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# A path-integral approach to Bayesian inference for inverse problems using the semiclassical approximation

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**Abstract** We demonstrate how path integrals often used in problems of theoretical physics can be adapted to provide a machinery for performing Bayesian inference in function spaces. Such inference comes about naturally in the study of inverse problems of recovering continuous (infinite dimensional) coefficient functions from ordinary or partial differential equations (ODE, PDE), a problem which is typically ill-posed. Regularization of these problems using $L^2$ function spaces (Tikhonov regularization) is equivalent to Bayesian probabilistic inference, using a Gaussian prior. The Bayesian interpretation of inverse problem regularization is useful since it allows one to quantify and characterize error and degree of precision in the solution of inverse problems, as well as examine assumptions made in solving the problem – namely whether the subjective choice of regularization is compatible with prior knowledge. Using path-integral formalism, Bayesian inference can be explored through various perturbative techniques, such as the semiclassical approximation, which we use in this manuscript. Perturbative path-integral approaches, while offering alternatives to computational approaches like Markov-Chain-Monte-Carlo (MCMC), also provide natural starting points for MCMC methods that can be used to refine approximations. In this manuscript, we illustrate a path-integral formulation for inverse problems and demonstrate it on an inverse problem in membrane biophysics as well as inverse problems in potential theories involving the Poisson equation.

**Keywords** Inverse problems · Bayesian inference · Field theory · Path integral · Potential theory · Semiclassical approximation

## 1 Introduction

One of the main conceptual challenges in solving inverse problems results from the fact that most interesting inverse problems are not well-posed. One often chooses a solution that is "useful," or that optimizes some regularity criteria. Such a task is commonly known as *regularization*, of which there are many variants. One of the most commonly used methods is *Tikhonov Regularization*, or $L^2$-penalized regularization [8, 9, 20, 32, 45].

Here we first demonstrate the concept behind Tikhonov regularization using one of the simplest inverse problems, the interpolation problem. Tikhonov regularization, when applied to interpolation, solves the inverse problem of

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constructing a continuous function $\varphi : \mathbb{R}^d \to \mathbb{R}$ from point-wise measurements $\varphi_{\text{obs}}$ at positions $\{\mathbf{x}_m\}$ by seeking minima with respect to a cost functional of the form

$$H[\varphi] = \underbrace{\frac{1}{2}\sum_{m=1}^{M} \frac{1}{s_m^2}\left(\varphi(\mathbf{x}_m) - \varphi_{\text{obs}}(\mathbf{x}_m)\right)^2}_{H_{\text{obs}}[\varphi]} + \underbrace{\frac{1}{2}\sum_{\alpha}\gamma_\alpha \int |D^\alpha \varphi|^2 \,\mathrm{d}\mathbf{x}}_{H_{\text{reg}}[\varphi]}, \tag{1}$$

where the constants $1/s_m^2, \gamma_\alpha > 0$ are weighting parameters, and $D^\alpha = \prod_{j=1}^d (-i\partial_{x_j})^{\alpha_j}$ is a differential operator of order $\alpha = (\alpha_1, \ldots, \alpha_d)$.

Assuming $D^\alpha$ is isotropic and integer-ordered, it is possible to invoke integration-by-parts to write $H[\varphi]$ in the quadratic form

$$H[\varphi] = \frac{1}{2}\sum_{m=1}^{M} \frac{1}{s_m^2}\left(\varphi(\mathbf{x}_m) - \varphi_{\text{obs}}(\mathbf{x}_m)\right)^2 + \frac{1}{2}\int \varphi(\mathbf{x}) P(-\Delta)\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}, \tag{2}$$

where $P(\cdot)$ is a polynomial of possibly infinite order, $\Delta$ is the Laplacian operator, and we have assumed that boundary terms vanish. In the remainder of this work, we will focus on energy functionals of this form. This expression is known in previous literature as the information Hamiltonian [11].

Using this form of regularization serves two primary purposes. First, it selects smooth solutions to the inverse problem, with the amount of smoothness controlled by $H_{\text{reg}}$. For example, if only $H_{\text{obs}}$ is used, the solution can be any function that connects the observations $\varphi_{\text{obs}}$ at the measured points $\mathbf{x}_j$, such as a piecewise affine solution. Yet, such solutions may be physically unreasonable (not smooth). Second, it transforms the original inverse problem into a convex optimization problem that possesses an unique solution [3, 10]. If all of the coefficients of $P$ are non-negative, then the pseudo-differential-operator $P(-\Delta)$ is positive-definite [22], guaranteeing uniqueness. These features of Tikhonov regularization make it attractive; however, one needs to make certain choices. In practical settings, one will need to chose both the degree of the differential operator and value of the parameters $\gamma_\alpha$. These two choices adjust the trade-off between data agreement and regularity.

### 1.1 Bayesian inverse problems

The problem of parameter selection for regularization is well-addressed in the context of *Bayesian* inference, where regularization parameters can be viewed probabilistically as prior-knowledge of the solution. Bayesian inference over continuous function spaces has been applied to inverse problems in several contexts. One of the first applications of Bayesian inference to inverse problems was in the study of quantum inverse problems [28], where it was noted that Gaussian priors could be used to formulate field theories. Subsequently, variants of this methodology have been used for model reduction [29] and applied to many interpolation problems and inverse problems in fluid mechanics [6, 19, 44], geology [13, 31, 38, 39], cosmology [11, 34], and biology [18].

There is a wealth of literature concerning the computational aspects of Bayesian inverse problems. Much of these works approach inverse problems through the framework and language of data assimilation through Markov Chain Monte Carlo approaches [4, 4, 37, 40, 41]. Approximation methods based on sparsity have also been developed [43]. Finally, there is a large body of work on the theoretical aspects of maximum aposteriori inference for Bayesian inverse problems including questions of existence of solutions and convergence to solutions [7, 25–27, 44]

## 2 Field-theoretic formulation

Bayesian inference on $\varphi$ entails the construction of a probability density $\pi$ known as the ***posterior distribution*** $\pi(\varphi)$ which obeys ***Bayes' rule,***

$$\pi(\varphi) = \frac{\overbrace{\Pr(\varphi_{\text{obs}}|\varphi)}^{\text{likelihood}}\overbrace{\Pr(\varphi)}^{\text{prior}}}{Z[0]}. \tag{3}$$

where $Z[0]$ is the partition function or normalization factor. The posterior density $\pi$ is a density in a space of functions. The inverse problem is then investigated by computing the statistics of the posterior probability density $\pi(\phi)$ through the evaluation of $Z[0]$. The solution of the inverse problem corresponds to the specific $\varphi$ that maximizes $\pi(\phi)$, subject to prior knowledge encoded in the prior probability density $\Pr(\varphi)$. This solution is known as the ***mean field*** solution. The variance, or error, of the mean field solution is found by computing the variance of the posterior distribution about the mean field solution.

This view of inverse problems also leads naturally to the use of functional integration and perturbation methods common in theoretical physics [24, 46]. Use of the probabilistic viewpoint allows for exploration of inverse problems beyond mean field, with the chief advantage of providing a method for uncertainty quantification.

As shown in [13, 28], Tikhonov regularization has the probabilistic interpretation of Bayesian inference with a Gaussian prior distribution. That is, the regularization term in Eq 2 combines with the data term to specify a posterior distribution of the form

$$\pi(\varphi|\varphi_{\mathrm{obs}}) = \frac{1}{Z[0]}e^{-H[\varphi]} = \frac{1}{Z[0]}\underbrace{\exp\left\{-\sum_{m=1}^{M}\frac{1}{s_m^2}\left(\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)\right)^2\right\}}_{\text{likelihood }(\exp\{-H_{\mathrm{obs}}\})}\underbrace{\exp\left\{-\frac{1}{2}\int\varphi(\mathbf{x})P(-\Delta)\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}\right\}}_{\text{prior }(\exp\{-H_{\mathrm{reg}}\})}. \tag{4}$$

where the partition function

$$Z[0] = \int\mathcal{D}\varphi e^{-H[\varphi]} = \int\underbrace{\mathcal{D}\varphi e^{-H_{\mathrm{reg}}[\varphi]}}_{dW[\varphi]}e^{-H_{\mathrm{obs}}[\varphi]} \tag{5}$$

is a sum over the contributions of all functions in the separable Hilbert space $\{\varphi : H_{\mathrm{reg}}[\varphi] < \infty\}$. This sum is expressed as a ***path integral***, which is an integral over a function space. The formalism for this type of integral came about first from high-energy theoretical physics [14], and then found application in nearly all areas of physics as well as in the representation of both Markovian [5, 15, 35], and non-Markovian [16, 36] stochastic processes. In the case of Eq. 5, where the field theory is real-valued and the operator $P(-\Delta)$ is self-adjoint, a type of functional integral based on abstract Wiener measure may be used [23]. The abstract Wiener measure $dW[\varphi]$ used for Eq. 5 subsumes the prior term $H_{\mathrm{reg}}$, and it is helpful to think of it as a Gaussian measure over lattice points taken to the continuum limit.

