

Bias-Variance Tradeoff in Numerical Solution to the Poisson Equation

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Jan 13, 2017



I L L I N O I S



Numerical solution to the Poisson equation

Problem formulation

Poisson equation:
$$-\frac{1}{\rho(x)} \nabla \cdot (\rho(x) \nabla \phi(x)) = h(x) - \hat{h}$$
$$\int_{\mathbb{R}^d} \phi(x) \rho(x) dx = 0$$

- $\rho : \mathbb{R}^d \rightarrow \mathbb{R}^+$ (prob. density)
- $h : \mathbb{R}^d \rightarrow \mathbb{R}$ (given function), $\hat{h} := \int h(x) \rho(x) dx$
- $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ (solution)

Problem:

Given: $\{X^1, \dots, X^N\} \stackrel{\text{i.i.d.}}{\sim} \rho$

Find: $\{\nabla \phi(X^1), \dots, \nabla \phi(X^N)\}$ (approximately)

Almost like a statistical learning problem



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Feedback Particle Filter

Generalization of the Kalman Filter

Kalman Filter:

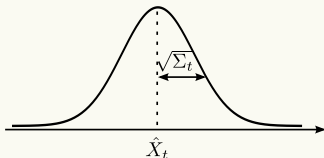
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$$dZ_t = HX_t dt + dW_t$$

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$$\frac{d\Sigma_t}{dt} = \dots \text{ (Riccati equation)}$$



Challenge: Compute the gain function $K_t := \nabla \phi$ from Poisson eq.

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$$+ K_t(X_t^i) \circ \left(dZ_t - \frac{h(X_t^i) + \hat{h}_t}{2} dt \right)$$



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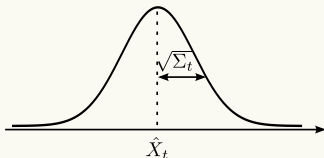
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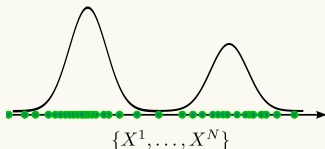
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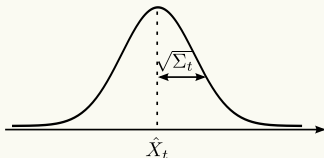
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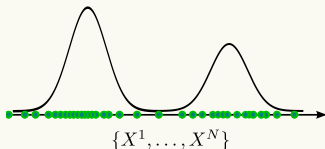
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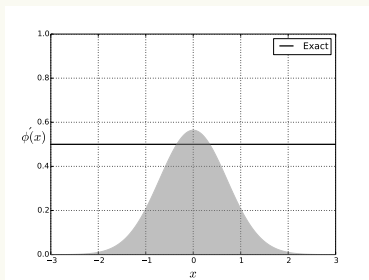
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Poisson equation

Examples

Gaussian distribution linear h



$$\nabla\phi(x) = \text{constant} \quad (\text{Kalman gain})$$

Bimodal distribution linear h

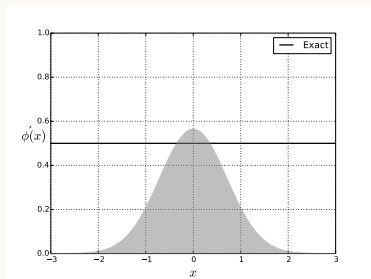
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Poisson equation

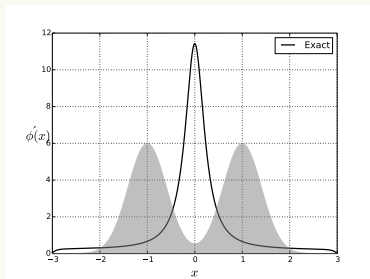
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Literature Review

Poisson equation and weighted Laplacian

Poisson equation:
$$-\frac{1}{\rho} \nabla \cdot (\rho \nabla \phi) = h - \hat{h}$$

Weighted Laplacian:
$$\Delta_{\rho} \phi := \frac{1}{\rho} \nabla \cdot (\rho \nabla \phi) = \Delta \phi + \nabla \log \rho \cdot \nabla \phi$$

PDE

- Markov Diffusion operators [D. Bakry, et. al. 2013]
- Heat kernels [A. Grigoryan, 2009]

