

Article

A Preliminary Analysis of a Physics-Informed Neural Network for the Forward Problem in EEG

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Abstract

The distributed inverse source problem in electroencephalography (EEG) requires the determination of a current-independent, geometry-dependent auxiliary function, which is defined by a Poisson partial differential equation (PDE), where its solution is referred to as the forward problem. In this study, we investigate the feasibility of employing a mesh-free Physics-Informed Neural Network (PINN) for obtaining this auxiliary function. The proposed architecture integrates Kolmogorov–Arnold Networks (KANs) into an extended PINN (XPINN) framework augmented with Multi-scale Fourier feature mappings to capture potential field discontinuities across piecewise-homogeneous tissue interfaces. The PINN loss functional incorporates the governing PDE, Neumann boundary conditions, flux continuity and reference data for specific neuronal source and electrode configurations. Numerical experiments on a three-layer spherical head model demonstrate that the XPIKAN surrogate achieves a relative L_2 error below 1% on unseen sensor coordinates. Factorial sensitivity analyses confirm stable model generalization across varying source-sensor configurations without the need for dense volumetric meshes. As a result, XPIKAN provides a meshless, continuous, and differentiable solution that offers faster inference time compared to classical solvers like finite element or boundary element methods and enables exact gradient computation for inverse source localization.

Keywords: physics-informed neural networks; electroencephalography; Kolmogorov–Arnold networks; medical imaging; inverse problems



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1. Introduction

Using EEG data, it is possible to estimate the neuronal current. This is known as solving the EEG inverse problem [1–3]. The usual approach to the solution of this inverse problem is the approximation of the neuronal current via a large number of dipoles. For a given dipole configuration, OpenMEEG solves the electric potential in Volts [4,5]. In particular, this approach is used by sLORETA [6]. An alternative approach, which is followed here, is treating the neuronal current as a continuous function [7–11]. The approach requires the solution of an auxiliary function, $v_s(\mathbf{r}, \boldsymbol{\tau})$; the determination of this function is known as the solution of the forward problem. A crucial step in the latter approach is the use of the so-called Helmholtz decomposition, namely the current is decomposed into an irrotational

and a solenoidal component [7,9–11]. In this setting, the current $\mathbf{J}$ at a source location $\boldsymbol{\tau} \in \Omega_c$ is given by:

$$\mathbf{J}^p(\boldsymbol{\tau}) = \nabla_{\boldsymbol{\tau}}\Psi(\boldsymbol{\tau}) + \nabla_{\boldsymbol{\tau}} \times \mathbf{A}(\boldsymbol{\tau}), \quad \boldsymbol{\tau} \in \Omega_c, \quad (1)$$

where $\mathbf{A}(\boldsymbol{\tau})$ represents the solenoidal part satisfying $\nabla \cdot \mathbf{A}(\boldsymbol{\tau}) = 0$, and $\Psi(\boldsymbol{\tau})$ describes the irrotational part. According to [12], the electric potential u_s measured at an observation point $\mathbf{r}$ on the scalp S_s is expressed as

$$u_s(\mathbf{r}) = -\frac{1}{4\pi} \int_{\Omega_c} \Delta_{\boldsymbol{\tau}}\Psi(\boldsymbol{\tau})v_s(\mathbf{r}, \boldsymbol{\tau})dV(\boldsymbol{\tau}) + \frac{1}{4\pi} \int_{S_c} v_s(\mathbf{r}, \boldsymbol{\tau})(\hat{\mathbf{n}}(\boldsymbol{\tau}) \cdot \mathbf{J}^p)dS(\boldsymbol{\tau}), \quad \mathbf{r} \in S_s, \quad (2)$$

where the auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ is independent of the current [9]. If $v_s(\mathbf{r}, \boldsymbol{\tau})$ is available, Equation (2) gives a direct relation between $u_s(\mathbf{r})$ and $\nabla_{\boldsymbol{\tau}}^2\Psi(\boldsymbol{\tau})$.

The EEG data acquisition system involves attaching a set of electrodes on the scalp. These electrodes are spatially distributed on the scalp at different coordinates [1–3]. The recorded potentials $u_s(\mathbf{r})$ at these electrode positions form the left-hand side of (2). Then, the process of reconstructing the irrotational component of the current $\nabla\Psi(\boldsymbol{\tau})$ involves constructing a system of linear equations given by the measurement Equation (2) [11]. To this end, we first need to obtain the solution to the auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$. If the conductivity profile of the brain is considered to be a piecewise homogeneous conductor, then $v_s(\mathbf{r}, \boldsymbol{\tau})$ is governed by a boundary value problem (BVP) [9,11]. The key feature of $v_s(\mathbf{r}, \boldsymbol{\tau})$ is that it is geometry-dependent and current independent. The geometry of the brain varies slightly from patient to patient. This in turn implies $v_s(\mathbf{r}, \boldsymbol{\tau})$ is patient specific and ideally, needs to be obtained for every patient under study. However, obtaining a patient-specific $v_s(\mathbf{r}, \boldsymbol{\tau})$ requires constructing a numerical head model from the patient's MRI. This process is computationally intensive: it involves segmenting the MRI to identify tissue compartments (scalp, skull, brain), and then generating surface or volume meshes for each compartment [13–23]. Once the mesh is built, $v_s(\mathbf{r}, \boldsymbol{\tau})$ is obtained by solving the boundary value problem numerically, typically with the boundary element method (BEM) [11] or the finite element method (FEM) [24]. Crucially, classical methods like FEM must repeat the entire solve for every new source location $\boldsymbol{\tau}$, which prevents real-time clinical application.

Physics-Informed Neural Networks (PINNs) provide a mesh-free framework for the solution of forward and inverse problems governed by partial differential equations [25–29]. Instead of discretizing the domain with a volumetric mesh, PINNs approximate the solution with a neural network and embed the governing PDE and boundary conditions directly into the loss function. Such physics-constrained formulation distinguishes PINNs from classical surrogate models that rely solely on data fitting [30–37], and from purely data-driven forward solvers that require extensive pre-computed training sets [11]; hence the model significantly reduces its dependency on large synthetic datasets. Furthermore, this paradigm shifts the computational burden from repeated numerical solves to a one-time offline training phase; once trained, the network delivers solutions at any query point in a fraction of a second. This speed is critical for the EEG inverse problem, where source localization algorithms may call the forward solver many times per iteration. In addition, the physics-constrained loss provides the PINN surrogate an inherent denoising ability to make it robust to experimental noise in EEG recordings.

For the EEG forward problem, where the auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ satisfies a linear elliptic boundary value problem on a three-layer head model, a standard PINN formulation would treat the entire domain as a single continuous region. However, the conductivity profile of the head is piecewise homogeneous, with sharp discontinuities at the inner skull and scalp interfaces. These jumps degrade the accuracy of a single global network. A natural

extension is the Extended Physics-Informed Neural Network (XPINN) framework, which decomposes the domain into sub-regions, assigns an independent sub-network to each compartment, and enforces interface conditions (continuity of the potential and normal current flux) as additional loss terms [38].

To further improve the representation capacity of each sub-network, we replace conventional multi-layer perceptrons with Kolmogorov–Arnold Networks (KANs). KANs place learnable activation functions on the edges of the network rather than on the nodes, and have been shown to achieve superior accuracy for PDE solutions while requiring substantially fewer parameters [39–41]. The combination of the XPINN decomposition strategy with KAN sub-networks yields the XPIKAN architecture employed in this work. In the XPIKAN surrogate, the entire head model geometry is parameterized once, the BVP and interface constraints are absorbed into the loss, and training is performed fully offline. At inference time, the network provides $v_s(\mathbf{r}, \tau)$ instantaneously for any source location τ without any mesh regeneration or iterative solving. To be specific, the contributions of this work are as follows:

1. We develop an XPIKAN forward solver enhanced with multi-scale Fourier features that serves as a mesh-free real-time surrogate.
2. We investigate the practical design factors that govern solution accuracy and robustness and quantify their effects through statistical comparisons.
3. We solve the forward problem on a spherical head model with an XPIKAN, using known reference values of v_s^* to guarantee uniqueness and simulate real-world data.

The remainder of the paper is organized as follows. Section 2 describes the three-layer head model and formulates the boundary value problem for the auxiliary function $v_s(\mathbf{r}, \tau)$. Section 3 details the multi-scale Fourier XPIKAN architecture, domain decomposition, and loss-function construction. Numerical experiments and a comprehensive analysis of the governing design factors are presented in Section 4. Conclusions and directions for future work are summarized in Section 5.