When the functional integral of the exponentiated energy functional can be written in the form

$$Z[0] = \int\mathcal{D}\varphi\exp\left\{-\frac{1}{2}\iint\varphi(\mathbf{x})A(\mathbf{x},\mathbf{x}')\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' + \int b(\mathbf{x})\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}\right\}, \tag{6}$$

then the probability density is Gaussian in function-space and the functional integral of Eq. 6 has the solution [46]

$$Z[0] = \exp\left\{\frac{1}{2}\iint b(\mathbf{x})A^{-1}(\mathbf{x},\mathbf{x}')b(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' - \frac{1}{2}\log\det A\right\}. \tag{7}$$

The operators $A(\mathbf{x},\mathbf{x}')$ and $A^{-1}(\mathbf{x},\mathbf{x}')$ are related through the relationship

$$\int A(\mathbf{x},\mathbf{x}')A^{-1}(\mathbf{x}',\mathbf{x}'')\,\mathrm{d}\mathbf{x}' = \delta(\mathbf{x}-\mathbf{x}''). \tag{8}$$

Upon neglecting $H_{\mathrm{obs}}$, the functional integral of Eq. 5 can be expressed in the form of Eq. 6 with $A(\mathbf{x},\mathbf{x}') = P(-\Delta)\delta(\mathbf{x}-\mathbf{x}')$. The pseudo-differential-operator $P(-\Delta)$ acts as an infinite-dimensional version of the inverse of a covariance matrix. It encodes the a-priori spatial correlation, implying that values of the function $\varphi$ are spatially correlated according to a correlation function (Green's function) $A^{-1}(\mathbf{x},\mathbf{y}) = G(\mathbf{x},\mathbf{y}) : \mathbb{R}^d\times\mathbb{R}^d\to\mathbb{R}$ through the relationship implied by Eq. 8, $P(-\Delta)G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})$ so that $G(\mathbf{x},\mathbf{y}) = \left(\frac{1}{2\pi}\right)^d\int_{\mathbb{R}^d}e^{-i\mathbf{k}\cdot(\mathbf{y}-\mathbf{x})}\frac{1}{P(|\mathbf{k}|^2)}\mathrm{d}\mathbf{k}$ where $P(|\mathbf{k}|^2)$ is the symbol of the pseudo-differential-operator $P(-\Delta)$. It is evident that when performing Tikhonov regularization, one should chose regularization that is reflective of prior knowledge of correlations, whenever available.

### 2.1 Mean field inverse problems

We turn now to the more-general problem, where one seeks recovery of a scalar function $\xi$ given measurements of a coupled scalar function $\varphi$ over interior points $\mathbf{x}_i$, and the relationship between the measured and desired functions is given by a partial differential equation

$$F(\varphi(\mathbf{x}),\xi(\mathbf{x})) = 0 \qquad \mathbf{x}\in\Omega\setminus\partial\Omega. \tag{9}$$

As before, we regularize $\xi$ using knowledge of its spatial correlation, and write a posterior probability density

$$\pi[\varphi,\xi|\varphi_{\mathrm{obs}}] = \frac{1}{Z[0]}\exp\left\{-\frac{1}{2}\int\sum_{m=1}^{M}\delta(\mathbf{x}-\mathbf{x}_m)\frac{(\varphi(\mathbf{x})-\varphi_{\mathrm{obs}}(\mathbf{x}))^2}{s_m^2}\,\mathrm{d}\mathbf{x} - \frac{1}{2}\int\xi(\mathbf{x})P(-\Delta)\xi(\mathbf{x})\,\mathrm{d}\mathbf{x}\right\}\boldsymbol{\delta}\left(F(\varphi,\xi)\right),$$

where we have used the Dirac-delta function $\delta$ to specify that our observations are taken with noise $s_m^2$ at certain positions $\mathbf{x}_m$, and an infinite-dimensional delta functional $\boldsymbol{\delta}$ to specify that $F(\varphi, \xi) = 0$ everywhere. Using the inverse Fourier-transformation, one can represent $\boldsymbol{\delta}$ in path-integral form as $\boldsymbol{\delta}\left(F(\varphi, \xi)\right) = \int \mathcal{D}\lambda e^{-i\int \lambda(x) F(\varphi(\mathbf{x}),\xi(\mathbf{x}))\,\mathrm{d}\mathbf{x}}$, where $\lambda(\mathbf{x})$, is a Fourier wavevector. The reason for this notation will soon be clear. We now have a posterior probability distribution of three functions $\varphi, \xi, \lambda$ of the form

$$\pi[\varphi, \xi, \lambda(\mathbf{x})|\varphi_{\text{obs}}] = \frac{1}{Z[0]} \exp\left\{-H[\varphi, \xi, \lambda]\right\}, \tag{10}$$

where the *partition functional* is

$$Z[0] = \iiint \mathcal{D}\varphi \mathcal{D}\xi \mathcal{D}\lambda \exp\left\{-H[\varphi, \xi, \lambda]\right\}, \tag{11}$$

and the *Hamiltonian*

$$H[\varphi, \xi, \lambda; \varphi_{\text{obs}}] = \frac{1}{2}\int \sum_{m=1}^{M} \delta(\mathbf{x}-\mathbf{x}_m)\frac{(\varphi(\mathbf{x}) - \varphi_{\text{obs}}(\mathbf{x}))^2}{s_m^2}\,\mathrm{d}\mathbf{x} + \frac{1}{2}\int \xi(\mathbf{x}) P(-\Delta)\xi(\mathbf{x})\,\mathrm{d}\mathbf{x} + i\int \lambda(\mathbf{x}) F(\varphi, \xi)\,\mathrm{d}\mathbf{x}, \tag{12}$$

is a functional of $\varphi, \xi$, and the Fourier wave vector $\lambda(\mathbf{x})$. Similar Hamiltonians, providing a probabalistic model for data in the context of inverse problems, have appeared in previous literature [11, 28, 44], where they have been referred to as "Information Hamiltonians."

Maximization of the posterior probability distribution, also known as Bayesian maximum a posteriori estimation (MAP) inference, is performed by minimization of the corresponding energy functional (Eq. 12) with respect to the functions $\varphi, \xi, \lambda$. One may perform this inference by solving the associated Euler-Lagrange equations

$$P(-\Delta)\xi + \frac{\delta}{\delta\xi(\mathbf{x})}\int \lambda(\mathbf{x}) F(\varphi, \xi)\,\mathrm{d}\mathbf{x} = 0, \tag{13}$$

$$\sum_{n=1}^{M} \delta(\mathbf{x}-\mathbf{x}_n)(\varphi(\mathbf{x}) - \varphi_{\text{obs}}(\mathbf{x})) + \frac{\delta}{\delta\varphi(\mathbf{x})}\int \lambda(\mathbf{x}) F(\varphi, \xi)\,\mathrm{d}\mathbf{x} = 0 \tag{14}$$

$$F(\varphi, \xi) = 0, \tag{15}$$

where $\lambda(\mathbf{x})$ here serves the role of a Lagrange multiplier. Solving this system of partial differential equations simultaneously allows one to arrive at the solution to the original Tikhonov-regularized inverse problem. Now, suppose one is interested in estimating the precision of the given solution. The field-theoretic formulation of inverse problems provides a way of doing so.

### 2.2 Beyond mean-field – semiclassical approximation

The functions $\varphi, \xi, \lambda : \mathbb{R}^d \to \mathbb{R}$ each constitute scalar fields[1]. ***Field theory*** is the study of statistical properties of such fields through evaluation of an associated ***path integral*** (functional integral). Field theory applied to Bayesian inference has appeared in prior literature under the names Bayesian Field theory [13, 28, 44], and Information Field Theory [11].

