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NUMERICAL SOLUTION OF THE CAUCHY PROBLEM FOR THE LAPLACE EQUATION: A DETERMINISTIC AND BAYESIAN APPROACH

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Abstract. The problem of determining a harmonic function in a bounded region from measurements on part of the boundary (Cauchy data) is called the *Cauchy problem for the Laplace equation*, it is ill-posed and arises in several applications. In this work we solve the problem in complex annular regions using statistical inversion models based on Bayes formula. We take advantage of the connection between the 'a priori' distribution and Tikhonov regularization to propose different models where smooth or non-smooth regularization is possible. In particular, the 'a priori' model is built up from Gaussian Markov random fields (GMRF) used in spatial statistics. The posterior distribution is explored by a MCMC sampling based on a Metropolis–Hasting algorithm known as the t-walk. Numerical results for noisy data are presented to illustrate the effectiveness of the proposed models.

1 INTRODUCTION

We present a numerical study for the solution of the following problem in an annular region Ω: Given a function V defined on the exterior boundary Γ_2, find a function $\varphi = u|_{\Gamma_1}$ defined on the interior boundary Γ_1, which is the trace of a function $u \in H^1(\Omega)$ that is the solution of

$$-\nabla \cdot (\sigma \nabla u) = 0 \quad \text{in} \quad \Omega, \quad u = V \quad \text{on} \quad \Gamma_2, \quad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Gamma_2. \tag{1}$$

This problem is ill-posed, arise in several applications, so many numerical solution techniques has been applied to solve it. Recently, it was solved with a variational approach based on its reformulation as a boundary control problem, for which the cost function φ incorporates a penalized term that includes the Cauchy data [1]. Lagrange linear finite elements are good enough to solve the forward problem. Here, we go beyond and consider a statistical inversion computational models based on Bayes formula.

2 VARIATIONAL DETERMINISTIC FORMULATION

We introduce the following auxiliary problem, named the state equation (SE) or forward problem (FP): Given $\varphi \in H^{1/2}(\Gamma_1)$ find $u \in H^1(\Omega)$ such that

$$(SE) \quad -\nabla \cdot (\sigma \nabla u) = 0 \quad \text{in } \Omega, \qquad u = \varphi \quad \text{on } \Gamma_1, \qquad \sigma \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \Gamma_2, \tag{2}$$

where σ is the electrostatic conductivity, and u denotes the electrostatic potential. For each $\varphi \in H^{1/2}(\Gamma_1)$ the weak solution $u \doteq u_\varphi$ exist, is unique and $\|u_\varphi\|_{H^1(\Omega)} \leq C \|\varphi\|_{H^{1/2}(\Gamma_1)}$ (C does not depend on φ). Thus, the linear operator $\mathcal{L} : H^{1/2}(\Gamma_1) \to H^1(\Omega)$, $\mathcal{L}(\varphi) = u_\varphi$ is injective and continuous. The operator $\mathcal{K} : H^{1/2}(\Gamma_1) \to L^2(\Gamma_2)$, $\mathcal{K}(\varphi) = \mathcal{L}(\varphi)|_{\Gamma_2} = u_\varphi|_{\Gamma_2}$ is lineal, injective and compact, since it is the composition of $\mathcal{L}$ and the trace operator $u \longrightarrow u|_{\Gamma_2}$, which is compact. A solution of (SE) is also solution of the Cauchy problem if we choose the boundary condition φ on Γ_1 in such a way that

$$\mathcal{K}\,\varphi = V. \tag{3}$$

This equation is satisfied if V is smooth enough ($V \in Im(\mathcal{K})$). However, since $\mathcal{K}$ is compact then $\mathcal{K}^{-1}$ is not continuous. Therefore, the problem is ill–posed, and we will obtain numerical instability when attempting to find approximated solutions.