2. Head Model and the Forward Problem

The accuracy of any EEG forward solver depends critically on how faithfully the head geometry and tissue conductivities are represented. In this section, we formalize the three-layer spherical head model and derive the transmission boundary value problem that governs the auxiliary function $v_s(\mathbf{r}, \tau)$.

2.1. Head Geometry

The different compartments of a spherical head model for a piecewise homogeneous conductor model are shown in Figure 1. Ω_c represents the cerebrum with conductivity σ_c . The cerebrospinal fluid (CSF) is represented by the domain Ω_f with conductivity σ_f . The skull is represented by the domain Ω_b with conductivity σ_b . The outermost shell, Ω_s , models the scalp and has conductivity σ_s . The boundaries are respectively denoted by $\partial\Omega_c, \partial\Omega_f, \partial\Omega_b, \partial\Omega_s$. The region outside the head, denoted by Ω_e , is assumed to have zero conductivity.

It can be observed from Table 1 that Ω_f (CSF) has a higher conductivity than the remaining three compartments but, it also has a very small thickness. It was shown in [42] that the brain-CSF interface has a negligible effect in the analysis. For this reason, Ω_f (CSF) is usually ignored during the numerical approximation of v_s . We therefore only consider the three layer head model involving the compartments Ω_c, Ω_b and Ω_s .

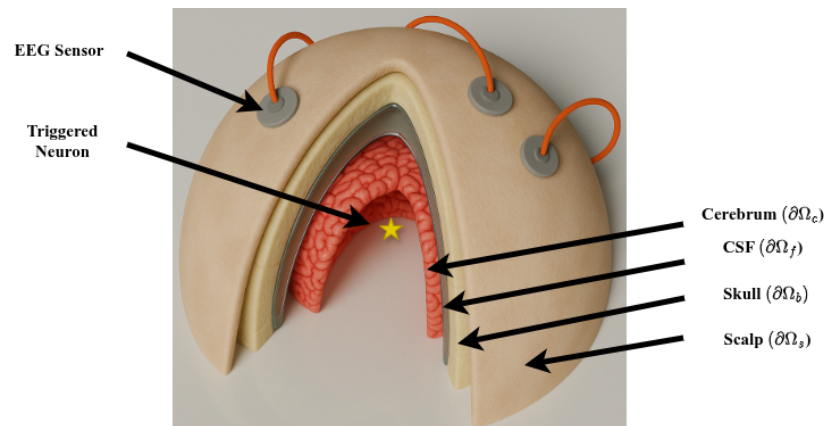


Figure 1. In the spherical head model, Ω_c denotes the cerebrum, surrounded in order by Ω_f , Ω_b , and Ω_s , which represent the cerebrospinal fluid, skull, and scalp, with conductivities σ_c , σ_f , σ_b , and σ_s , respectively.

Table 1. The radii and conductivity values for the different compartments of the head model.

Domain Ω	Conductivity σ (S/m)	Radius [43]
Scalp Ω_s	0.33	0.90
Skull Ω_b	0.0042	0.85
CSF Ω_f	1.0	0.80
Cerebrum Ω_c	0.33	0.79

2.2. The Auxiliary Function and the Transmission BVP

Low-frequency neuronal activity follows the quasi-static approximation of Maxwell's equations, where the inductive effect is negligible ($\nabla_{\mathbf{r}} \times \mathbf{E} \approx 0$). This allows the representation of the electric field by a scalar potential $\mathbf{E} = -\nabla_{\mathbf{r}} u$. The total current density is decomposed into $\mathbf{J} = \mathbf{J}^p + \mathbf{J}^v$, where $\mathbf{J}^p$ is the primary impressed neuronal current and $\mathbf{J}^v$ is the passive volume current. Applying Ohm's law ($\mathbf{J}^v = \sigma \mathbf{E}$) and the principle of charge conservation ($\nabla_{\mathbf{r}} \cdot \mathbf{J} = 0$) yields the fundamental variable-coefficient elliptic equation:

$$\nabla_{\mathbf{r}} \cdot (\sigma(\mathbf{r}) \nabla_{\mathbf{r}} u(\mathbf{r})) = \nabla_{\mathbf{r}} \cdot \mathbf{J}^p(\mathbf{r}), \quad \mathbf{r} \in \Omega. \quad (3)$$

To reduce this continuous problem to a computationally tractable form, we model the head as a bounded set $\Omega \subset \mathbb{R}^3$ partitioned into N nested, mutually disjoint open subdomains Ω_k , such that Ω_1 (cerebrum) is the innermost compartment and Ω_N (scalp) is the outermost. The global volume is $\Omega = \bigcup_{k=1}^N \Omega_k \cup \bigcup_{k=1}^{N-1} \Gamma_k$, where $\Gamma_k = \partial\Omega_k \cap \partial\Omega_{k+1}$ denotes the interface between adjacent layers. The isotropic conductivity $\sigma(\mathbf{r})$ is defined as a piecewise-constant scalar field $\sigma(\mathbf{r}) = \sum_{k=1}^N \sigma_k \chi_{\Omega_k}(\mathbf{r})$, where χ is the indicator function.

In accordance with the framework established by Fokas [9] and Dassios [7], the forward-inverse mapping is decoupled from the source dynamics by shifting the analytical burden onto a current-independent, geometry-dependent auxiliary function $v(\mathbf{r}, \boldsymbol{\tau})$. This function represents the potential at $\mathbf{r}$ due to a singular point source at $\boldsymbol{\tau} \in \Omega_1$ and is governed by the BVP:

$$\begin{cases} -\nabla_{\mathbf{r}} \cdot (\sigma(\mathbf{r}) \nabla_{\mathbf{r}} v(\mathbf{r}, \boldsymbol{\tau})) = \delta(\mathbf{r} - \boldsymbol{\tau}) - \frac{1}{|\Omega|}, & \mathbf{r} \in \Omega, \\ \nabla_{\mathbf{r}} v(\mathbf{r}, \boldsymbol{\tau}) \cdot \hat{\mathbf{n}} = 0, & \mathbf{r} \in S_s = \partial\Omega. \end{cases} \quad (4)$$

The term $1/|\Omega|$ ensures the compatibility condition for the Neumann problem, which is defined only up to an additive constant. Stability in the quotient space $H^1(\Omega)/\mathbb{R}$ is guaranteed by the Poincaré-Wirtinger inequality; we therefore normalize the field to

obtain the zero-mean auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ satisfying the surface integral condition $\int_{\partial\Omega_s} v_s(\mathbf{r}, \boldsymbol{\tau}) dS = 0$.

The structure of BVP (4) makes it particularly well-suited for solution with PINNs. Because the primary current is compactly supported inside the cerebrum ($\text{supp}(\mathbf{J}^p) \subseteq \Omega_1$), the governing equation reduces to the Laplace equation $\Delta_{\mathbf{r}} v_k = 0$ in all exterior regions $k > 1$. The only non-harmonic contribution is the point source at $\boldsymbol{\tau} \in \Omega_1$. Rather than approximating a Dirac delta in the volumetric loss, which is numerically challenging for neural networks, we decompose the innermost potential into a known singular free-space kernel and a regular harmonic correction. This translocates the volumetric singularity onto the interface transmission conditions, where it can be enforced through standard continuity and flux-matching terms in the PINN loss (See Section 3). The resulting system is linear in the transmission and boundary data, which yields an adjoint Green kernel relating the scalp potential $u_s(\mathbf{r})$ to the neuronal source:

$$u_s(\mathbf{r}) = - \int_{\Omega_c} v_s(\mathbf{r}, \boldsymbol{\tau}) \nabla_{\boldsymbol{\tau}} \cdot \mathbf{J}^p(\boldsymbol{\tau}) dV(\boldsymbol{\tau}). \quad (5)$$

As noted in [42], the high conductivity and minimal thickness of the CSF (Ω_f) have a negligible effect on this distribution. Thus, the forward problem reduces to determining $v_s(\mathbf{r}, \boldsymbol{\tau})$ for $\boldsymbol{\tau} \in \Omega_c$ and $\mathbf{r} \in \partial\Omega_s$ using a 3-layer model comprising the cerebrum (Ω_c), skull (Ω_b), and scalp (Ω_s).