In general, field theory deals with functional integrals of the form

$$Z[J] = \int \mathcal{D}\varphi \exp\Bigg\{ -\underbrace{\left[\frac{1}{2}\iint \varphi(\mathbf{x}) A(\mathbf{x}, \mathbf{x}')\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' + \int V[\varphi(\mathbf{x})]\,\mathrm{d}\mathbf{x}\right]}_{H[\varphi]} + \int J(\mathbf{x})\varphi(\mathbf{x})\Bigg\}, \tag{16}$$

where the Hamiltonian of interest is recovered when the "source" $J = 0$, and the potential function $V$ is nonlinear in $\varphi$. Assuming that after non-dimensionalization, $V[\varphi]$ is relatively small in comparison to the other terms, one is then able to expand the last term in formal Taylor series so that after completing the Gaussian part of the integral as in Eq. 7,

[1] We will use Greek letters to denote fields

$$Z[J] = \int \underbrace{\mathcal{D}\varphi \exp\left\{-\frac{1}{2}\iint \varphi(\mathbf{x})A(\mathbf{x},\mathbf{x}')\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' + \int J(\mathbf{x})\varphi(\mathbf{x})\right\}}_{\text{Gaussian}} \left(1 - \int V[\varphi]\,\mathrm{d}\mathbf{x} + \dots\right)$$

$$\propto \exp\left[-V\left(\frac{\delta}{\delta J}\right)\right] \exp\left(\frac{1}{2}\iint J(\mathbf{x})A^{-1}(\mathbf{x},\mathbf{x}')J(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'\right). \tag{17}$$

In this way, $Z[J]$ can be expressed in series form as moments of a Gaussian distribution. The integral is of interest because one can use it to recover moments of the desired field through functional differentiation,

$$\left\langle \prod_k \varphi(\mathbf{x}_k) \right\rangle = \frac{1}{Z[0]} \prod_k \frac{\delta}{\delta J(\mathbf{x}_k)} Z[J] \Bigg|_{J=0}. \tag{18}$$

This approach is known as the *weak-coupling approach* [46]. For this expansion to hold, however, the external potential $V$ must be small in size compared to the quadratic term. This assumption is not generally valid during Tikhonov regularization, as common rules of thumb dictate that the data fidelity and the regularization term should be of similar order of magnitude [2, 42]. Another perturbative approach – the one that we will take in this manuscript – is to expand the Hamiltonian in a functional Taylor series

$$H[\varphi] = H[\varphi^\star] + \frac{1}{2}\iint \frac{\delta^2 H[\varphi^\star]}{\delta\varphi(\mathbf{x})\varphi(\mathbf{x}')} (\varphi(\mathbf{x}) - \varphi^\star(\mathbf{x}))(\varphi(\mathbf{x}') - \varphi^\star(\mathbf{x}'))\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' + \dots \tag{19}$$

about its extremal point $\varphi^\star$. To the second order (as shown), the expansion is known as the *semiclassical approximation* [17] which provides an approximate Gaussian density for the field $\varphi$. Corrections to the semiclassical expansion can be evaluated by continuing this expanion to higher orders, where evaluation of the functional integral can be aided by the use of Feynman diagrams [14].

### 2.3 Monte-Carlo for refinement of approximations

The Gaussian approximation is useful because Gaussian densities are easy to sample. One may sample a random field $\varphi(\mathbf{x})$ from a Gaussian distribution with inverse-covariance $A(\mathbf{x},\mathbf{x}')$ by solving the stochastic differential equation

$$\frac{1}{2}\int A(\mathbf{x},\mathbf{x}')\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}' = \eta(\mathbf{x}), \tag{20}$$

where $\eta$ is the unit white noise process which has mean $\langle\eta(\mathbf{x})\rangle = 0$, and spatial correlation $\langle\eta(\mathbf{x})\eta(\mathbf{x}')\rangle = \delta(\mathbf{x}-\mathbf{x}')$. With the ability to sample from the approximating Gaussian distribution of Eq. 19, one may use Monte-Carlo simulation to sample from the true distribution by weighting the samples obtained from the Gaussian distribution. Such an approach is known as *importance sampling* [30], where samples $\varphi_i$ are given importance weights $w_i$ according to the ratio $w_i = \exp\left(-H_{\text{approx}} + H_{\text{true}}\right) / \sum_j w_j$. Statistics of $\varphi$ may then be calculated using the weighted samples; for instance expectations can be approximated as $\langle g(\varphi(\mathbf{x}))\rangle \approx \sum_i w_i g(\varphi_i(\mathbf{x}))$. Using this method, one can refine the original estimates of the statistics of $\varphi$.

## 3 Examples

### 3.1 Interpolation of the height of a rigid membrane or plate

We first demonstrate the field theory for inverse problems on an interpolation problem where one is able to determine the regularizing differential operator based on prior knowledge. This example corresponds to the interpolation example mentioned in the Introduction. Consider the problem where one is attempting to identify in three-dimensions the position of a membrane. For simplicity, we assume that one is interested in obtaining the position of the membrane only over a restricted spatial domain, where one can use the Monge parameterization to reduce the problem to two-dimensions and define the height of the membrane $\varphi : \mathbb{R}^2 \to \mathbb{R}$.

Suppose one is able to measure the membrane in certain spatial locations $\{\mathbf{x}_m\}$, but one seeks to also interpolate the membrane in regions that are not observable. Physically, models for fluctuations in membranes are well known, for instance the Helfrich free-energy [12] suggests that one should use a regularizing differential operator

$$P(-\Delta) = \beta(\kappa\Delta^2 - \sigma\Delta) \qquad \beta,\sigma,\kappa > 0, \tag{21}$$

where $\sigma$ and $\kappa$ are the membrane tension and bending rigidity, respectively. The Hamiltonian associated with the Helfrich operator is

$$H[\varphi;\varphi_{\text{obs}}] = \frac{1}{2}\int\sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right)^2 \mathrm{d}\mathbf{x} + \frac{1}{2}\int\varphi(\mathbf{x})P(-\mathit{\Delta})\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}, \tag{22}$$

and the mean-field solution for $\varphi$ corresponds to the extremal point of the Hamiltonian, which is the solution of the corresponding Euler-Lagrange equation

$$\frac{\delta H}{\delta\varphi} = \sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right) + P(-\mathit{\Delta})\varphi(\mathbf{x}) = 0. \tag{23}$$

To go beyond mean-field, one may compute statistics of the probability distribution $\Pr(\varphi)\propto e^{-H[\varphi]}$, using the generating functional which is expressed as a functional integral

$$\begin{aligned} Z[J] \propto \int\mathcal{D}\varphi\exp\Bigg\{ -\frac{1}{2}\iint\varphi(\mathbf{x})\underbrace{\left[\delta(\mathbf{x}-\mathbf{x}')\sum_{m=1}^{M}\frac{\delta(\mathbf{x}'-\mathbf{x}_m)}{s_m^2} + P(-\mathit{\Delta})\delta(\mathbf{x}-\mathbf{x}')\right]}_{A(\mathbf{x},\mathbf{x}')}\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' \\ + \int\left[\sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2} + J(\mathbf{x})\right]\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}\Bigg\}, \end{aligned} \tag{24}$$

where we have completed the square. According to Eq. 7, Eq. 24 has the solution

$$Z[J] \propto \exp\left\{\frac{1}{2}\iint J(\mathbf{x})A^{-1}(\mathbf{x},\mathbf{x}')J(\mathbf{x}')\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{x} + \int J(\mathbf{x})\sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}\,\mathrm{d}\mathbf{x}\right\}. \tag{25}$$

Through functional differentiation of Eq. 25, Eq. 18 implies that the mean-field solution is

$$\langle\varphi(\mathbf{x})\rangle = \sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}, \tag{26}$$

and variance in the solution is

$$\Big\langle\varphi(\mathbf{x})-\langle\varphi(\mathbf{x})\rangle\,,\varphi(\mathbf{x}')-\langle\varphi(\mathbf{x}')\rangle\Big\rangle = A^{-1}(\mathbf{x},\mathbf{x}'). \tag{27}$$