2.1 Min-norm solution and properties

Since $Im(\mathcal{K})$ is dense in $L^2(\Gamma_2)$, we can obtain a well defined solution by finding the minimal norm solution: $\min_\varphi J(\varphi) = \frac{1}{2} \int_{\Gamma_1} |\varphi|^2 dS$, subject to $\mathcal{K}\,\varphi = V$. The solution may be obtained by penalization, as in [1], or equivalently by solving the regularized problem

$$\min_\varphi J_\alpha(\varphi) = \frac{\alpha}{2} \|\varphi\|^2_{L^2(\Gamma_1)} + \frac{1}{2} \|\mathcal{K}\,\varphi - V\|^2_{L^2(\Gamma_2)}. \tag{4}$$

For each α the unique solution φ_α satisfies

$$DJ_\alpha(\varphi) = \alpha\,\varphi + \mathcal{K}^*\left(\mathcal{K}\,\varphi - V\right) = 0, \tag{5}$$

where $\mathcal{K}^* : L^2(\Gamma_2) \to L^2(\Gamma_1)$ is defined as $\mathcal{K}^* \upsilon = \sigma \left.\frac{\partial p}{\partial \mathbf{n}}\right|_{\Gamma_2}$, with p solution of the adjoint problem:

$$-\nabla \cdot (\sigma \nabla p) = 0 \quad \text{in } \Omega, \quad p = 0 \quad \text{on } \Gamma_1, \quad \sigma \frac{\partial p}{\partial \mathbf{n}} = \upsilon \quad \text{on } \Gamma_2. \tag{6}$$

Some important properties proved in [1] are: $\langle \mathcal{K}\varphi, V\rangle_{L^2(\Gamma_2)} = \langle \varphi, \mathcal{K}^* V\rangle_{L^2(\Gamma_1)}$, if $V \in Im(\mathcal{K})$ then $\lim_{\alpha\longrightarrow 0} \mathcal{K}\,\varphi_\alpha = V$ in $L^2(\Gamma_2)$, $\lim_{\alpha\longrightarrow 0} \varphi_\alpha = \varphi$ in $L^2(\Gamma_1)$. If we have noisy data V_δ where $\|V_\delta - V\| \le \delta\,\|V\|$, δ being the amount of perturbation, then the regularization parameter can be elected as $\alpha(\delta) \propto \delta$. If n conjugate gradient iterations are employed to solve (4) or (5) with regularization parameter $\alpha(\delta)$ and finite element approximation (with discretization parameter h) of the elliptic subproblems at each iteration, then

$$\lim_{\delta\to 0} \|\varphi^n_{h,\alpha(\delta)} - \varphi\|_{L^2(\Gamma_1)} = 0$$

when $\{h, \delta\} \to \{0, 0\}$ along trajectories that satisfy $h^{1/2} \le \delta^{1+\epsilon}$, with $\epsilon \ge 0$.

3 BAYESIAN APPROACH

Information is available through some measurements or data with error o uncertainty and all variables in the problem are considered as random. We first discretize (3): Let $\mathcal{T}_h$ be a triangular mesh of Ω, h being the characteristic size, V_h be the finite element discretization of V and let φ_h be the corresponding finite element solution of (3). Thus, the discrete analogue of (3) can be represented by

$$\mathcal{K}_h\,\varphi_h = u_h|_{\Gamma_2} = V_h. \tag{7}$$

We define the following vector values: $\mathbf{x} = (x_i)_{i=1}^n \in \mathbb{R}^n$ with $x_i = \varphi_h(P_i)$ and $\{P_i\}_{i=1}^n$ are the nodes of the FE mesh on Γ_1, $\mathbf{y} = (x_i)_{i=1}^m \in \mathbb{R}^m$ with $y_j = V_h(Q_j)$,and $\{Q_j\}_{j=1}^m$ are the nodes of the FE mesh on Γ_2. Then, the relation between these nodal values in equation (7) is better represented by a linear equation of the form

$$A\,\mathbf{x} = \mathbf{y}, \qquad A \in \mathbb{R}^{m\times n} \text{ and } \mathbf{y} \in \mathbb{R}^m \text{ given.} \tag{8}$$

The min-norm solution of (8) is obtained from the quadratic function $F_\alpha(\mathbf{x}) = \frac{\alpha}{2}\|\mathbf{x}\|^2_{\mathbb{R}^n} + \frac{1}{2}\|A\,\mathbf{x} - \mathbf{y}\|^2_{\mathbb{R}^m}$ and satisfies $DF_\alpha(\mathbf{x}) = \alpha\,\mathbf{x} + A^T(A\,\mathbf{x} - \mathbf{y}) = \mathbf{0}$. Table 1 shows the analogy between the continuous and discrete regularized optimization problems.