The 3-Layer Piecewise Homogeneous BVP

We model the head as a 3-layer medium comprising the cerebrum (Ω_c), skull (Ω_b), and scalp (Ω_s) with constant conductivities σ_c, σ_b , and σ_s . To resolve the spatial singularity analytically and establish a framework suitable for neural operator approximations, we decompose the total potential in the innermost layer Ω_c into the sum of an unbounded free-space singular potential $u^\infty(\mathbf{r}, \boldsymbol{\tau})$ and a regular auxiliary potential $v_c(\mathbf{r}, \boldsymbol{\tau})$. The component $u^\infty = 1/(4\pi|\mathbf{r} - \boldsymbol{\tau}|)$ represents the Newtonian potential generated by a singular point source embedded within an unbounded, homogeneous space of conductivity σ_c . By exploiting the linearity of the Laplacian, the volumetric source term is canceled such that $\Delta_{\mathbf{r}} v_c(\mathbf{r}, \boldsymbol{\tau}) = 0$.

Consequently, the physical requirements of potential continuity and normal current flux conservation translocate the source influence entirely to the boundary transmission conditions across the first interface $\partial\Omega_c$. The determination of the scalp auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ thus constitutes the forward problem, governed by a globally harmonic system for observation points $\mathbf{r}$ and source points $\boldsymbol{\tau} \in \Omega_c$:

$$\nabla_{\mathbf{r}}^2 v_i(\mathbf{r}, \boldsymbol{\tau}) = 0, \quad \mathbf{r} \in \Omega_i, \quad i \in \{c, b, s\}, \quad (6)$$

$$v_b(\mathbf{r}, \boldsymbol{\tau}) - v_c(\mathbf{r}, \boldsymbol{\tau}) = \frac{1}{4\pi\sigma_c} \frac{1}{|\mathbf{r} - \boldsymbol{\tau}|}, \quad \mathbf{r} \in \partial\Omega_c, \quad (7)$$

$$\sigma_b \frac{\partial v_b(\mathbf{r}, \boldsymbol{\tau})}{\partial n} - \sigma_c \frac{\partial v_c(\mathbf{r}, \boldsymbol{\tau})}{\partial n} = \frac{\partial}{\partial n} \left(\frac{1}{4\pi|\mathbf{r} - \boldsymbol{\tau}|} \right), \quad \mathbf{r} \in \partial\Omega_c, \quad (8)$$

$$v_s(\mathbf{r}, \boldsymbol{\tau}) - v_b(\mathbf{r}, \boldsymbol{\tau}) = 0, \quad \mathbf{r} \in \partial\Omega_b, \quad (9)$$

$$\sigma_s \frac{\partial v_s(\mathbf{r}, \boldsymbol{\tau})}{\partial n} - \sigma_b \frac{\partial v_b(\mathbf{r}, \boldsymbol{\tau})}{\partial n} = 0, \quad \mathbf{r} \in \partial\Omega_b, \quad (10)$$

$$\frac{\partial v_s(\mathbf{r}, \boldsymbol{\tau})}{\partial n} = 0, \quad \mathbf{r} \in \partial\Omega_s. \quad (11)$$

Here, $\partial/\partial n$ denotes the outward normal derivative. Equations (7)–(10) enforce the continuity of potential and flux, while Equation (11) imposes the insulating Neumann condition at

the air-scalp interface. To satisfy the Neumann gauge, the solution is made unique by the zero-mean condition $\int_{\partial\Omega_s} v_s dS = 0$.

To provide an analytical foundation for the ground truth used in validating the XPIKAN, we specialize the BVP to concentric spherical geometry with radii $r_c < r_b < r_s$. Due to the azimuthal symmetry about the axis defined by τ , the functional dependence of the field collapses to the observation radius r , the source depth $\|\tau\|$, and the subtended angle γ , where $\cos \gamma = \hat{\mathbf{r}} \cdot \hat{\boldsymbol{\tau}}$. In this setting, the singular kernel is expanded for $r > \|\tau\|$ as $1/|\mathbf{r} - \boldsymbol{\tau}| = \sum_{n=0}^{\infty} (\|\tau\|^n / r^{n+1}) P_n(\cos \gamma)$. The harmonic auxiliary fields within each layer Ω_k take the spectral form $v_k = \sum (A_{k,n} r^n + B_{k,n} r^{-(n+1)}) P_n(\cos \gamma)$.

The coefficients are propagated from the innermost core to the scalp using a transfer matrix approach [7]. By enforcing boundedness at the origin ($B_{c,n} = 0$) and excluding the $n = 0$ monopole mode to satisfy the zero-mean gauge, the spectral solution on the scalp ($r = r_s$) is given by

$$v_s(\mathbf{r}, \boldsymbol{\tau}) = \frac{1}{\sigma_s} \sum_{n=1}^{\infty} \left[\frac{2n+1}{nM_{2,2} + (n+1)M_{2,1}} \right] \frac{|\tau|^n}{r_s^{n+1}} P_n(\cos \gamma), \quad (12)$$

where the propagation matrix $\mathbf{M} = \prod_{k=1}^{N-1} \mathbf{T}_{k,n}$ is the product of interface transition matrices:

$$\mathbf{T}_{k,n} = \frac{1}{2n+1} \begin{bmatrix} n + (n+1) \frac{\sigma_k}{\sigma_{k+1}} & (n+1) \left(\frac{\sigma_k}{\sigma_{k+1}} - 1 \right) \left(\frac{r_s}{r_k} \right)^{2n+1} \\ n \left(\frac{\sigma_k}{\sigma_{k+1}} - 1 \right) \left(\frac{r_k}{r_s} \right)^{2n+1} & (n+1) + \frac{n\sigma_k}{\sigma_{k+1}} \end{bmatrix}. \quad (13)$$

3. XPIKAN Surrogate for the Forward Problem

The central computational challenge identified in Section 2 is the need for a fast, mesh-free, and case-specific evaluation of the auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ that appears in the measurement Equation (2). Since v_s must be evaluated at many source-sensor pairs during source localization, we approximate it with a neural network surrogate that, once trained, delivers solutions instantaneously.

A single neural network defined over the entire head volume would, however, encounter severe difficulties in approximating the potential fields v_c, v_b, v_s . The conductivity $\sigma(\mathbf{r})$ is piecewise constant and undergoes sharp jumps at the interfaces $\partial\Omega_c$ and $\partial\Omega_b$; these jumps induce C^1 discontinuities in the derivative of the auxiliary function that a globally smooth network cannot easily capture. To resolve this, we adopt the XPINN strategy [38]. Instead of a single network, we decompose the domain into the three physical compartments and assign an independent neural network to each region. Each sub-network is responsible for approximating the auxiliary harmonic function within one homogeneous compartment; the interface conditions that couple the compartments are enforced through dedicated loss terms (Section 3).

For the individual sub-networks, we choose the Kolmogorov–Arnold network, an architecture that has demonstrated superior accuracy for PDE solutions while using substantially fewer parameters than conventional multi-layer perceptrons [39–41]. The KAN is grounded in the Kolmogorov–Arnold representation theorem, which guarantees that any smooth multivariate continuous function $f : [0, 1]^n \rightarrow \mathbb{R}$ on a compact domain can be expressed as a finite superposition of univariate functions and additions:

$$f(\mathbf{y}) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^n \phi_{q,p}(y_p) \right), \quad (14)$$

where $\phi_{q,p} : [0, 1]^n \rightarrow \mathbb{R}$ and $\Phi_q : \mathbb{R} \rightarrow \mathbb{R}$. A deep KAN generalizes this structure to L layers, each containing a matrix of learnable univariate functions $\Phi_l = \{\phi_{l,j,i}\}$. The network

output is the composition $\hat{v}(\mathbf{y}) = (\Phi_{L-1} \circ \Phi_{L-2} \circ \dots \circ \Phi_0)(\mathbf{y})$, where the elements of the l th matrix Φ_l can be computed as

$$[\Phi_l]_{j,i} = \phi_{l,j,i}(\cdot) \quad i = 1, 2, \dots, d_{l-1}, j = 1, 2, \dots, d_l, \quad (15)$$

in which d_l denotes network width of layer l with $d_{L-1} = 1$.