Stochastic analysis

- Simulation and optimization theory for Markov models [S. Meyn, R. Tweedie, 2012]

Statistical learning

- Nonlinear dimensionality reduction [M. Belkin, 2003]
- Diffusion maps [R. Coifman, S. Lafon, 2006]
- Spectral clustering [M. Hein, et. al. 2006]



Three Formulations of the Poisson Equation

P) Weak formulation: (Galerkin)

$$\langle \nabla \phi, \nabla \psi \rangle = \langle h - \hat{h}, \psi \rangle, \quad \forall \psi \in H^1(\mathbb{R}^d, \rho)$$

where $\langle f, g \rangle := \int f(x)g(x)\rho(x) dx$

S) Semigroup formulation: (kernel-based)

$$\phi = P\phi + \tilde{h}$$

where $P := e^{\epsilon \Delta_\rho}$ and $\tilde{h} := \int_0^t e^{s \Delta_\rho} (h - \hat{h}) ds$

3) Variational formulation: (Neural net ?)

$$\min_{\phi \in H_0^1(\mathbb{R}^d, \rho)} \mathbb{E} \left[\frac{1}{2} |\nabla \phi(X)|^2 - \phi(X)(h(X) - \hat{h}) \right]$$

where $X \sim \rho$



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Galerkin Approximation

Concept

Strong form:

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$$\langle \nabla \phi^{(M)}, \nabla \psi \rangle = \langle h - \hat{h}, \psi \rangle, \quad \forall \psi \in S$$

where $S = \text{span}\{\psi_1, \dots, \psi_M\}$

Empirical approximation

$$\frac{1}{N} \sum_{i=1}^N \nabla \phi^{(M)}(X^i) \cdot \nabla \psi(X^i) = \frac{1}{N} \sum_{i=1}^N (h(X^i) - \hat{h}) \psi(X^i), \quad \forall \psi \in S$$

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Galerkin Approximation Algorithm

- Select basis functions $\{\psi_1, \dots, \psi_M\}$
- Express the approximate solution as

$$\phi^{(M,N)}(x) = \sum_{m=1}^M c_m \psi_m(x)$$

- Obtain $c = (c_1, \dots, c_M)$ by solving

$$Ac = b$$

where

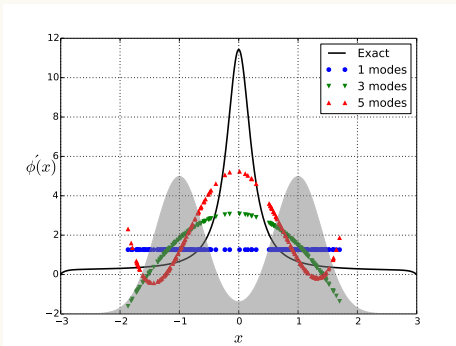
$$A_{ml} = \langle \nabla \psi_m, \nabla \psi_l \rangle \approx \frac{1}{N} \sum_{i=1}^N \nabla \psi_m(X^i) \cdot \nabla \psi_l(X^i)$$

$$b_m = \langle \psi_m, h \rangle \approx \frac{1}{N} \sum_{i=1}^N \psi_m(X^i) h(X^i) - \hat{h}$$



Galerkin Approximation

Numerical result



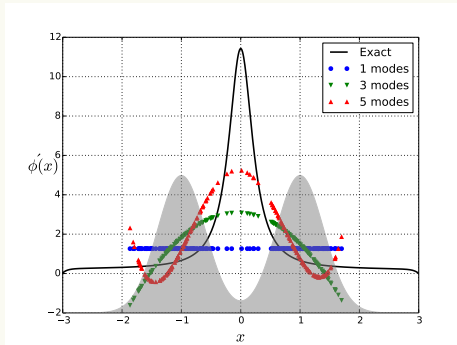
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- Choice of basis functions
- Singularity of A
- Computationally scales with $O(Nd^P)$



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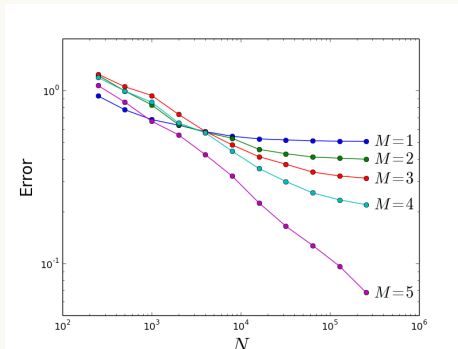