Table 1: Analogy between continuous and discrete regularized problems

	Continuous	Discrete
Problem	$\mathcal{K}\,\varphi = V$	$A\,\mathbf{x} = \mathbf{y}$
Quadratic Function	$\frac{\alpha}{2}\|\varphi\|^2_{L^2(\Gamma_1)} + \frac{1}{2}\|\mathcal{K}\,\varphi - V\|^2_{L^2(\Gamma_2)}$	$\frac{\alpha}{2}\|\mathbf{x}\|^2_{\mathbb{R}^n} + \frac{1}{2}\|A\,\mathbf{x} - \mathbf{y}\|^2_{\mathbb{R}^m}$
Derivative	$\alpha\,\varphi + \mathcal{K}^*(\mathcal{K}\varphi - V)$	$\alpha\,\mathbf{x} + A^T(A\,\mathbf{x} - \mathbf{y})$

3.1 Statistical model

Considering additive noise $\mathbf{e} \in \mathbb{R}^m$, our model is $\mathbf{y} = A\,\mathbf{x} + \mathbf{e}$ and the probability distributions of $\mathbf{X} = (X_i)_{i=1}^n$, $\mathbf{Y} = (Y_j)_{j=1}^m$ and $\mathbf{E} = (E_j)_{j=1}^m$ are tied together by the equation $\mathbf{Y} = A\,\mathbf{X} + \mathbf{E}$. The random variable $\mathbf{Y}$ denotes our data (measurements) and a realization is $\mathbf{Y} = \mathbf{y}$, finally $\mathbf{X}$ denotes the unobservable quantities. The full probability model can always be factored into components: $p(\mathbf{x},\mathbf{y}) = p(\mathbf{y}\,|\,\mathbf{x})\,p(\mathbf{x}) = p(\mathbf{x}\,|\,\mathbf{y})\,p(\mathbf{y})$. Applying Bayes' Rule, we obtain

$$p(\mathbf{x}\,|\,\mathbf{y}) = \frac{p(\mathbf{y}\,|\,\mathbf{x})\,p(\mathbf{x})}{p(\mathbf{y})} \quad \text{provided} \quad 0 < p(\mathbf{y}) < \infty. \tag{9}$$

The likelihood function $p(\mathbf{y}\,|\,\mathbf{x})$ is associated to the discrete state equation (SE), and takes in account the noise associated to error. We assume $\mathbf{E} \sim N(0, \sigma^2_{noise}\mathcal{I})$ and that $\mathbf{E}$, $\mathbf{X}$ are independent. If we set $\mathbf{X} = \mathbf{x}$, then $\mathbf{Y}$ conditioned on $\mathbf{X} = \mathbf{x}$ is distributed as $\mathbf{E}$, whose probability density is translated by $A\,\mathbf{x}$, that is

$$p(\mathbf{y}\,|\,\mathbf{x}) \propto p(\mathbf{e}) = p(\mathbf{y} - A\,\mathbf{x}) = \exp\left(-\frac{1}{2\,\sigma^2_{noise}}\|\mathbf{y} - A\,\mathbf{x}\|^2_{\mathbb{R}^m}\right). \tag{10}$$