Inside a KAN, each univariate edge function $\phi_{l,j,i}(y_i)$ is constructed as a weighted sum of a smooth residual branch and a B-spline branch:

$$\phi_{l,j,i}(y_i) = \theta'_{l,j,i} \text{SiLU}(y_i) + \theta''_{l,j,i} B_{l,j,i}(y_i), \quad (16)$$

where $\text{SiLU}(x) = x/(1 + e^{-x})$ provides a stable gradient flow and $\theta'_{l,j,i}$ and $\theta''_{l,j,i}$ are learnable network weights. The spline term $B_{l,j,i}(y_i)$ is expressed as

$$B_{l,j,i}(y_i) = \sum_{m=1}^{k+G} \beta_{l,j,i,m} B_{m,k}(y_i; \mathbf{t}), \quad (17)$$

where k is the basis function order, G is the number of grid intervals, $\beta_{l,j,i,m}$ are learnable B-spline coefficients, and $B_{m,k}(x; \mathbf{t})$ denotes the basis function of order k . In this setting, a knot vector, $\mathbf{t} = (t_1, t_2, \dots, t_{G+2k+1})$ is a set of equidistant points over the domain $|x| < 1$. The values t_i mark where curve segments connect, satisfying $t_i \leq t_{i+1}$ for all i . The basis functions $B_{m,k}(x)$ depend on k and the knot vector and are defined recursively via the Cox-de Boor formula:

$$B_{m,0}(y) = \begin{cases} 1, & t_m \leq y < t_{m+1}, \\ 0, & \text{otherwise,} \end{cases} \quad (18)$$

and for $k > 0$:

$$B_{m,k}(y) = \frac{y - t_m}{t_{m+k} - t_m} B_{m,k-1}(y) + \frac{t_{m+k+1} - y}{t_{m+k+1} - t_{m+1}} B_{m+1,k-1}(y). \quad (19)$$

The set of coefficients $\Theta = \{\beta_{l,j,i,m}, \theta'_{l,j,i}, \theta''_{l,j,i}\}$ constitutes the learnable parameters of the network, to be optimized by minimizing a suitable loss function over the training dataset.

The raw coordinates that describe a source-sensor pair form a 6-dimensional vector $\mathbf{x} = [\mathbf{r}, \boldsymbol{\tau}]^T$. Before feeding this vector into the KAN, we transform it to better expose the high-frequency content and the underlying spherical geometry. Standard coordinate-based networks often suffer from spectral bias, favoring low frequencies [44]; to overcome this we apply a multi-scale Fourier feature mapping $\gamma(\cdot)$:

$$\gamma(\mathbf{x}) = \bigoplus_{s \in \mathfrak{S}} \left[\cos(2\pi \mathbf{B}_s \mathbf{x}), \sin(2\pi \mathbf{B}_s \mathbf{x}) \right]^T, \quad (20)$$

where $\bigoplus$ is the concatenation operator, $\mathfrak{S}$ is a set of frequency scales and $\mathbf{B}_s \in \mathbb{R}^{\mathfrak{M} \times 6}$ with $\mathfrak{M}$ random frequencies are static projection matrices with entries drawn from $\mathcal{N}(0, s^2)$.

Because the head is modeled as a set of concentric spheres, the solution depends on the geometry only through rotationally invariant quantities. We therefore augment the Fourier features with several scalar invariants: the radial distances $\|\mathbf{r}\|$ and $\|\boldsymbol{\tau}\|$, the Euclidean source-sensor separation $\|\mathbf{r} - \boldsymbol{\tau}\|$ along with its inverse $\|\mathbf{r} - \boldsymbol{\tau}\|^{-1}$, and the cosine of the subtended angle $\cos \gamma = (\mathbf{r} \cdot \boldsymbol{\tau}) / (\|\mathbf{r}\| \|\boldsymbol{\tau}\|)$. The final input vector $\mathbf{y} \in \mathbb{R}^{2|\mathfrak{S}|+5}$ to each KAN is

$$\mathbf{y} = \left[\gamma(\mathbf{x})^T, \|\mathbf{r}\|, \|\boldsymbol{\tau}\|, \|\mathbf{r} - \boldsymbol{\tau}\|, \|\mathbf{r} - \boldsymbol{\tau}\|^{-1}, \cos \gamma \right]^T. \quad (21)$$

With the XPIKAN surrogate architecture fully defined, the remaining task is to specify how the governing physics and available reference data are used to train the parameter sets $\Theta_c, \Theta_b, \Theta_s$. This is accomplished by minimizing a composite physics-informed loss function, which is the subject of the next section.

Physics-Informed Loss Formulation

The sub-networks representing the three compartments are trained jointly by minimizing a multi-objective composite loss functional. Let $\Theta = \{\Theta_c, \Theta_b, \Theta_s\}$ denote the set of all learnable parameters. The total loss functional is defined as

$$\mathcal{L}_{\text{Total}}(\Theta) = \lambda_{\text{PDE}} \mathcal{L}_{\text{PDE}}(\Theta) + \lambda_{\text{BC}} \mathcal{L}_{\text{BC}}(\Theta) + \lambda_{\text{Flux}} \mathcal{L}_{\text{Flux}}(\Theta) + \lambda_{\text{Data}} \mathcal{L}_{\text{Data}}(\Theta), \quad (22)$$

where $\lambda_{\text{PDE}}, \lambda_{\text{BC}}, \lambda_{\text{Flux}}$, and λ_{Data} are hyper-parameters that balance the contributions of the Laplacian, boundary values, interface fluxes, and reference data points. In the following we define each term and explain its role in embedding the physics of the forward problem. To simplify notation in what follows, we write the three KAN surrogates compactly as $\hat{v}_c(\mathbf{y}) = \text{KAN}_c(\mathbf{y}; \Theta_c)$, $\hat{v}_b(\mathbf{y}) = \text{KAN}_b(\mathbf{y}; \Theta_b)$, and $\hat{v}_s(\mathbf{y}) = \text{KAN}_s(\mathbf{y}; \Theta_s)$.

Let N_Ω be the number of interior collocation points sampled within each compartment, N_Γ the number of interface sampling points, and N_d the number of sparse analytical anchor points. To satisfy Laplace's equation in the source-free regions, we apply automatic differentiation to evaluate the spatial Laplacian $\nabla_{\mathbf{r}}^2$ of the network outputs at internal collocation points. This gives the PDE loss

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_\Omega} \sum_{i=1}^{N_\Omega} \left[\left(\nabla_{\mathbf{r}}^2 \hat{v}_c(\mathbf{y}_i^c) \right)^2 + \left(\nabla_{\mathbf{r}}^2 \hat{v}_b(\mathbf{y}_i^b) \right)^2 + \left(\nabla_{\mathbf{r}}^2 \hat{v}_s(\mathbf{y}_i^s) \right)^2 \right], \quad (23)$$

where $\mathbf{y}_i^c, \mathbf{y}_i^b, \mathbf{y}_i^s$ are inputs corresponding to points sampled inside the cerebrum Ω_c , skull Ω_b , and scalp Ω_s , respectively.

Potential continuity and the singularity decomposition on the interfaces are enforced directly through the boundary-condition loss. Let $f_1(\mathbf{r}, \boldsymbol{\tau}) = \frac{1}{\|\mathbf{r} - \boldsymbol{\tau}\|}$ be the singular free-space potential. At the brain–skull interface $\partial\Omega_c$ (radius $r_c = 0.79$) and the skull–scalp interface $\partial\Omega_b$ (radius $r_b = 0.85$), the required matchings yield

$$\begin{aligned} \mathcal{L}_{\text{BC}} = & \frac{1}{N_{\Gamma_c}} \sum_{i=1}^{N_{\Gamma_c}} \left(\hat{v}_b(\mathbf{y}_i^{\Gamma_c}) - \left[\frac{1}{4\pi\sigma_c} f_1(\mathbf{r}_i, \boldsymbol{\tau}_i) + \hat{v}_c(\mathbf{y}_i^{\Gamma_c}) \right] \right)^2 \\ & + \frac{1}{N_{\Gamma_b}} \sum_{j=1}^{N_{\Gamma_b}} \left(\hat{v}_s(\mathbf{y}_j^{\Gamma_b}) - \hat{v}_b(\mathbf{y}_j^{\Gamma_b}) \right)^2. \end{aligned} \quad (24)$$

