné dosáhnout požadované přesnosti s výrazně menším počtem kvadraturních bodů?

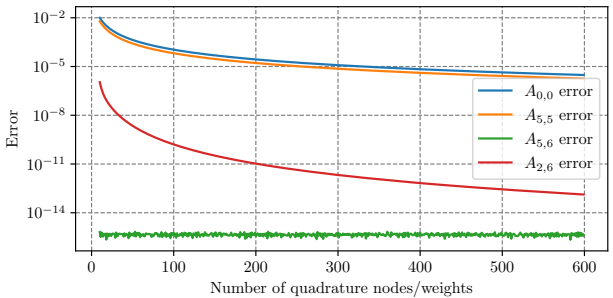

Figure 7: Error of entries $A_{k,l}$ obtained from exponential covariance

Answer

Rozdělíme na část pod $y = x$ a část nad $y = x$, tím vzniknou dva trojúhelníky.

Poté aplikujeme substituci na čtverec kde $x = u, y = \frac{1}{2}(u+1)(v+1) - 1$ a $|J| = (u+1)/2$. Substituce v integrálu pak je:

$$\int_{-1}^{1}\int_{-1}^{1} \psi_k\left(\frac{(u+1)(v+1)}{2} - 1\right) c\left(u, \frac{(u+1)(v+1)}{2} - 1\right) \psi_j(u)\,(u+1)/2\,dudv$$

Na vrchní trojúhelník použijeme podobnou substituci $x = \frac{1}{2}(u+1)(v+1) - 1, y = v$ a $|J| = (v+1)/2$

Opponent questions

Odkud v důkazu věty 15 plyne, že $\langle x\pi_k, \pi_{k-1}\rangle = \langle \pi_k, \pi_k\rangle$?

Answer

$$\langle x\pi_k, \pi_{k-1}\rangle = \langle \pi_k, x\pi_{k-1}\rangle$$

π_{k-1} je monický $\implies x\pi_{k-1}$ je monický

$$\begin{aligned} \exists p_{k-1} \in P_{k-1} : x\pi_{k-1} &= x^k + p_{k-1} \\ \exists q_{k-1} \in P_{k-1} : \pi_k &= x^k + q_{k-1} \end{aligned}$$

$$x\pi_{k-1} - \pi_k = p_{k-1} - q_{k-1} = r_{k-1} \in P_{k-1}$$

$$x\pi_{k-1} = \pi_k + x\pi_{k-1} - \pi_k = \pi_k + r_{k-1} = \pi_k + \sum_{i=0}^{k-1} c_i\pi_i, \quad r_{k-1} \in P_{k-1}$$

$$\langle \pi_k, x\pi_{k-1}\rangle = \langle \pi_k, \pi_k + \sum_{i=0}^{k-1} c_i\pi_i\rangle = \langle \pi_k, \pi_k\rangle + \sum_{i=0}^{k-1} c_i \langle \pi_k, \pi_i\rangle = \langle \pi_k, \pi_k\rangle$$

Opponent questions

Na straně 32 píšete, že efektivita Gaussovské kvadratury závisí na hladkosti integrované funkce. Z čeho toto tvrzení vychází?

Answer

Pozorování vychází z Remark 25: The n-point Gauss quadrature rule integrates polynomials of degree up to $2n-1$ exactly. Efektivita Gaussové kvadratury poté závisí na nepřesnosti aproximace polynomem. Existují odhady chyby polynomiální aproximace v závislosti na hladkosti aproximované funkce, například: *The $h-p$ version of the finite element method with quasiuniform meshes by I. Babuška, Manil Suri*, Lemma 4.1:

LEMMA 4.1 : *Let $S = Q$ or $S = T$ be the standard square or triangle. Then there exists a family of operators $\{\hat{\pi}_p\}$, $p = 1, 2, 3, \ldots$, $\hat{\pi}_p : H^k(S) \to \mathscr{P}_p(S)$ such that for any $0 \leqslant q \leqslant k$, $u \in H^k(S)$*

$$\|u - \hat{\pi}_p u\|_{q,S} \leqslant C p^{-(k-q)} \|u\|_{k,S}, \qquad k \geqslant 0 \tag{4.1a}$$

Opponent questions

Jak by Vaše implementace KL rozkladu fungovala ve více než dvou prostorových dimenzích?

Answer

Implementace KL by fungovala podobným způsobem.

Bázové funkce $\psi(\boldsymbol{x})$ by byly násobky orthonormálních polynomů
$(\psi_{i,j,k,l}(\boldsymbol{x}) = \tilde{\pi}_i(x_1)\tilde{\pi}_j(x_2)\tilde{\pi}_k(x_3)\tilde{\pi}_l(x_4))$

Tensor A by měl více dimenzí, pro spektralní rozklad by se A převedlo na matici.

Opponent questions

Bylo by možné provést KL rozklad i na jiných doménách než kartézských součinech intervalů?

Answer

Ano, ale ne s mojí implementací. Neměli bysme bázy orthogonálních polynomů a W by poté nebyla jednotková matice.