On the other hand, concerning the construction of the 'a priori' model we can assume the following properties for the random variables $\mathbf{X}$ y $\mathbf{Y}$: (i) Each element x_i, defined on Γ_1, is related with its neighbours. At least it depends on x_{i-1} and x_{i+1}, but generally it may depend on $\mathbf{x}_{-i} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$. A similar property is valid for Y; (ii) Both boundaries, Γ_1 and Γ_2, are closed curves, so that $x_{n+1} = x_1$ and $y_{m+1} = y_1$. Therefore we can use concepts of spatial statistics to generate the prior distribution. Good models for the 'a priori' distribution of the spatially distributed parameter vector $\mathbf{x} = (x_1, \dots, x_n)$ are *Gaussian Markov random fields* (GMRF), where Gaussian probability distributions are assigned for the full conditionals $x_i\,|\,\mathbf{x}_{-i} \sim N\left(\sum_{j\neq i}\beta_{ij}\,x_j,\ k_i^{-1}\right)$, with parameters $\beta_{ij}\ \ k_i = \beta_{ji}\,k_j$, see [2]. The joint density function for $\mathbf{x}$ is the Gaussian

$$p(\mathbf{x}) = (2\pi)^{-\frac{n}{2}}|Q|^{\frac{1}{2}}\exp\left(-\frac{1}{2}\mathbf{x}^T Q\,\mathbf{x}\right), \quad Q_{ij} = \begin{cases} k_i, & \text{si } i = j, \\ -k_i\,\beta_{ij}, & \text{si } i \neq j. \end{cases} \tag{11}$$

To have a proper probability distribution $p(\mathbf{x})$, Q must be symmetric and positive definite. if Q is symmetric positive semi-definite the GMRF is called intrinsic and is denoted by IGMRF. An important class of GMRF are those in which the *precision matrix* Q is the numerical discretization of the *diffusion operator*. So we discretize $-\partial^2\varphi/\partial s^2$ along Γ_1 to obtain Q. We first introduce the basic forward dicretization: $\frac{\partial\varphi}{\partial s}(P_i) \approx \frac{\varphi_{i+1}-\varphi_i}{h_i}$ for $i = 1, \dots n$ (any other discretization is also valid). Considering periodicity ($\varphi_{n+1} = \varphi_1$), the associated matrix D, such that $\frac{\varphi_{i+1}-\varphi_i}{h_i} = (D\,\mathbf{x})_i$, $1 \leq i \leq n$, is:

$$D = \begin{bmatrix} -\frac{1}{h_1} & \frac{1}{h_1} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{h_2} & \frac{1}{h_2} & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\frac{1}{h_{n-1}} & \frac{1}{h_{n-1}} \\ \frac{1}{h_n} & 0 & 0 & \dots & 0 & -\frac{1}{h_n} \end{bmatrix}. \tag{12}$$

Then we may propose $Q = \frac{1}{\gamma^2}D^T D$. We observe that $\left\langle -\frac{\partial^2\varphi}{\partial s^2}, \eta\right\rangle_{L^2(\Gamma_1)} = \left\langle \frac{\partial\varphi}{\partial s}, \frac{\partial\eta}{\partial s}\right\rangle_{L^2(\Gamma_1)}$, $\forall\ \varphi, \eta \in H^1(\Gamma_1)$ has the discrete analogue $\langle D^T D\,\mathbf{x},\,\mathbf{w}\rangle_{\mathbb{R}^n} = \langle D\,\mathbf{x},\,D\,\mathbf{w}\rangle_{\mathbb{R}^n}$, $\forall\ \mathbf{x}, \mathbf{w} \in \mathbb{R}^n$ in this case. However, we want to show that $Q = \frac{1}{\gamma^2}DD^T$ also works. In this case

$$Q = \frac{1}{\gamma^2}\begin{bmatrix} \frac{2}{h_1^2} & -\frac{1}{h_1h_2} & 0 & \cdots & 0 & -\frac{1}{h_1h_n} \\ -\frac{1}{h_1h_2} & \frac{2}{h_2^2} & -\frac{1}{h_2h_3} & \cdots & 0 & 0 \\ 0 & -\frac{1}{h_2h_3} & \frac{2}{h_3^2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & -\frac{1}{h_{n-1}h_n} \\ -\frac{1}{h_1h_n} & 0 & 0 & \cdots & -\frac{1}{h_{n-1}h_n} & \frac{2}{h_n^2} \end{bmatrix}. \tag{13}$$