The transmission conditions also require continuity of the normal current flux. Because the skull conductivity is much lower than that of the surrounding tissues, the raw flux residuals differ by orders of magnitude across interfaces, which can destabilize training. We therefore normalize each flux residual by the local average of the normal current density. The scale factors are defined as

$$J_{\text{scale},c} = \epsilon + \frac{1}{N_{\Gamma_c}} \sum_{i=1}^{N_{\Gamma_c}} \left| \frac{1}{4\pi} \frac{\partial f_1}{\partial n} + \sigma_c \frac{\partial \hat{v}_c}{\partial n} \right|, \quad J_{\text{scale},b} = \epsilon + \frac{1}{N_{\Gamma_b}} \sum_{j=1}^{N_{\Gamma_b}} \left| \sigma_b \frac{\partial \hat{v}_b}{\partial n} \right|, \quad (25)$$

where $\epsilon = 10^{-8}$ prevents division by zero. With these, the flux loss, which also includes the zero-flux insulation condition on the outer scalp boundary $\partial\Omega_s$ (radius $r_s = 0.90$), is

$$\begin{aligned}\mathcal{L}_{\text{Flux}} = & \frac{1}{J_{\text{scale},c}} \left[\frac{1}{N_{\Gamma_c}} \sum_{i=1}^{N_{\Gamma_c}} \left(\sigma_b \frac{\partial \hat{v}_b}{\partial n} - \left[\frac{1}{4\pi} \frac{\partial f_1}{\partial n} + \sigma_c \frac{\partial \hat{v}_c}{\partial n} \right] \right)^2 \right] \\ & + \frac{1}{J_{\text{scale},b}} \left[\frac{1}{N_{\Gamma_b}} \sum_{j=1}^{N_{\Gamma_b}} \left(\sigma_s \frac{\partial \hat{v}_s}{\partial n} - \sigma_b \frac{\partial \hat{v}_b}{\partial n} \right)^2 \right] \\ & + \frac{1}{N_{\Gamma_s}} \sum_{k=1}^{N_{\Gamma_s}} \left(\frac{\partial \hat{v}_s}{\partial n} \right)^2.\end{aligned}\quad (26)$$

Here $\partial/\partial n$ denotes the outward normal derivative, computed via automatic differentiation as $\nabla_{\mathbf{r}} v \cdot \frac{\mathbf{r}}{\|\mathbf{r}\|}$.

Neumann boundary value problems are unique only up to an additive constant. To eliminate this gauge freedom and accelerate convergence, we introduce a small set of sparse scalp potential evaluations obtained from the analytic spherical harmonic solution $v_s^*(\mathbf{r}, \boldsymbol{\tau})$. These evaluations are structured as a pairing of N_{sens} sensor locations on the scalp and N_{src} source locations within the cerebrum, such that $N_d = N_{\text{sens}} \times N_{\text{src}}$. The data loss is defined as

$$\mathcal{L}_{\text{Data}} = \frac{1}{N_d} \sum_{m=1}^{N_d} \left(\hat{v}_s(\mathbf{y}_m^d) - v_s^*(\mathbf{r}_m, \boldsymbol{\tau}_m) \right)^2. \quad (27)$$

The total loss functional $\mathcal{L}_{\text{Total}}$ is then optimized using the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm. The complete computational procedure for the proposed XPIKAN framework is illustrated in Figure 2. In the next section, we provide numerical results and key findings derived from this forward model.

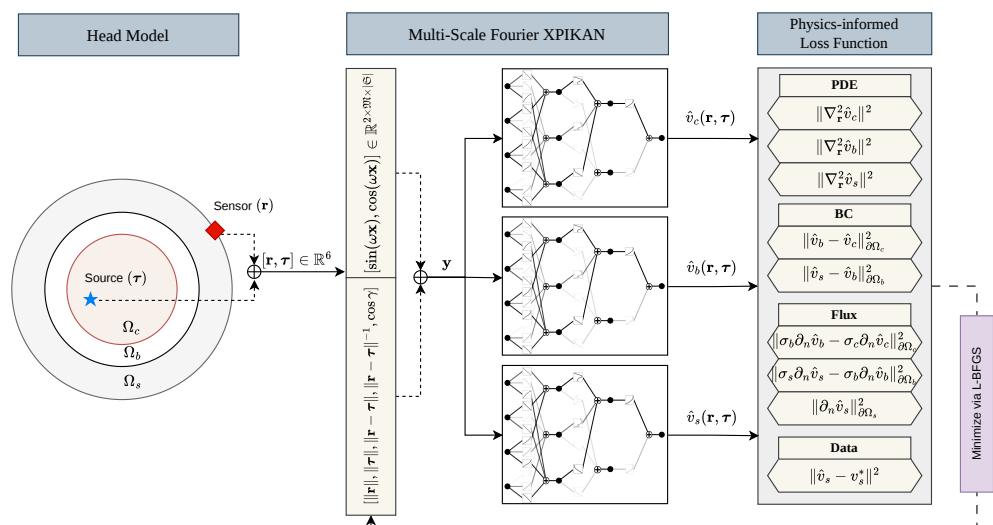


Figure 2. Schematic of the XPIKAN framework for the EEG forward problem. **(Left)** The three-layer head model defines the spatial domains for source $\boldsymbol{\tau}$ and sensor $\mathbf{r}$. **(Center)** Raw coordinates undergo multi-scale Fourier feature mapping and augmentation with geometric invariants before processing through the KAN architecture. **(Right)** The training process is governed by a composite loss function that enforces the interior Poisson/Laplace equations, interface transmission conditions (BC), Flux, and data fidelity. The entire system is optimized via the L-BFGS algorithm to update the network parameters Θ .

4. Numerical Results

In this section, we evaluate the performance of the XPIKAN surrogate in solving the three-layer spherical EEG forward problem. To ensure the model achieves optimal

accuracy with minimal parameterization, we first perform a systematic hyperparameter optimization, followed by a statistical analysis of the prediction accuracy.

The hyperparameter optimization strategy involves embedding the L-BFGS minimization algorithm into the Tree Parzen Estimator (TPE) algorithm. More precisely, for each candidate configuration proposed by the TPE, the three sub-networks (Cerebrum $\hat{v}_c$, Skull $\hat{v}_b$, and Scalp $\hat{v}_s$) are trained jointly by minimizing the loss functional (22), after which the prediction error on a hold-out validation set is evaluated. The result is fed back to the TPE, and the loop is repeated for a pre-specified number of trials ($N_{\text{TPE}} = 150$ in our experiments). The architecture that yields the lowest validation error is then selected as the base model for all subsequent assessments.

The search space covers the network depth $L \in \{1, \dots, 5\}$, the hidden-layer width $d_l \in \{16, 32, 64, 128\}$, the B-spline order $k \in \{2, 3, 4\}$, and the number of grid points $G \in \{5, 10, \dots, 50\}$. For the Fourier feature mapping $\gamma(\mathbf{x})$, the TPE explores subsets $\mathfrak{S} \subseteq \{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$ and mapping dimensions $\mathfrak{M} \in \{8, 16, 32\}$. The penalty weights $\lambda_{\text{PDE}}, \lambda_{\text{BC}}, \lambda_{\text{Flux}}, \lambda_{\text{Data}}$ are sampled log-uniformly from $\{1, 10, 100, 1000\}$ to identify the optimal balance between physics enforcement and data fitting.

Consistent with the high expressive power of Kolmogorov–Arnold networks, the TPE search, conducted on a Kaggle T4 GPU, identified that relatively shallow architectures achieve the highest efficiency. The optimal configuration determined by the search uses a network depth of $L = 2$, a uniform hidden-layer width of $d_l = 64$, B-spline order $k = 3$, and $G = 30$ grid points. The Fourier feature mapping operates with the scale set $\mathfrak{S} = \{10^{-4}, 10^{-3}\}$ and a mapping dimension $\mathfrak{M} = 16$. The loss components are balanced with the penalty weights $\lambda_{\text{PDE}} = 1$, $\lambda_{\text{BC}} = 10$, $\lambda_{\text{Flux}} = 10$, and $\lambda_{\text{Data}} = 100$.

With the optimal architecture fixed, we now detail the data generation and training procedure. The training process requires three families of collocation points. Interior PDE points are drawn with Latin Hypercube Sampling (LHS) to achieve a quasi-uniform coverage of the 6D source-sensor space within each homogeneous shell $\Omega_c, \Omega_b, \Omega_s$. Interface points are sampled uniformly on the spherical boundaries $\partial\Omega_c$ and $\partial\Omega_b$, and N_{Γ} points are also placed on the outer scalp surface $\partial\Omega_s$ to enforce the insulation condition. To fix the gauge and to provide a sparse reference signal, N_d source-sensor pairs with exact values v_s^* computed from the analytical spherical-harmonic expansion (12) are employed as data anchors. All training is performed offline with the L-BFGS optimizer, using a tolerance of 10^{-9} and at most 500 epochs. A separate validation set of N_{val} independent source-sensor pairs is generated from the same analytical solution and remains unseen during training; it serves exclusively for hyperparameter selection.