To solve for these quantities, we compute the operator $A^{-1}$, which according to Eq. 8, satisfies the partial differential equation

$$\sum_{m=1}^{M}\frac{\delta(\mathbf{x}_m-\mathbf{x})}{s_m^2}A^{-1}(\mathbf{x},\mathbf{x}'') + P(-\mathit{\Delta})A^{-1}(\mathbf{x},\mathbf{x}'') = \delta(\mathbf{x}-\mathbf{x}''). \tag{28}$$

Using the Green's function for $P(-\mathit{\Delta})$,

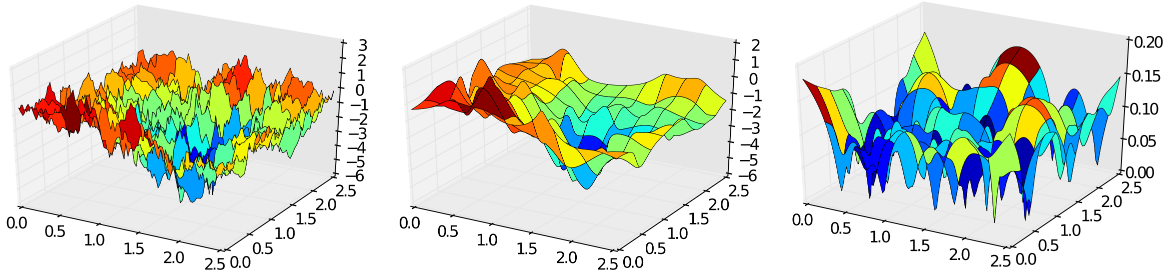
$$G(\mathbf{x},\mathbf{x}') = \frac{-1}{2\pi\beta\sigma}\left[\log\left(|\mathbf{x}-\mathbf{x}'|\right) + K_0\left(\sqrt{\frac{\sigma}{\kappa}}|\mathbf{x}-\mathbf{x}'|\right)\right], \tag{29}$$

we find

$$A^{-1}(\mathbf{x},\mathbf{x}'') = \overbrace{G(\mathbf{x},\mathbf{x}'')}^{\text{known}} - \sum_{m=1}^{M}\frac{\overbrace{G(\mathbf{x},\mathbf{x}_m)}^{\text{known}}\,\overbrace{A^{-1}(\mathbf{x}_m,\mathbf{x}'')}^{\text{unknown}}}{s_m^2}. \tag{30}$$

To calculate $A^{-1}(\mathbf{x},\mathbf{x}')$, we need $A^{-1}(\mathbf{x}_m,\mathbf{x}')$, for $m\in\{1,\ldots,M\}$. Solving for each of these simultaneously yields the equation

$$A^{-1}(\mathbf{x},\mathbf{x}') = G(\mathbf{x},\mathbf{x}') - \mathbf{G}_s(\mathbf{x})\left(\mathbf{I}+\boldsymbol{\mathit{\Lambda}}\right)^{-1}\mathbf{G}(\mathbf{x}'), \tag{31}$$




(a) $\varphi(\mathbf{x})$ (b) $\langle\varphi(\mathbf{x})\rangle$ (c) $\sqrt{\langle(\varphi(\mathbf{x}) - \langle\varphi(\mathbf{x})\rangle)^2\rangle}$

Fig. 1: **Interpolation of a membrane.** (a) A simulated membrane undergoing thermal fluctuations is the object of reconstruction. (b) Mean-field reconstruction of the membrane using 100 randomly-placed measurements with noise. (c) Pointwise standard error in the reconstruction of the membrane. Parameters used: $\sigma = 10^{-2}, \beta = 10^3, \kappa = 10^{-4}, s_m = 10^{-2}$.

where $\mathbf{G}_s(\mathbf{x}) \equiv \left[\frac{G(\mathbf{x},\mathbf{x}_1)}{s_1^2}, \frac{G(\mathbf{x},\mathbf{x}_2)}{s_2^2}, \ldots, \frac{G(\mathbf{x},\mathbf{x}_M)}{s_M^2}\right]$, $\mathbf{G}(\mathbf{x}) \equiv [G(\mathbf{x},\mathbf{x}_1), G(\mathbf{x},\mathbf{x}_2), \ldots, G(\mathbf{x},\mathbf{x}_M)]$, and $\mathbf{\Lambda}_{ij} \equiv G(\mathbf{x}_i,\mathbf{x}_j)/s_i^2$.

Fig. 1 shows an example of the use of the Helfrich free energy for interpolation. A sample of a membrane undergoing thermal fluctuations was taken as the object of recovery. Uniformly, 100 randomly-placed, noisy observations of the height of the membrane were taken. The mean-field solution for the position of the membrane and the standard error in the solution are presented. The standard error is not uniform and dips to approximately the measurement error at locations where measurements were taken.

### 3.2 Source recovery for the Poisson equation

Now consider an example where the function to be recovered is not directly measured. This type of inverse problem often arises when considering the Poisson equation in isotropic medium:

$$\Delta\varphi(\mathbf{x}) = \rho(\mathbf{x}). \tag{32}$$

Measurements of $\varphi$ are taken at points $\{\mathbf{x}_i\}$ and the objective is to recover the source function $\rho(\mathbf{x})$. Previous researchers have explored the use of Tikhonov regularization to solve this problem [1, 21]; here we quantify the precision of such solutions.

Making the assumption that $\rho$ is correlated according to the Green's function of the pseudo-differential-operator $P(-\Delta)$, we write the Hamiltonian

$$\begin{aligned} H[\varphi,\rho,\lambda;\varphi_{\text{obs}}] = \frac{1}{2}\int\sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x}))^2\,\mathrm{d}\mathbf{x} + \frac{1}{2}\int\rho(\mathbf{x})P(-\Delta)\rho(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ + i\int\lambda(\mathbf{x})\left(\Delta\varphi(\mathbf{x})-\rho(\mathbf{x})\right)\,\mathrm{d}\mathbf{x}. \end{aligned} \tag{33}$$

The extremum of $H[\varphi,\rho,\lambda;\varphi_{\text{obs}}]$ occurs at $(\varphi^\star,\rho^\star)$, which are found through the corresponding Euler-Lagrange equations $\left(\frac{\delta H}{\delta\varphi} = 0, \frac{\delta H}{\delta\rho} = 0, \frac{\delta H}{i\delta\lambda} = 0\right)$,

$$\begin{aligned} \sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}(\varphi^\star(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})) + P(-\Delta)\Delta^2\varphi^\star(\mathbf{x}) = 0, \\ \rho^\star = \Delta\varphi^\star. \end{aligned} \tag{34}$$

In addition to the extremal solution, we can also evaluate how precisely the source function has been recovered by considering the probability distribution given by the exponentiated Hamiltonian,

$$\pi(\rho(\mathbf{x})|\{\varphi_{\text{obs}}(\mathbf{x}_i)\}) = \frac{1}{Z[0]}\exp\left\{-\frac{1}{2}\int\sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x}))^2\,\mathrm{d}\mathbf{x} - \frac{1}{2}\int\Delta\varphi(\mathbf{x})P(-\Delta)\Delta\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}.\right\}, \tag{35}$$

where we have integrated out the $\lambda$ and $\rho$ variables by making the substitution $\rho = \Delta\varphi$. To compute the statistics of $\varphi$, we first compute $Z[J]$, the generating functional which by Eq. 7 has the solution

$$Z[J] \propto \exp\left\{\frac{1}{2}\iint \Delta J(\mathbf{x})A^{-1}(\mathbf{x},\mathbf{x}')\Delta_{\mathbf{x}'}J(\mathbf{x}')\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{x} + \int J(\mathbf{x})\Delta\sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}\,\mathrm{d}\mathbf{x}\right\}, \tag{36}$$

where

$$A(\mathbf{x},\mathbf{x}') = \Delta^2 P(-\Delta)\delta(\mathbf{x}-\mathbf{x}') + \delta(\mathbf{x}-\mathbf{x}')\sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2} \tag{37}$$

and $A^{-1}$ is defined as in Eq. 8. The first two moments have the explicit solution given by the generating functional,

$$\left.\frac{\delta Z[J]}{\delta J(\mathbf{x})}\right|_{J=0} = \left(\sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)\Delta A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}\right)Z[0]$$

$$\left.\frac{\delta^2 Z[J]}{\delta J(\mathbf{x})\delta J(\mathbf{x}')}\right|_{J=0} = \left(\Delta\Delta_{\mathbf{x}'}A^{-1}(\mathbf{x},\mathbf{x}') + \left(\sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)\Delta A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}\right)\left(\sum_{k=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_k)\Delta_{\mathbf{x}'}A^{-1}(\mathbf{x}',\mathbf{x}_k)}{s_k^2}\right)\right)Z[0].$$