Galerkin Approximation

Error analysis

Special case: The basis functions are eigenfunctions of Δ_ρ

$$\underbrace{\mathbb{E} \left[\|\nabla\phi - \nabla\phi^{(M,N)}\|_{L^2} \right]}_{\text{Total error}} \leq \underbrace{\frac{1}{\sqrt{\lambda_M}} \|h - \Pi_S h\|_{L^2}}_{\text{Bias}} + \underbrace{\frac{1}{\sqrt{N}} \|h\|_\infty \sqrt{\sum_{m=1}^M \frac{1}{\lambda_m}}}_{\text{Variance}}$$





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Semigroup identity: $e^{\epsilon \Delta_\rho} = I + \int_0^\epsilon e^{s \Delta_\rho} \Delta_\rho ds$

Semigroup formulation:

$$\phi = e^{\epsilon \Delta_\rho} \phi + \tilde{h}$$

where $\tilde{h} := \int_0^\epsilon e^{s \Delta_\rho} (h - \hat{h}) ds$

Kernel representation:

$$\phi(x) = \int \tilde{k}_\epsilon(x, y) \phi(y) \rho(y) dy + \tilde{h}(x)$$

Empirical approximation:

$$\phi(x) = \frac{1}{N} \sum_{i=1}^N \tilde{k}_\epsilon(x, X^i) \phi(X^i) + \tilde{h}(x)$$

But $\tilde{k}_\epsilon(x, y) = ?$



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Kernel-based Approximation

Special case: $\rho = 1$

$$e^{\epsilon \Delta} f(x) = \int g_{\epsilon}(x, y) f(y) dy. \quad (\text{for all } \epsilon > 0)$$

where g_{ϵ} is the Gaussian kernel.

In general:

$$e^{\epsilon \Delta_{\rho}} f(x) \approx \int \frac{1}{n_{\epsilon}(x)} \frac{g_{\epsilon}(x, y)}{\sqrt{\int g_{\epsilon}(y, z) \rho(z) dz}} f(y) \rho(y) dy := T_{\epsilon} f(x) \quad (\text{for } \epsilon \downarrow 0)$$

where n_{ϵ} is normalizing constant.

Empirical approximation:

$$e^{\epsilon \Delta_{\rho}} f(x) \approx \sum_{j=1}^N \frac{1}{n_{\epsilon}^{(N)}(x)} \frac{g_{\epsilon}(x, X^j)}{\sqrt{\frac{1}{N} \sum_{l=1}^N g_{\epsilon}(X^j, X^l)}} f(X^j) := T_{\epsilon}^{(N)} f(x)$$

where $n_{\epsilon}^{(N)}$ is normalizing constant.

R. Coifman, S. Lafon, Diffusion maps, *Applied and computational harmonic analysis*, 2006,
M. Hein, J. Audibert, U. Von Luxburg, Convergence of graph Laplacians on random neighborhood graphs, *JLMR*, 2007



Kernel-based Approximation

Special case: $\rho = 1$

$$e^{\epsilon \Delta} f(x) = \int g_{\epsilon}(x, y) f(y) dy. \quad (\text{for all } \epsilon > 0)$$

where g_{ϵ} is the Gaussian kernel.

In general:

$$e^{\epsilon \Delta \rho} f(x) \approx \int \frac{1}{n_{\epsilon}(x)} \frac{g_{\epsilon}(x, y)}{\sqrt{\int g_{\epsilon}(y, z) \rho(z) dz}} f(y) \rho(y) dy := T_{\epsilon} f(x) \quad (\text{for } \epsilon \downarrow 0)$$

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Kernel-based Approximation Algorithm

Exact solution:

$$\phi(x) = e^{\epsilon \Delta_\rho} \phi(x) + \tilde{h}(x)$$

where $\tilde{h} := \int_0^\epsilon e^{s \Delta_\rho} (h - \hat{h}) ds$

Approximation:

$$\phi_\epsilon^{(N)}(x) := T_\epsilon^{(N)} \phi_\epsilon^{(N)}(x) + \epsilon(h(x) - \hat{h}),$$