To quantify the accuracy of the XPIKAN surrogate against the analytical reference v_s^* , we employ three different metrics. We first evaluate the Mean Absolute Error, $\text{MAE} = \frac{1}{n} \sum_{i=1}^n |\hat{v}_s(\mathbf{y}_i) - v_s^*(\mathbf{r}_i, \boldsymbol{\tau}_i)|$, which reports the typical magnitude of the prediction residual. To complement this absolute measure, we also report the Relative Root Mean Square Error (or simply Relative L2):

$$\text{RRMSE}(\%) = \frac{\sqrt{\sum_{i=1}^n (\hat{v}_s(\mathbf{y}_i) - v_s^*(\mathbf{r}_i, \boldsymbol{\tau}_i))^2}}{\sqrt{\sum_{i=1}^n (v_s^*(\mathbf{r}_i, \boldsymbol{\tau}_i))^2}} \times 100, \quad (28)$$

which quantifies the error relative to the signal magnitude, and the Coefficient of Determination:

$$R^2 = 1 - \frac{\sum_{i=1}^n (\hat{v}_s(\mathbf{y}_i) - v_s^*(\mathbf{r}_i, \boldsymbol{\tau}_i))^2}{\sum_{i=1}^n (v_s^*(\mathbf{r}_i, \boldsymbol{\tau}_i) - \bar{v}_s^*)^2}, \quad (29)$$

with $\bar{v}_s^*$ denoting the sample mean of the reference values, that captures how well the model reproduces the spatial variation of the reference solution. All metrics are evaluated on a test set of source-sensor pairs that were not used during training or validation.

Beyond reporting pointwise accuracy metrics, we subjected the XPIKAN surrogate to a comprehensive battery of statistical validations designed to probe its robustness and physical reliability. These tests span four critical domains: predictive validity, which examines the absolute agreement with the analytical reference solution; architectural sensitivity, which quantifies how prediction quality varies with hyperparameter choices and how computational resources interact with model capacity; geometric robustness, which verifies that accuracy remains invariant across the entire spherical domain without systematic spatial bias; and physical fidelity, which directly measures adherence to Maxwell’s equations and the interface transmission conditions. The central physical evaluations are detailed below, and the Appendix A compiles the secondary sensitivity metrics. Table 2 summarizes all tests in the overall validation architecture.

Table 2. Statistical and physical validation scheme for the XPIKAN model.

Observations	Validation Domain	Key Finding	Statistical Method & Analysis
Observation 1	Global Accuracy	Generalization on unseen sensors with minimal bias	OLS regression (R^2), Pearson (r), CCC (ρ_c), Bland-Altman
Observation 2	Physical Fidelity	Sub-network adherence to interior elliptic PDEs	Normalized Laplacian residuals, MVP correlation (R^2)
Observation 3	Flux Continuity	Interface continuity & Neumann gauge preservation	TOST equivalence framework, Pearson correlation, t -test
Observation 4	Sensor & Source Density	Monotonic error reduction; 5-sensor spatial limit	Spearman, Power-law, Tukey’s HSD, interaction analysis
Observation 5	Source Depth Invariance	Depth-invariant predictive fidelity across shells	Jonckheere-Terpstra (JT) test
Observation 6	Noise Robustness	Decoupled predictive accuracy from target noise	Spearman correlation (ρ), linear regression
Observation 7	PI vs. Data-Driven	Robust regularization over data-driven baseline	Wilcoxon signed-rank, Mean RRMSE
Observation 8	Transfer Learning	Rapid conductivity adaptation via warm-start	Multi-objective loss convergence comparison
Observation A1	Loss Weight Sensitivity	λ_{Data} and λ_{Flux} dominate model accuracy	4-way ANOVA, Scheirer-Ray-Hare, Tukey’s HSD
Observation A2	Collocation Point Density	Discretization invariance across point densities	Multi-factorial variance decomposition
Observation A3	Fourier Feature Spectrum	Scale configuration is the primary accuracy driver	Two-way ANOVA, Tukey’s HSD
Observation A4	Spatial Generalization	Log-linear error decay with angular distance	Spearman correlation, Mann-Whitney U, Log-linear Reg.
Observation A5	Proximity Error	U-shaped error profile across source-sensor distance	Mann-Whitney U, pointwise error vs. D

Observation 1 (Global Accuracy & Agreement). *The model demonstrates stable generalization capabilities across both trained and completely unseen scalp sensors. On the independent evaluation set of 5000 coordinate pairs, the overall RRMSE error is 0.2572%. This level of performance is consistent with the individual sensor tracking curves shown in Figures 3 and 4. Ordinary Least Squares (OLS) regression of the predicted values against the analytical ground truth yields a highly aligned fit ($\hat{v}_s = 0.99979 v_s^* + 9.28059 \times 10^{-5}$), with a coefficient of determination $R^2 = 0.99999$. The estimated slope $\beta_1 = 0.99979$ is highly congruent with the ideal value of 1.0. Crucially, the OLS intercept ($\beta_0 = 9.28059 \times 10^{-5}$) is statistically non-significant ($p = 0.3223$), indicating the absence of any systematic offset or global translation bias in the network’s predictions. To ensure that the strong linear fit is not masking scaling or translation errors, we evaluated both the Pearson correlation coefficient (r) and Lin’s Concordance Correlation Coefficient (CCC, ρ_c). The Pearson correlation is $r \approx 1.00000$, and the concordance coefficient is $\rho_c = 0.99980$. Because ρ_c strictly penalizes deviations from the 45° identity line, this value confirms strong absolute agreement across the entire dynamic range of the scalp potentials. Furthermore, Bland-Altman agreement analysis reveals a negligible mean prediction bias of 9.24098×10^{-5} with a standard deviation of differences of 6.65079×10^{-3} . The 95% limits of agreement (LoA) span narrowly from -1.29431×10^{-2} to 1.31280×10^{-2} . Again, this tight boundary confirms that the prediction residuals remain small and uniformly distributed across the scalp domain, without presenting localized regions of high error variance.*

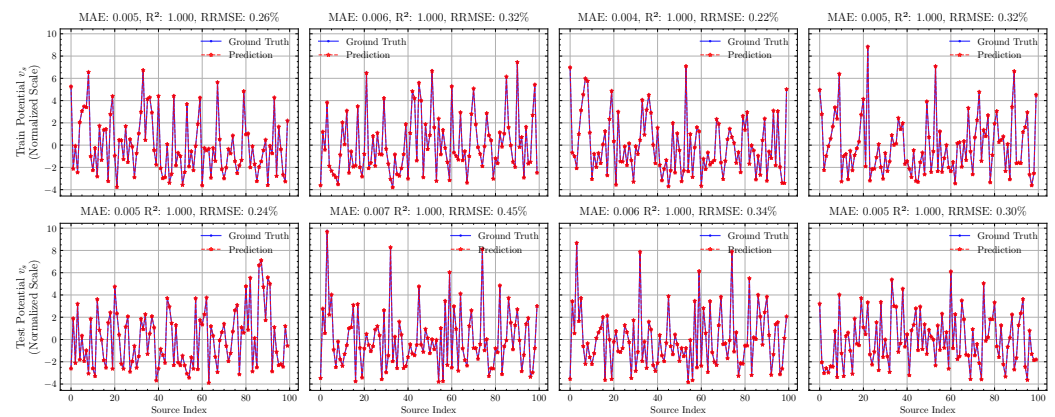


Figure 3. Spatial reconstruction performance of the XPIKAN model for a set of source locations within the brain. The top row displays the potential curves for sensors included in the training set, while the bottom row evaluates the model's generalization capabilities on completely unseen test sensors. Blue markers represent the analytical ground truth potential, which is compared against the red dashed lines representing the neural network predictions. Quantitative metrics, including the MAE and RRMSE, are provided for each subplot. The results demonstrate high-fidelity tracking of the auxiliary function across both training and testing regimes.

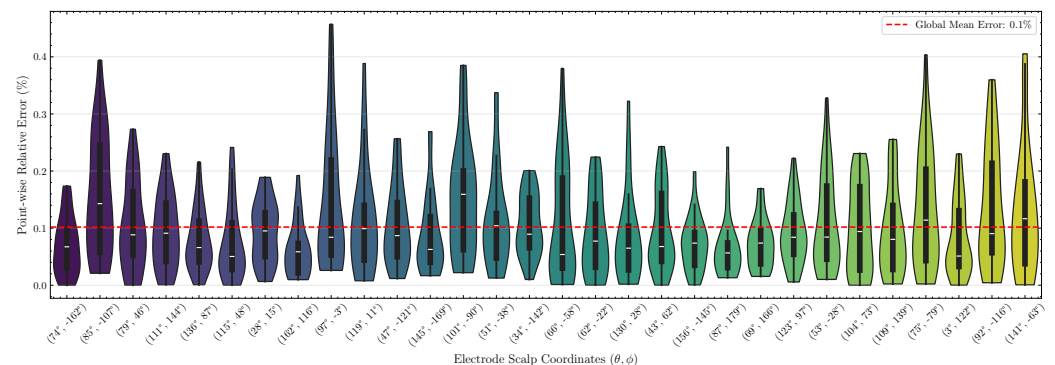


Figure 4. Spatial distribution of point-wise relative errors across the set of unseen test electrodes on the scalp. Each violin plot represents the error density for a specific electrode coordinate (θ, ϕ) , aggregated over multiple independent source locations within the cerebrum to demonstrate local reconstruction stability. The internal black box plots indicate the quartiles and median error values, while the outer kernel density estimate highlights the consistency of the model across varying source depths. A global mean error of approximately 0.1% is indicated by the red dashed line.