These formulae imply that our mean-field source has the solution

$$\langle\rho(\mathbf{x})\rangle = \sum_{m=1}^{M}\frac{\varphi_{\text{obs}}(\mathbf{x}_m)\Delta A^{-1}(\mathbf{x},\mathbf{x}_m)}{s_m^2}, \tag{38}$$

subject to the weighted unbiasedness condition $\sum_m \varphi(\mathbf{x}_m)/s_m^2 = \sum_m \varphi_{\text{obs}}(\mathbf{x}_m)/s_m^2$, and the variance in the source has the solution

$$\Big\langle \rho(\mathbf{x}) - \langle\rho(\mathbf{x})\rangle\,, \rho(\mathbf{x}') - \langle\rho(\mathbf{x}')\rangle\Big\rangle = \Delta\Delta_{\mathbf{x}'}A^{-1}(\mathbf{x},\mathbf{x}'). \tag{39}$$

The inverse operator $A^{-1}$ is solved in the same way as in the previous section, yielding for the fundamental solution $G$ satisfying $P(-\Delta)\Delta^2 G(\mathbf{x}) = \delta(\mathbf{x})$,

$$A^{-1}(\mathbf{x},\mathbf{x}') = G(\mathbf{x},\mathbf{x}') - \mathbf{G}_s(\mathbf{x})\left(\mathbf{I}+\boldsymbol{\Lambda}\right)^{-1}\mathbf{G}(\mathbf{x}'), \tag{40}$$

where $\mathbf{G}, \mathbf{G}_s$ and $\boldsymbol{\Lambda}$ are defined as they are in Eq. 31.

As an example, we recover the source function in $\mathbb{R}^2$ shown in Fig. 2a. This source was used along with a uniform unit dielectric coefficient to find the solution for the Poisson equation that is given in Fig. 2b. Noisy samples of the potential field were taken at 125 randomly-placed locations (depicted in Fig. 2c). For regularization, we sought solutions for $\rho$ in the Sobolev space $H^2(\mathbb{R}^2)$. Such spaces are associated with the Bessel potential operator $P(-\Delta) = \beta(\gamma-\Delta)^2$. Using 125 randomly placed observations, reconstructions of both $\varphi$ and $\rho$ were performed. The standard error of the reconstruction is also given.

### 3.3 Recovery of a spatially-varying dielectric coefficient field

Finally, consider the recovery of a spatially varying dielectric coefficent $\epsilon(\mathbf{x})$ by inverting the Poisson equation

$$\nabla\cdot(\epsilon\nabla\varphi) - \rho = 0, \tag{41}$$

where $\rho$ is now known, and $\varphi$ is measured. This problem is more difficult than the problems in the previous sections. While Eq. 41 is bilinear in $\epsilon$ and $\varphi$, the associated inverse problem of the recovery of $\epsilon$ given measurements of $\varphi$ is nonlinear, since $\epsilon$ does not relate linearly to data in $\varphi$. This situation is also exacerbated by the fact that no closed-form solution for $\epsilon$ as a function of $\varphi$ exists.

Assuming that the gradient of the dielectric coefficient is spatially correlated according to the Gaussian process given by $P(-\Delta)$, we work with the Hamiltonian

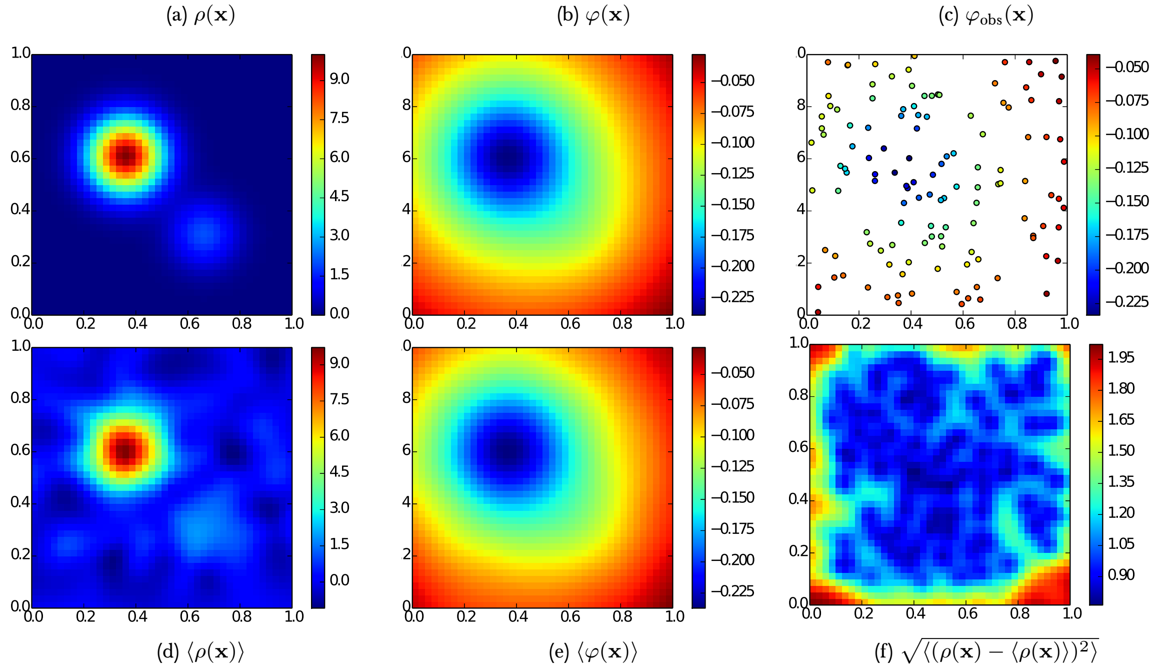



Fig. 2: **Source inversion for Poisson's equation in isotropic medium in $\mathbb{R}^2$.** (a) Synthetic source function that is the object of recovery. (b) A solution to Poisson's equation on the infinite domain corresponding to this source. (c) 125 randomly-placed observations of $\varphi$ taken with noise. (d) Reconstruction of the source. (e) Reconstruction of the potential. (f) Pointwise standard error in the reconstruction of the source. Parameters used: $\beta = 10^{-4}, s_m = 10^{-3}, \gamma = 10^2$.

$$H[\varphi,\epsilon,\lambda;\rho,\varphi_{\text{obs}}] = \frac{1}{2}\sum_{m=1}^{M}\int \frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}|\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})|^2\,\mathrm{d}\mathbf{x} - \frac{1}{2}\int \epsilon(\mathbf{x})\Delta P(-\Delta)\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} + i\int \lambda(\mathbf{x})\left[\nabla\cdot(\epsilon\nabla\varphi)-\rho\right]\,\mathrm{d}\mathbf{x}, \tag{42}$$

which yields the Euler-Lagrange equations

$$\nabla\cdot(\epsilon\nabla\varphi)-\rho = 0, \tag{43}$$

$$-\Delta P(-\Delta)\epsilon - \nabla\lambda\cdot\nabla\varphi = 0, \tag{44}$$

$$\sum_{j=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_j)}{s_j^2}(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})) + \nabla\cdot(\epsilon\nabla\lambda) = 0. \tag{45}$$

We have assumed that $\epsilon$ is sufficiently regular such that $\int \nabla\epsilon(\mathbf{x})\cdot P(-\Delta)\nabla\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} < \infty$, thereby imposing vanishing boundary-conditions at $|\mathbf{x}|\to\infty$. The Lagrange multiplier $\lambda$ satisfies the Neumann boundary conditions $\nabla\lambda = 0$ outside of the convex hull of the observed points. In order to recover the optimal $\epsilon$, one must solve these three PDEs simultaneously. A general iterative strategy for solving this system of partial differential equations is to use Eq. 43 to solve for $\varphi$, use Eq 44 to solve for $\epsilon$, and use Eq. 45 to solve for $\lambda$. Given $\lambda$ and $\varphi$, The left-hand-side of Eq 44 provides the gradient of the Hamiltonian with respect to $\epsilon$ which can be used for gradient descent. Eqs. 43 and 45 are simply the Poisson equation.