The full Bayesian model is described with the resultant posterior distribution $p(\mathbf{x}\,|\,\mathbf{y}) \propto p(\mathbf{x})\,p(\mathbf{y}\,|\,\mathbf{x}) = \exp\left(-\frac{1}{2\gamma^2}\|D\,\mathbf{x}\|^2_{\mathbb{R}^n} - \frac{1}{2\sigma^2_{noise}}\|\mathbf{y} - A\,\mathbf{x}\|^2_{\mathbb{R}^m}\right)$, which is also Gaussian:

$$p(\mathbf{x}\,|\,\mathbf{y}) \propto \mathcal{N}(\overline{\mathbf{x}}, \Sigma), \quad \text{with} \quad \overline{\mathbf{x}} = \Sigma A^T\mathbf{y}, \quad \Sigma = \left(Q + \frac{1}{\sigma^2_{noise}}A^TA\right)^{-1}. \tag{14}$$

The inverse exists, since $\mathrm{Ker}(D) \cap \mathrm{Ker}(A) = \mathbf{0}$.

3.2 Relation with Tikhonov regularization

If we define $\alpha = \sigma^2_{noise}/\gamma^2$, then the potential $V(\mathbf{x}\,|\,\mathbf{y})$ defines the quadratic function $\frac{\alpha}{2}\|D\,\mathbf{x}\|^2_{\mathbb{R}^n} + \frac{1}{2}\|\mathbf{y} - A\,\mathbf{x}\|^2_{\mathbb{R}^m}$. If further, we replace D by the identity matrix $\mathcal{I}$, we recover the quadratic function in Table 1 from which the min-norm solution is obtained. Then the 'a priori' distribution plays the role of regularization in the statistical model and corresponds to the regularization term in the Tikhonov quadratic function. The relation $\alpha = \sigma^2_{noise}/\gamma^2$ indicates that the regularization parameter in the deterministic approach to solve ill-posed problems should be proportional to the level of noise of the perturbed data, and this is consistent with a result in [1]. Thus, different precision matrices Q for statistical inversion define different Tikhonov regularization strategies for traditional inversion techniques. Table 2 shows several Tikhonov regularizations and their corresponding precision matrices for GMRF defined on irregular meshes. In that table $W = \mathrm{diag}(w_1, \ldots, w_n)$, $w_i = |\epsilon + (D\mathbf{x})_i|^{-1/2}$, $0 < \epsilon < 1$, actually w_i is a discretization of $\omega(P_i) = |\partial\varphi(P_i)/\partial s|^{-1/2}$.

3.3 Sampling the posterior

We employ a general purpose MCMC sampler for arbitrary continuous distributions, that requires no tuning, known as the *t-walk* (for 'traverse' or 'thoughtful' walk, as opposed to a random-walk). The t-walk maintains two independent points in the sample space, and all moves are based on proposals that are then accepted with a standard Metropolis-Hastings acceptance probability on the product space. For more details see [3].

4 NUMERICAL RESULTS

Synthetic data is obtained from the 2D-harmonic function $u(x,y) = \exp(x)\sin(y)$ defined in the bounded annular domain given in Figure 1 below, that is $V = u|_{\Gamma_2}$. White noise is added: $V_\delta = V + \mathcal{N}(0,\sigma)$ with $\sigma = \max V(P_i)/p$, where $p = 10$, 20 or 100. The real noise level is given by $\delta = \|V_\delta - V\|_{L^2(\Gamma_2)}/\|V\|_{L^2(\Gamma_2)} \doteq ER(V_\delta, V)_{\Gamma_2}$. The forward

Table 2: Tikhonov regularizations and corresponding precision matrices for GMRF on irregular meshes