Observation 2 (Physical Fidelity). To ensure the validity of the network is not limited to arbitrary data fitting and that the model actively preserves the core PDEs, we evaluated both the local Laplacian residuals and the global Mean Value Property (MVP) across the three head compartments. As shown in Figure 5, the normalized Laplacian residuals are symmetrically centered around zero with tightly bounded variance, which confirms that the sub-networks satisfy the interior elliptic PDEs ($\Delta v_i = 0$) within their respective homogeneous domains. Furthermore, the harmonic nature of the learned potentials is verified by the strong alignment of the center potentials with the spherical shell averages, yielding a coefficient of determination of $R^2 = 0.9954$ in the cerebrum and $R^2 = 1.0000$ in the skull and scalp layers.

Observation 3 (Flux Continuity). To evaluate the physical fidelity of the XPIKAN model across the multi-compartment domain, we subjected the interface continuity jumps and boundary conditions to some statistical tests. Using the Two One-Sided Tests (TOST) equivalence framework with a strict 1% tolerance threshold (potential equivalence bound: $\pm 2.06 \times 10^{-2}$; flux equivalence bound: $\pm 7.56 \times 10^{-3}$), the model demonstrated significant mathematical continuity. At the brain–skull

interface, both the potential jump (mean: -1.71×10^{-3} , $p = 0.0061$) and the flux jump (mean: 1.47×10^{-3} , $p < 0.0001$) successfully rejected the non-equivalence null hypothesis. The physical compatibility extended to the skull–scalp interface, yielding equivalent potential (mean jump: -5.00×10^{-3} , $p = 0.0101$) and flux (mean jump: 7.51×10^{-4} , $p < 0.0001$) distributions. Analysis of the flux topology at the brain–skull boundary confirmed strong alignment between the input and output current fields (Pearson $r = 0.8169$, $R^2 = 0.6673$, intercept: -6.15×10^{-4}), with the linear slope of 0.0206 correctly reflecting the scaling behavior dictated by the low-conductivity skull compartment. While the standard deviation of the localized potential discontinuities at this interface was 2.46×10^{-1} , the high skewness (16.45) and kurtosis (385.50) of the distribution indicate that these larger residuals are highly isolated, occurring primarily near singular sources, rather than representing systematic boundary offsets. Finally, a one-sample t -test verified the stability of the Neumann gauge on the outer scalp boundary; the mean scalp potential (-8.89×10^{-3}) was statistically indistinguishable from zero ($t = -0.1623$, $p = 0.8711$, RMS: 2.45, bias-to-RMS ratio: 3.63×10^{-3}), confirming that the optimization process successfully preserves the zero-mean physical constraint without global drift.

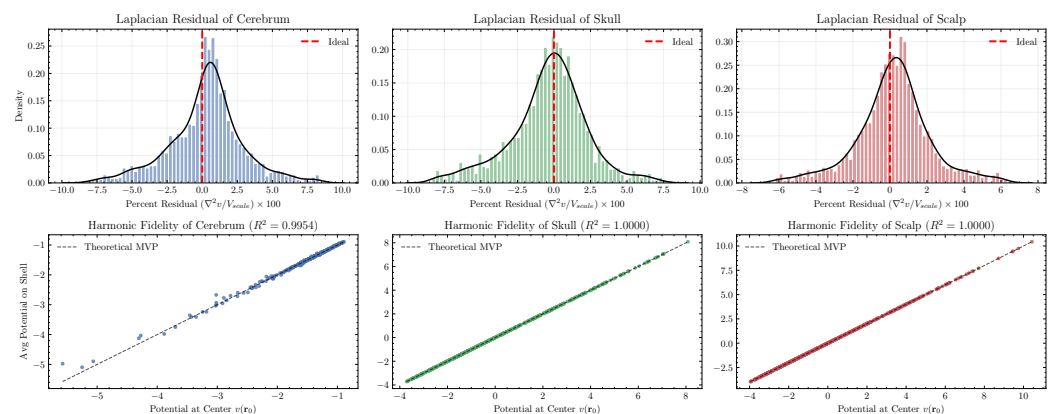


Figure 5. The physical consistency of the XPIKAN architecture is evaluated across the three head compartments: the cerebrum, skull, and scalp. The top row provides histograms and kernel density estimates of the normalized Laplacian residuals, verifying that the networks satisfy the governing Poisson/Laplace equations within their respective domains. In the bottom row, the harmonic nature of the learned fields is validated via the MVP, comparing the potential at a central point to the average potential on a surrounding shell. The high correlation ($R^2 \approx 1.0$) between the center potentials and shell averages across all layers indicates that the sub-networks have converged to a physically valid harmonic solution.

Observation 4 (Sensor & Source Density Scaling). *The model’s performance is robustly governed by the resolution of the observational and training data. We observe a strong, statistically significant monotonic relationship between resource density and error reduction. Spearman rank correlation coefficients confirm that increasing both the number of scalp sensors ($\rho = -0.60$, $p < 0.001$) and the number of training sources ($\rho = -0.60$, $p < 0.001$) consistently drives the reconstruction error down. Power-law fitting across the log-log resource domain reveals convergence rates of $\alpha_{\text{sens}} = 0.86$ and $\alpha_{\text{src}} = 0.99$. The near-linear scaling with respect to training sources indicates that the network’s expressive capacity is efficiently utilized to map the diverse dipolar configurations within the cerebrum. Detailed marginal gain analysis identifies a resolution threshold at 5 scalp sensors. The transition from 4 to 5 sensors yields the most substantial localized performance jump, with a 67.23% reduction in the median Test MAE. This threshold likely represents the spatial Nyquist limit required to resolve the low-frequency potential distributions on the scalp after the spatial low-pass filtering effect of the low-conductivity skull. While minor stochastic fluctuations are observed at intermediate densities, the overall trend follows a robust decay toward a global error floor at 25 sensors (maximum considered value for N_{sens}). Tukey’s HSD post-hoc testing confirms that*

beyond 5 sensors, the model enters a saturation phase where further increases in electrode density do not yield statistically significant improvements in reconstruction fidelity ($p > 0.09$ for comparisons between 5, 10, and 25 sensors). Furthermore, interaction analysis ($F = 182.96$, $p < 0.001$) confirms that the benefit of source density is strictly coupled to sensor resolution, suggesting that increasing source diversity can partially compensate for sparse sensor arrays in low-density setups.

Observation 5 (Source Depth Invariance). To establish a continuous profile of the model's predictive fidelity across the cerebral volume, we performed an ordered trend analysis using the Jonckheere-Terpstra (JT) test. The radial distance $\|\tau\|$ was partitioned into ten concentric decile shells, and the distribution of relative errors was evaluated for monotonic trends from the deep core to the cortical surface. The analysis yielded a JT statistic of 2356.0 with a corresponding p -value of 0.1793, failing to reject the null hypothesis of uniform error distribution. The median error slope in log-space was found to be negligible, indicating that the XPIKAN framework maintains strict depth invariance (Figure 6). The result demonstrates that the architecture successfully mitigates the near-field singularities associated with shallow cortical sources and provides statistically equivalent precision for both deep-seated and superficial neural activity.