For quantifying error in the mean-field recovery, we seek a formulation of the problem of recovering $\epsilon$ using the path integral method. We are interested in the generating functional $Z[J] = \iiint \mathcal{D}\varphi\mathcal{D}\epsilon\mathcal{D}\lambda \exp\left(-H[\varphi,\epsilon,\lambda] + \int J\epsilon\,\mathrm{d}\mathbf{x}\right)$. Integrating in $\lambda$ and $\varphi$, yields the marginalized generating functional

$$
\begin{aligned}
Z[J] &= \int \mathcal{D}\epsilon \exp\left\{-H[\epsilon;\rho,\varphi_{\text{obs}}] + \int J(\mathbf{x})\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x}\right\} \\
&= \int \mathcal{D}\epsilon \exp\left\{-\frac{1}{2}\sum_{m=1}^{M}\int \frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left[\varphi(\epsilon(\mathbf{x})) - \varphi_{\text{obs}}(\mathbf{x})\right]^2\,\mathrm{d}\mathbf{x} - \frac{1}{2}\int \epsilon(\mathbf{x})(-\Delta)P(-\Delta)\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int J(\mathbf{x})\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x}\right\}. \quad (46)
\end{aligned}
$$

To approximate this integral, one needs an expression for the $\varphi$ as a function of $\epsilon$. To find such an expression, one can use the product rule to write Poisson's equation as $\epsilon\Delta\varphi + \nabla\epsilon\cdot\nabla\varphi = \rho$. Assuming that $\nabla\epsilon$ is small, one may solve Poisson's equation in expansion of powers of $\nabla\epsilon$ by using the Green's function $L(\mathbf{x},\mathbf{x}')$ of the Laplacian operator to write $\varphi(\mathbf{x}) = \int L(\mathbf{x},\mathbf{x}')\frac{\rho(\mathbf{x}')}{\epsilon(\mathbf{x}')}\,\mathrm{d}\mathbf{x}' - \int L(\mathbf{x},\mathbf{x}')\nabla_{\mathbf{x}'}\log\epsilon(\mathbf{x}')\cdot\nabla_{\mathbf{x}'}\varphi(\mathbf{x}')\,\mathrm{d}\mathbf{x}'$, which is a Fredholm integral equation of the second kind. The function $\varphi$ then has the Liouville-Neumann series solution

$$\varphi(\mathbf{x}) = \sum_{n=0}^{\infty}\varphi_n(\mathbf{x}) \tag{47}$$

$$\varphi_n(\mathbf{x}) = \int K(\mathbf{x},\mathbf{y})\varphi_{n-1}(\mathbf{y})\,\mathrm{d}\mathbf{y} \qquad n\geq 1 \tag{48}$$

$$\varphi_0(\mathbf{x}) = \int L(\mathbf{x},\mathbf{y})\frac{\rho(\mathbf{y})}{\epsilon(\mathbf{y})}\,\mathrm{d}\mathbf{y} \tag{49}$$

$$K(\mathbf{x},\mathbf{y}) = \nabla_{\mathbf{y}}\cdot\Big[L(\mathbf{x},\mathbf{y})\nabla_{\mathbf{y}}\log\epsilon(\mathbf{y})\Big], \tag{50}$$

where $\nabla\epsilon$ is assumed to vanish at the boundary of reconstruction. Taken to two terms in the expansion of $\varphi(\epsilon)$ given in Eqs. 47-50, the second-order term in the Taylor expansion of Eq. 46 is of the form (see Appendix A)

$$\frac{\delta^2 H}{\delta\epsilon(\mathbf{x})\delta\epsilon(\mathbf{x}')} \sim -\Delta P(-\Delta)\delta(\mathbf{x}-\mathbf{x}') + \sum_{m=1}^{M} a_m(\mathbf{x},\mathbf{x}').$$

This expression, evaluated at the solution of the Euler-Lagrange equations $\epsilon^\star,\varphi^\star$, provides an an approximation of the original probability density from which the posterior variance $\big\langle\epsilon(\mathbf{x})-\epsilon^\star(\mathbf{x}),\epsilon(\mathbf{x}')-\epsilon^\star(\mathbf{x}')\big\rangle = A^{-1}(\mathbf{x},\mathbf{x}')$ can be estimated. To find this inverse operator, we discretize spatially and compute the matrix $\mathbf{A}^{-1}_{ij} = A^{-1}(\mathbf{x}_i,\mathbf{x}_j)$,

$$\mathbf{A}^{-1} = (\mathbf{I} + \mathbf{G}\mathbf{A}_m^{-1})^{-1}\mathbf{G},$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{G}$ is a matrix of values $[(-\Delta)P(-\Delta)\delta(\mathbf{x},\mathbf{x}')]^{-1}$, $\mathbf{A}_m^{-1} = \left[\delta\mathbf{x}\sum_m a_m(\mathbf{x},\mathbf{x}')\right]^{-1}$, and $\delta\mathbf{x}$ is the volume of a lattice coordinate.

As an example, we present the recovery of a dielectric coefficient in $\mathbb{R}^1$ over the compact interval $x\in[0,1]$ of a dielectric coefficient shown in Fig. 3a given a known source function $(10\times\mathbf{1}_{x\in[0,1]})$. A solution to the Poisson equation given Eq. 41 is shown in Fig. 3b. For regularization, we use the operator $P(-\Delta) = \beta(\gamma-\Delta)$, and assume that $\nabla\epsilon\to 0$ at the boundaries of the recovery, which are outside of the locations where measurements are taken. For this reason, we take the Green's function $G$ of the differential operator $-\frac{d^2}{dx^2}P(-\frac{d^2}{dx^2}) = -\frac{d^2}{dx^2}\beta(\gamma-\frac{d^2}{dx^2})$ to vanish along with its first two derivatives at the boundary of recovery.

The point-wise standard error and the posterior covariance are shown in Figs. 3c and 3d, respectively. Monte-Carlo corrected estimates are also shown. Note that approximate point-wise errors are much larger than the Monte-Carlo point-wise errors. This fact is due in-part to inaccuracy in using the series solution for the Poisson equation given in Eq 47, which relies on $\nabla\epsilon$ to be small. While the approximate errors were inaccurate, the approximation was still useful in providing a sampling density for use in importance sampling.

## 4 Discussion

In this paper we have presented a general method for regularizing ill-posed inverse problems based on the Bayesian interpretation of Tikhonov regularization, which we investigated through the use of field-theoretic approaches. We demonstrated the approach by considering two linear problems – interpolation (Sec. 3.1) and source inversion (Sec. 3.2), and a non-linear problem – dielectric inversion (Sec. 3.3). For linear problems Tikhonov regularization yields Gaussian functional integrals, where the moments are available in closed-form. For non-linear problems, we demonstrated a perturbative technique based on functional Taylor series expansions, for approximate local density estimation near the maximum a-posteriori solution of the inverse problem. We also discussed how such approximations can be improved based on Monte-Carlo sampling (Sec. 2.3).