Numerics:

$$\Phi = \mathbf{T}\Phi + \epsilon(\mathbf{h} - \hat{h})$$

- $\Phi = (\Phi_\epsilon^{(N)}(X^1), \dots, \Phi_\epsilon^{(N)}(X^N))$
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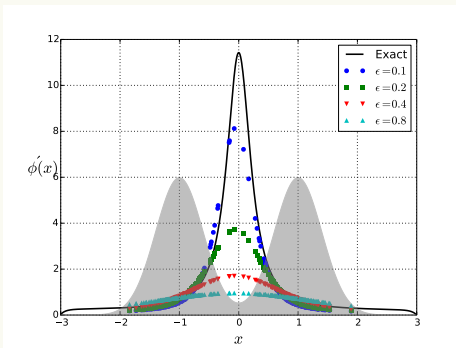
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Kernel-based approximation

Numerical result



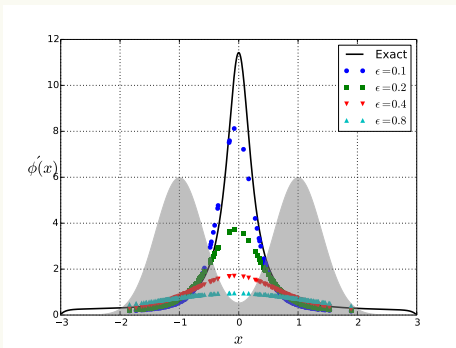
Properties

- 1 No singularity
- 2 Easy extension to Manifolds [C. Zhang, et. al. CDC 2015]
- 3 Better error bounds
- 4 Computational cost $O(N^2)$ (good in high dimensions)



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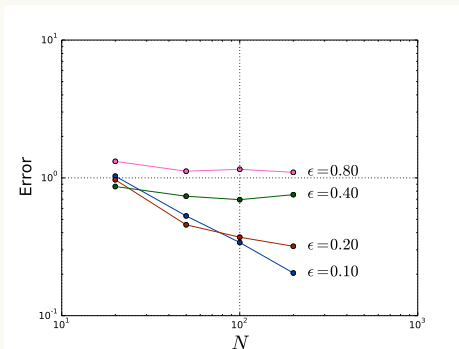


Kernel-based approximation

Error Analysis

Special case: Bounded domain

$$\underbrace{\mathbb{E} \left[\|\nabla\phi - \nabla\phi_\epsilon^{(N)}\|_2 \right]}_{\text{Total error}} \leq \underbrace{O(\epsilon)}_{\text{Bias}} + \underbrace{O\left(\frac{1}{\epsilon^{1+d/4}\sqrt{N}}\right)}_{\text{Variance}}$$



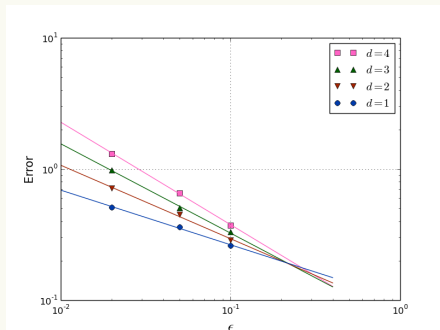
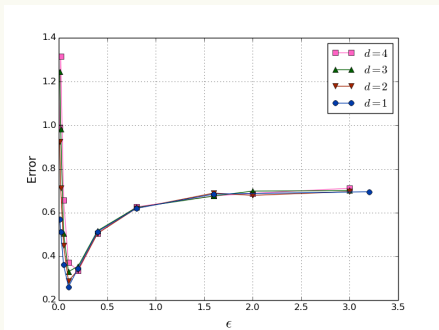


Kernel-based approximation

Error Analysis

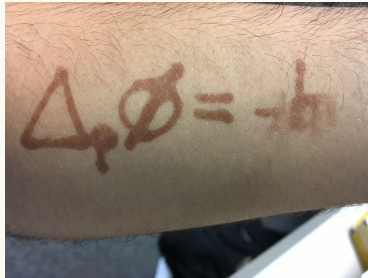
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Thank you for your attention!



Poisson equation, almost everywhere