Case	Tikhonov regularization	GMRF precision matrix
Min-norm	$\frac{\alpha}{2}\,\|\varphi\|^2_{L^2(\Gamma_1)}$	$Q = \alpha\, I$
Smooth	$\frac{\alpha}{2}\left\|\frac{\partial\varphi}{\partial s}\right\|^2_{L^2(\Gamma_1)}$	$Q = \alpha D^T D = \alpha\, L$ (Laplacian)
Smoother	$\frac{\alpha}{2}\left\|\frac{\partial^2\varphi}{\partial s^2}\right\|^2_{L^2(\Gamma_1)}$	$Q = \alpha\, L^T L$ (Biharmonic)
TV-reg	$\frac{\alpha}{2}\left\|\frac{\partial\varphi}{\partial s}\right\|_{L^1(\Gamma_1)}$	$Q = \alpha\, D^T W\, D$ (Anisotropy)

problem (SE) is solved with a linear FEM using the software FEniCS and integrated with the *t-walk* algorithm through the Phyton environment. All numerical computations were done with an HP portable personal computer with an Ubuntu 16.04 operative system, 4GB RAM, and an AMD A8-7410 processor.

Figures 2 and 3 show graphs with the numerical results when the perturbation added to data is 5% ($p = 20$) and 10% ($p = 10$), respectively. The left graph in each figure shows the exact data V (red line) and the perturbed data V_δ (blue dots) vs angle; the right graph in each figure shows the exact solution φ (red line) along with the conditional mean $\overline{\varphi}$ (blue line), the MAP $\varphi_{_{MAP}}$ (black line) and the deterministic (variational) numerical solution $\hat{\varphi}$ (green line). Parameters (function values on each boundary) generated by the random sample are shown in gray in each figure. Numerical values for these results are shown in Table 3 where we have included also the case with 1% ($p = 100$) perturbation on V. In that table ER denotes the relative error of the corresponding values in the L^2-norm. Values like $f(\hat{\varphi})$ denote the image of $\hat{\varphi}$ under the forward map. This table shows that the numerical results are very satisfactory and all of them are obtained in an stable way.

Optimal low rank approximation of the Bayesian inverse problem, described in [4], is also employed in this work, mainly on the covariance matrix, in order to reduce computational storage and to enable fast computation on the numerical solutions. The informed dimension obtained on our problem is between 40 and 45, instead of the 156 nodal values of V_δ on Γ_2.

5 CONCLUSIONS

We have extended the work in [1] (based on variational techniques) to statistical inversion via Bayes rule with algorithms based on MCMC, obtaining excellent numerical results. The relation between Tikhonov regularization and the prior distribution, allow the design of different models to solve inverse and control problems modelled by differential equations. Concepts of spatial statistics are employed to built up the prior distri-

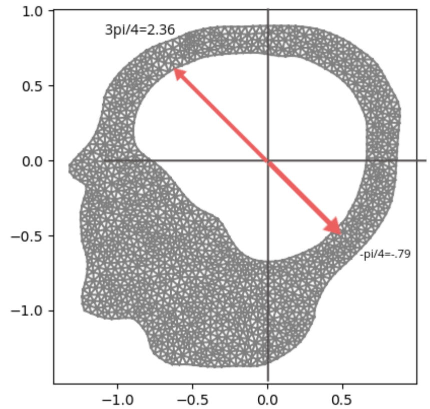

Figure 1: Mesh with 2908 triangular elements, 1454 nodes: 98 on Γ_1, 156 on Γ_2.