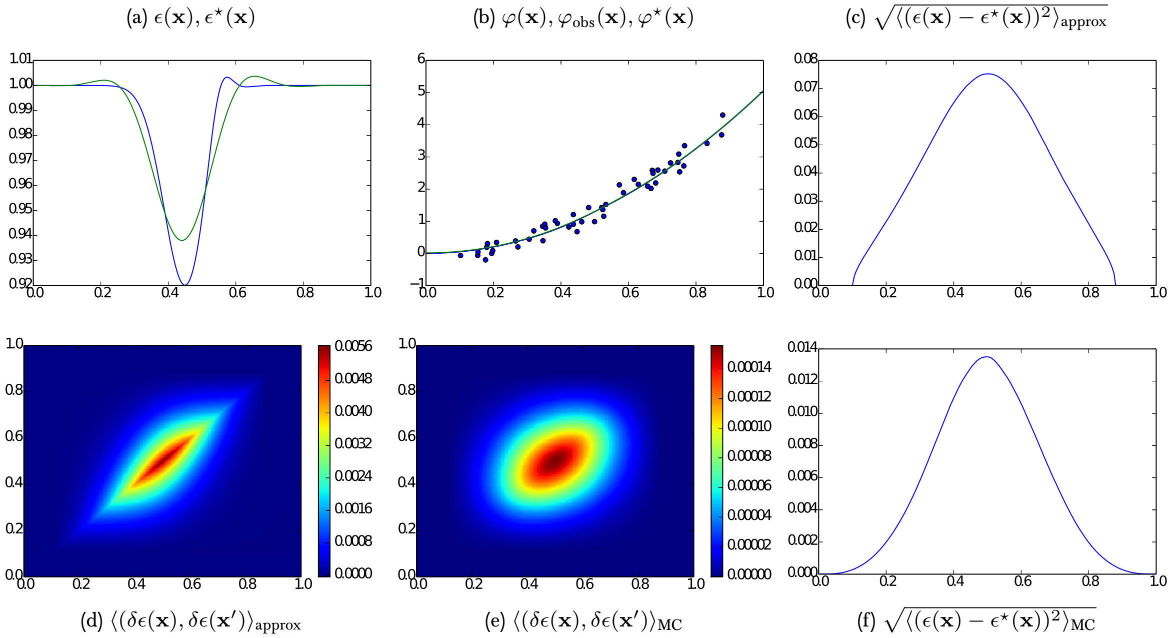



Fig. 3: **Dielectric inversion for Poisson's equation in** $\mathbb{R}^1$. (a) (blue) Spatially-varying dielectric coefficient $\epsilon$ that is the object of recovery, and the mean field recovery $\epsilon^\star$ (green). (b) A solution $\varphi$ (blue) to Poisson's equation given a known step-source supported on $[0, 1]$ and the spatially-varying dielectric coefficient, $50$ randomly placed samples of the solution taken with error, and the mean field recovery of the potential function $\varphi^\star$ (green). (c) Standard error in the mean-field recovery of the dielectric field. (d) Approximate posterior variance in the recovery of the dielectric field. ($\delta\epsilon = \epsilon - \epsilon^\star$). (e) Monte-Carlo corrected covariance field estimate (f) Monte-Carlo corrected point-wise error estimate. Parameters used: $s_m = 0.2, \beta = 2.5, \gamma = 100$.

Our first example problem was that of membrane or plate interpolation. In this problem the regularization term is known based on a priori knowledge of the physics of membranes with bending rigidity. The Helfrich free energy describes the thermal fluctuations that are expected of rigid membranes, and provided us with the differential operator to use for Tikhonov regularization. Using the path integral, we were able to calculate an analytical expression for the error in the reconstruction of the membrane surface. It is apparent that the error in the recovery depends on both the error of the measurements and the distance to the nearest measurements. Surprisingly, the reconstruction error did not explicitly depend on the misfit error.

The second example problem was the recontruction of the source term in the Poisson equation given measurements of the field. In this problem, the regularization is not known from physical constraints and we demonstrated the use of a regularizer chosen from a general family of regularizers. This type of regularization is equivalent to the notion of weak solutions in Sobolev spaces. Since the source inversion problem is linear, we were able to analytically calculate the solution as well as the error of the solution. Again, the reconstruction error did not explicitly depend on the misfit error.

The last example problem we demonstrated was the inversion of the dielectric coefficient of Poisson's equation from potential measurements. This problem was nonlinear, yielding non-Gaussian path-integrals. We used this problem to demonstrate the technique of semiclassical approximation for use in Bayesian inverse problems.

The reliability of the semiclassical approximation depends on how rapidly the posterior distribution falls off from the extremum or mean field solution. Applying the semiclassical approximation to the information Hamiltonian (Eq 12), one sees that the regularization only contributes to terms up to second order. Higher-order terms in the expansion rely only on the likelihood term in the Hamiltonian. Since the data error is assumed to be normally distributed with variance $s_m^2$, one expects each squared residual $(\varphi(\mathbf{x}_m) - \varphi_{\text{obs}}(\mathbf{x}_m))^2$ to be $\mathcal{O}(s_m^2)$. For this reason, each observation contributes a term of $O(1)$ to the Hamiltonian. As a result, there is an implicit large prefactor of $O(M)$ in the Hamiltonian, where $M$ is defined as before as the number of observations. The first order correction to the semiclassical method is then expected to be $\mathcal{O}(1/M)$.

### 4.1 Future directions

By putting inverse problems into a Bayesian framework, one gains access to a large toolbox of methodology that can be used to construct and verify models. In particular, Bayesian model comparison [33] methods can be used for identifying the regularization terms to be used when one does not have prior information available about the solution. Such methods can also be used when one has some knowledge of the object of recovery, modulo the knowledge of some parameters. For instance, one may seek to recover the height of a plate or membrane but not know the surface tension or elasticity. Then, Bayesian methods can be used to recover probability distributions for the regularizers along with the object of recovery.

Finally, Tikhonov regularization works naturally in the path integral framework because it involves quadratic penalization terms which yield Gaussian path integrals. It would be interesting to examine other forms of regularization over function spaces within the path integral formulation, such as $L^1$ regularization.

## 5 Acknowledgements

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## A Functional Taylor approximations for the dielectric field problem

We wish to expand the Hamiltonian

$$H[\epsilon;\rho,\varphi_{\text{obs}}] = \frac{1}{2}\sum_{m=1}^{M}\int \frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left[\sum_{n=0}^{\infty}\varphi_n(\epsilon(\mathbf{x})) - \varphi_{\text{obs}}(\mathbf{x})\right]^2 \mathrm{d}\mathbf{x} + \frac{1}{2}\int \epsilon(\mathbf{x})(-\Delta)P(-\Delta)\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} \tag{51}$$

about its extrema $\epsilon^*$. We take variations with respect to $\epsilon(\mathbf{x})$ to calculate its first functional derivative,

$$\begin{aligned}
\int \frac{\partial H}{\partial \epsilon(\mathbf{x})}\phi(\mathbf{x})\,\mathrm{d}\mathbf{x} &= \int (-\Delta)P(-\Delta)\epsilon(x)\phi(\mathbf{x})\,\mathrm{d}\mathbf{x} + \lim_{h\to 0}\frac{\mathrm{d}}{\mathrm{d}h}\frac{1}{2}\sum_{m=1}^{M}\int\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left[\sum_{n=0}^{\infty}\varphi_n(\epsilon(\mathbf{x})+h\phi(\mathbf{x})) - \varphi_{\text{obs}}(\mathbf{x})\right]^2\mathrm{d}\mathbf{x}\\
&= \int(-\Delta)P(-\Delta)\epsilon\phi\,\mathrm{d}\mathbf{x} + \lim_{h\to 0}\sum_{m=1}^{M}\int\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right)\frac{\mathrm{d}}{\mathrm{d}h}\varphi_0(\epsilon(\mathbf{x})+h\phi(\mathbf{x}))\,\mathrm{d}\mathbf{x}\\
&\quad + \lim_{h\to 0}\sum_{m=1}^{M}\int\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right)\frac{\mathrm{d}}{\mathrm{d}h}\varphi_1(\epsilon(\mathbf{x})+h\phi(\mathbf{x}))\,\mathrm{d}\mathbf{x}\\
&\quad + \underbrace{\lim_{h\to 0}\sum_{m=1}^{M}\int\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right)\sum_{n=2}^{\infty}\frac{\mathrm{d}}{\mathrm{d}h}\varphi_n(\epsilon(\mathbf{x})+h\phi(\mathbf{x}))\,\mathrm{d}\mathbf{x}}_{I_1}
\end{aligned}\tag{52}$$

Let us define the quantities

$$\begin{aligned}
\tilde{K}(\mathbf{y},\mathbf{z}) &= \nabla_{\mathbf{z}}\cdot\left[L(\mathbf{y},\mathbf{z})\nabla_{\mathbf{z}}\left(\frac{\phi(\mathbf{z})}{\epsilon(\mathbf{z})}\right)\right]\\
\tilde{\varphi}_0(\mathbf{x}) &= -\int L(\mathbf{x},\mathbf{y})\frac{\rho(\mathbf{y})\phi(\mathbf{y})}{\epsilon^2(\mathbf{y})}\,\mathrm{d}\mathbf{y}\\
\Psi(\mathbf{x}) &= \sum_{m=1}^{M}\frac{\delta(\mathbf{x}-\mathbf{x}_m)}{s_m^2}\left(\varphi(\mathbf{x})-\varphi_{\text{obs}}(\mathbf{x})\right).
\end{aligned}$$

Through direct differentiation we find that

$$\begin{aligned}
I_1 &= \sum_{n=2}^{\infty}\int\Psi(\mathbf{x})K(\mathbf{x},\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\tilde{\varphi}_0(\mathbf{y}_1)\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k\\
&\quad + \sum_{n=2}^{\infty}\int\Psi(\mathbf{x})\tilde{K}(\mathbf{x},\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k\\
&\quad + \sum_{n=2}^{\infty}\int\Psi(\mathbf{x})K(\mathbf{x},\mathbf{y}_n)\sum_{k=0}^{n-1}\left(\tilde{K}(\mathbf{y}_{k+1},\mathbf{y}_k)\prod_{\substack{j=1\\ j\neq k}}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k.
\end{aligned}$$

Integrating in $\mathbf{x}$:

$$
\begin{aligned}
I_1 &= \sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int K(\mathbf{x}_m,\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\tilde{\varphi}_0(\mathbf{y}_1)\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int \tilde{K}(\mathbf{x}_m,\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int K(\mathbf{x}_m,\mathbf{y}_n)\sum_{k=1}^{n-1}\left(\tilde{K}(\mathbf{y}_{k+1},\mathbf{y}_k)\prod_{\substack{j=1\\ j\neq k}}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k.
\end{aligned}
$$

We shift $\phi(\cdot)\to\phi(\mathbf{x})$, and integrate-by-parts to find

$$
\begin{aligned}
I_1 = &-\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int K(\mathbf{x}_m,\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)L(\mathbf{y}_1,\mathbf{x})\frac{\rho(\mathbf{x})}{\epsilon^2(\mathbf{x})}\phi(\mathbf{x})\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int\frac{\phi(\mathbf{x})}{\epsilon(\mathbf{x})}\nabla\cdot\left[L(\mathbf{x}_m,\mathbf{x})\nabla\left(K(\mathbf{x},\mathbf{y}_{n-1})\right)\right]\left(\prod_{j=1}^{n-2}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int K(\mathbf{x}_m,\mathbf{y}_n)\sum_{k=1}^{n-1}\left(\frac{\phi(\mathbf{x})}{\epsilon(\mathbf{x})}\nabla\cdot\left[L(\mathbf{y}_{k+1},\mathbf{x})\nabla K(\mathbf{x},\mathbf{y}_{k-1})\right]\prod_{\substack{j=1\\ j\neq k}}^{n-2}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\,\mathrm{d}\mathbf{x}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k.
\end{aligned}
$$

Note that all boundary terms disappear since we can take $\phi$ to disappear on the boundary. With $I_1$ computed, we find

$$
\begin{aligned}
\frac{\delta H}{\delta\epsilon(\mathbf{x})} = &(-\mathit{\Delta})P(-\mathit{\Delta})\epsilon(\mathbf{x})-\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\left[L(\mathbf{x}_m,\mathbf{x})\frac{\rho(\mathbf{x})}{\epsilon^2(\mathbf{x})}\right] \\
&+\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2\epsilon(\mathbf{x})}\nabla\cdot\left[L(\mathbf{x}_m,\mathbf{x})\nabla\varphi_0(\mathbf{x})\right]-\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\left(\frac{\rho(\mathbf{x})}{\epsilon^2(\mathbf{x})}\right)\int K(\mathbf{x}_m,\mathbf{y}_1)L(\mathbf{x},\mathbf{y}_1)\,\mathrm{d}\mathbf{y}_1 \\
&-\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\int K(\mathbf{x}_m,\mathbf{y}_n)\left(\prod_{j=1}^{n-1}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)L(\mathbf{y}_1,\mathbf{x})\frac{\rho(\mathbf{x})}{\epsilon^2(\mathbf{x})}\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2\epsilon(\mathbf{x})}\int\nabla\cdot\left[L(\mathbf{x}_m,\mathbf{x})\nabla\left(K(\mathbf{x},\mathbf{y}_{n-1})\right)\right]\left(\prod_{j=1}^{n-2}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k \\
&+\sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2\epsilon(\mathbf{x})}\int K(\mathbf{x}_m,\mathbf{y}_n)\sum_{k=1}^{n-1}\left(\nabla\cdot\left[L(\mathbf{y}_{k+1},\mathbf{x})\nabla K(\mathbf{x},\mathbf{y}_{k-1})\right]\prod_{\substack{j=1\\ j\neq k}}^{n-2}K(\mathbf{y}_{j+1},\mathbf{y}_j)\right)\varphi_0(\mathbf{y}_1)\prod_{k=1}^{n}\mathrm{d}\mathbf{y}_k.
\end{aligned}
\tag{53}
$$

Taken to two terms in the series expansion for $\varphi$, the first variation is

$$
\frac{\delta H}{\delta\epsilon(\mathbf{x})}\sim(-\mathit{\Delta})P(-\mathit{\Delta})\epsilon(\mathbf{x})+\sum_{m=1}^{M}\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2\epsilon(\mathbf{x})}\left[\nabla L(\mathbf{x},\mathbf{x}_m)\cdot\nabla\varphi_0(\mathbf{x})-\frac{\rho(\mathbf{x})}{\epsilon(\mathbf{x})}\int K(\mathbf{x}_m,\mathbf{y}_1)L(\mathbf{x},\mathbf{y}_1)\,\mathrm{d}\mathbf{y}_1\right]. \tag{54}
$$

To calculate the second-order term in the Taylor-expansion, we take another variation. Truncated at two terms in the expansion for $\varphi$:

$$
\frac{\delta^2 H}{\delta\epsilon(\mathbf{x})\delta\epsilon(\mathbf{x}')}=(-\mathit{\Delta})P(-\mathit{\Delta})\delta(\mathbf{x}-\mathbf{x}')+\sum_{m=1}^{M}a_m(\mathbf{x},\mathbf{x}'), \tag{55}
$$

where after canceling like terms,

$$
\begin{aligned}
a_m(\mathbf{x},\mathbf{x}') = &\,\delta(\mathbf{x}-\mathbf{x}')\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2\epsilon^2(\mathbf{x}')}\left[\frac{2\rho(\mathbf{x}')}{\epsilon(\mathbf{x}')}\int K(\mathbf{x}_m,\mathbf{y}_1)L(\mathbf{x}',\mathbf{y}_1)\,\mathrm{d}\mathbf{y}_1-\nabla_{\mathbf{x}'}L(\mathbf{x}',\mathbf{x}_m)\cdot\nabla_{\mathbf{x}'}\varphi_0(\mathbf{x}')-L(\mathbf{x}_m,\mathbf{x}')\frac{\rho(\mathbf{x}')}{\epsilon(\mathbf{x}')}\right] \\
&-\frac{\varphi(\mathbf{x}_m)-\varphi_{\mathrm{obs}}(\mathbf{x}_m)}{s_m^2}\left\{\nabla L(\mathbf{x},\mathbf{x}_m)\cdot\nabla_{\mathbf{x}'}L(\mathbf{x},\mathbf{x}')\frac{\rho(\mathbf{x}')}{\epsilon(\mathbf{x})\epsilon^2(\mathbf{x}')}+\frac{\rho(\mathbf{x})}{\epsilon^2(\mathbf{x})\epsilon(\mathbf{x}')}\nabla L(\mathbf{x},\mathbf{x}')\cdot\nabla_{\mathbf{x}'}L(\mathbf{x}_m,\mathbf{x}')\right\} \\
&+\left[\nabla L(\mathbf{x},\mathbf{x}_m)\cdot\nabla\varphi_0(\mathbf{x})-\frac{\rho(\mathbf{x})}{\epsilon(\mathbf{x})}\int K(\mathbf{x}_m,\mathbf{y}_1)L(\mathbf{x},\mathbf{y}_1)\,\mathrm{d}\mathbf{y}_1\right] \\
&\times\frac{1}{s_m^2\epsilon(\mathbf{x})\epsilon(\mathbf{x}')}\left[\nabla_{\mathbf{x}'}L(\mathbf{x}',\mathbf{x}_m)\cdot\nabla_{\mathbf{x}'}\varphi_0(\mathbf{x}')-\frac{\rho(\mathbf{x}')}{\epsilon(\mathbf{x}')}\int K(\mathbf{x}_m,\mathbf{y}_1)L(\mathbf{x}',\mathbf{y}_1)\,\mathrm{d}\mathbf{y}_1\right].
\end{aligned}
$$

It is using this expression that we can construct an approximating probability density for our field $\epsilon$.

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