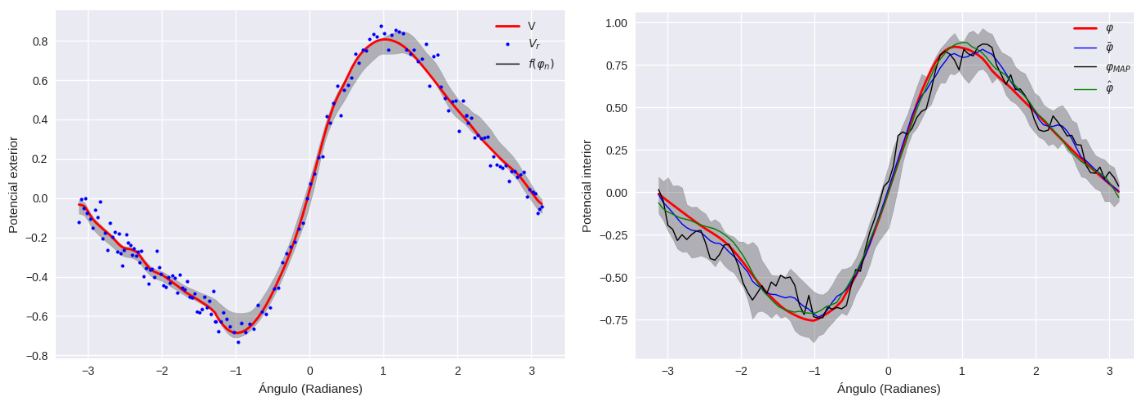

Figure 2: **Left**: $ER(V_\delta, V) = 0.10$. **Right:** $ER(\hat{\varphi}, \varphi) = 0.056$, $ER(\bar{\varphi}, \varphi) = 0.087$, $ER(\varphi_{MAP}, \varphi) = 0.167$

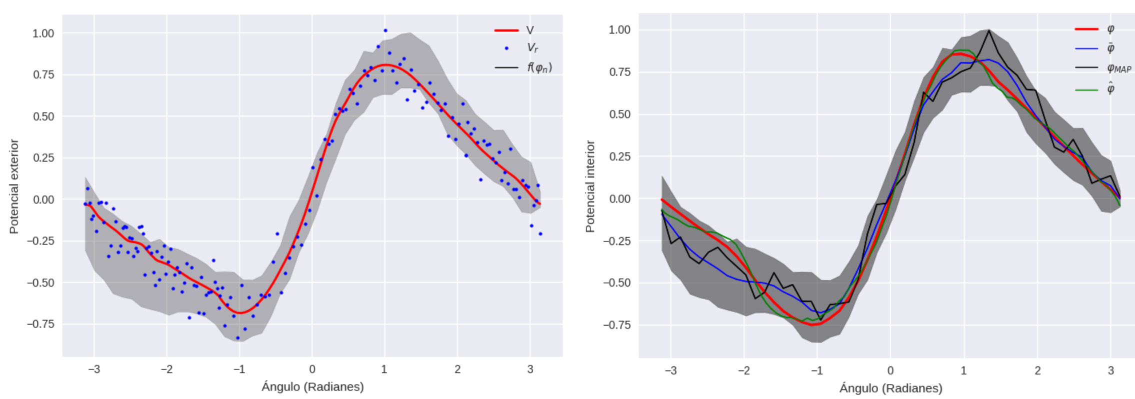

Figure 3: **Left:** $ER(V_\delta, V) = 0.18$. **Right**: $ER(\hat{\varphi}, \varphi) = 0.063$, $ER(\bar{\varphi}, \varphi) = 0.169$, $ER(\varphi_{MAP}, \varphi) = 0.226$.

Table 3: Data errors and their propagation to the interior and exterior electric potentials.

p (perturbation %)	100 (1%)	20 (5%)	10 (10%)
Noise level = $ER(V_\delta, V)_{\Gamma_2}$	0.0181	0.1001	0.1815
$ER(\hat{\varphi}, \varphi)_{\Gamma_1}$	0.0198	0.0563	0.0630
$ER(\bar{\varphi}, \varphi)_{\Gamma_1}$	0.0313	0.0870	0.1687
$ER(\varphi_{MAP}, \varphi)_{\Gamma_1}$	0.0862	0.1671	0.2259
$ER(f(\hat{\varphi}), V)_{\Gamma_2}$	0.0123	0.0353	0.0337
$ER(f(\bar{\varphi}), V)_{\Gamma_2}$	0.0133	0.0546	0.0935
$ER(f(\varphi_{MAP}), V)_{\Gamma_2}$	0.0150	0.0703	0.1299

bution through *Gaussian Markov random fields* based on discretizations of the diffusion operator. These connections between deterministic and statistical approaches allow the identification of the regularization parameter as it is related to the covariance of the prior distribution, which is consistent with a previous result in [1] where the regularization parameter is shown to be proportional to the level of noise of the perturbed data. Extensions to 3D problems or to problemas with non-smooth solutions, as well applications to other ill-posed problems, may give a deeper insight into these methods and techniques.

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