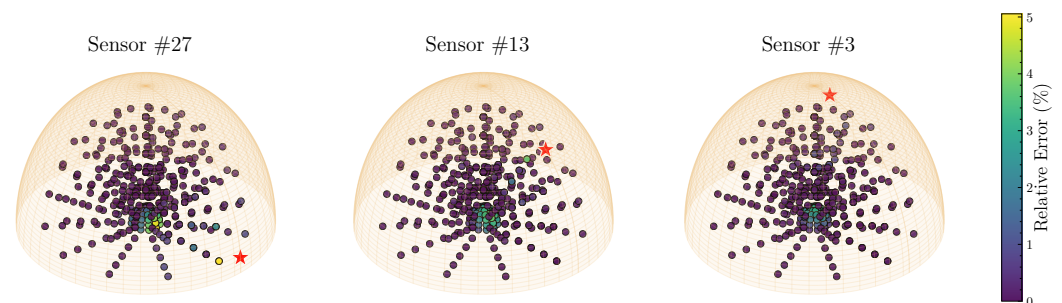


Figure 6. This visualization depicts the 3D distribution of relative reconstruction errors within the cerebrum for three specific scalp sensor locations. Each panel represents the upper hemisphere of the head model, where the red star indicates the registered position of the scalp electrode. The internal grid points represent potential source locations, colored according to their individual relative error percentages. It can be observed that the error remains low and uniformly distributed throughout the volume, with no significant inflation near the compartment interfaces or the coordinate center. The spatial stability validates that the inclusion of radial invariants and multi-scale Fourier features successfully mitigates the numerical singularities typical of EEG forward modeling. The shared colorbar confirms that the localized errors for all evaluated sensors remain well within acceptable clinical tolerances for source imaging.

Observation 6 (Noise Robustness). The regularizing efficacy of the XPIKAN framework was subjected to a large-scale robustness evaluation across a set of independent configurations, with target noise levels scaled from 0.5% up to 30% of the signal's standard deviation. Statistical analysis reveals a near-total immunity to target perturbations; the Spearman rank correlation between noise intensity and reconstruction error is notably weak ($\rho = 0.1785$), and linear regression yields a negligible error inflation slope of 0.0742%. The metrics indicate that the predictive accuracy of the model remains effectively decoupled from the noise floor of the training data ($R^2 = 0.0004$). With a mean Robustness Ratio of 1.20, the architecture demonstrates a self-correcting behavior where the physics-informed Laplacian and boundary constraints act as a rigorous spatial filter.

Observation 7 (Physics-Informed vs. Pure Data-Driven). To demonstrate the advantage of the XPIKAN framework over standard neural approximations, we performed a head-to-head comparison of XPIKAN against a pure data-driven surrogate model under a noise level of 5% and different numbers of training sensors. The results of the Wilcoxon signed-rank test ($p = 1.57 \times 10^{-3}$) confirm the statistical superiority of the XPIKAN, showing an average error reduction of 37.50% across

various sensor configurations. While the pure surrogate model relied solely on data interpolation, leading to a high Mean RRMSE of 33.17% at sparse sensor densities, the XPIKAN effectively utilized the embedded physical laws to regularize the solution, reducing the error to 13.14%.

Observation 8 (Transfer Learning for Conductivity Adaptation). To evaluate the model's adaptability to physiological variations, we implemented a transfer learning paradigm designed to address uncertainties in tissue conductivities, such as the $\pm 20\%$ variance for the skull-to-brain conductivity ratio [45–47]. In this setting, when a new personalized conductivity profile (σ) is introduced, the interior harmonic properties ($\Delta v_i = 0$) remain invariant, while only the transmission conditions at the compartment boundaries are perturbed. Utilizing a warm-start approach, the XPIKAN is initialized with the weights of a pre-trained baseline model rather than random values [48]. Because the network has already learned the underlying geometric invariants and spatial coordinate mappings, the optimization process only needs to adjust the parameters corresponding to the updated potential and flux gradients at the interface boundaries. As shown in Figure 7, this transfer learning strategy allows the network to adapt to a perturbed physical state in a fraction of the original training time.

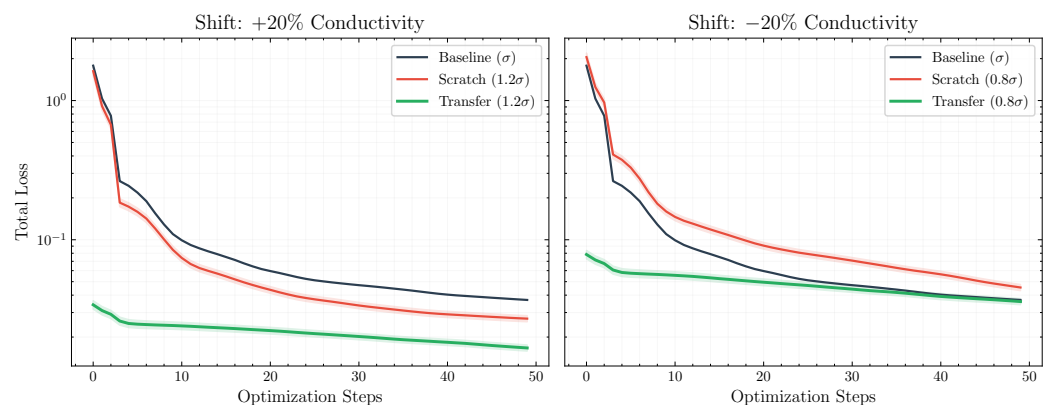


Figure 7. Robustness to Conductivity Uncertainty and Transfer Learning Efficiency. Convergence of the total loss functional is shown for a $\pm 20\%$ variation in the tissue conductivity ratio. The blue curve represents the baseline model (σ), while the red curves show optimization from scratch for the perturbed physical systems (1.2σ and 0.8σ). The green curves demonstrate the “warm-start” capability of the XPIKAN; by initializing weights from the baseline pre-trained state, the model converges to the new physical solution significantly faster than training from scratch. Shaded areas indicate the standard deviation of the loss.

Performance and Robustness Comparison

To evaluate the practical viability of the proposed model, we benchmarked the XPIKAN framework against both a standard FEM solver (constructed with 34,026 nodes) and a conventional, single-domain MLP-based PINN architecture. Table 3 summarizes these results. The XPIKAN architecture offers a highly competitive balance between physical accuracy and online computational throughput. While traditional numerical techniques such as the FEM are mathematically reliable for isolated, stationary solves, their execution latency per forward solve scales unfavorably when deployed in iterative inverse source localization routines that require millions of evaluations. Conversely, while MLP-PINNs offer faster evaluation times and lower memory requirements, they suffer from spectral bias. Because a standard single-domain MLP acts as a globally smooth function, it fails to resolve the sharp C^1 discontinuities in the potential field at the interfaces between tissue layers with highly contrasting conductivities.

In contrast, the XPIKAN surrogate achieves high accuracy at the tissue boundaries and delivers real-time inference throughput. This accuracy requires a larger offline training

overhead, which demands a higher initial memory footprint and longer training periods than standard MLPs. Because this computational cost remains entirely within an offline initialization phase, the overhead does not limit the potential real-time utility of the framework in future clinical settings. We performed a stability analysis across five independent optimization runs with randomized parameter initializations, which showed that the XPIKAN is highly stable. The model achieved a standard deviation in relative evaluation error of only $\pm 0.04\%$. This high stability, combined with an online evaluation throughput that is several orders of magnitude faster than traditional solvers, shows that the model can serve as a fast, meshless continuous surrogate. Therefore, it removes the necessity of solving large linear systems on discretized grids and prevents topological meshing failures, such as boundary intersections, which commonly destabilize BEM under personalized head configurations.

Table 3. Performance comparison across classical (FEM), conventional neural (MLP-PINN), and proposed (XPIKAN) frameworks. Metrics include inference throughput, memory overhead, and robustness statistics derived from five randomized training sessions. Memory values represent peak system (CPU) RAM usage during inference to ensure clinical relevance. PINN training was performed on a GPU; inference on 10^4 points was benchmarked on CPU for a fair comparison with FEM. For applications that require rapid offline training with acceptable accuracy, an extended MLP-PINN (XPIMLP) with augmented features represents a viable alternative, although its accuracy remains lower than the proposed XPIKAN. Bold cells indicate the best-performing framework for each metric.

Aspect	Metric	Sparse FEM	MLP-PINN	XPIKAN
Computational Efficiency	Peak Inference Memory	~ 10.0 MiB	~ 25.0 MiB	~ 300.0 MiB
	Inference Time	~ 60 s	0.5 s	2.0 s
	Scalability (Mesh Density)	Linear ($O(N)$)	Independent	Independent
Accuracy & Robustness	MAE	Reference	5.1×10^{-3}	2.7×10^{-3}
	R^2	Reference	0.980	0.999
	Relative L2 Error	Reference	3%	<1%
	Std. Dev.	Deterministic	$\pm 1.8\%$	$\pm 0.05\%$
Practical Utility	Mesh Dependency	Required	Meshless	Meshless
	Online Real-time Suitability	No	Yes	Yes

5. Conclusions

In this study, we presented a preliminary analysis of an extended physics-informed Kolmogorov–Arnold network to solve the geometry-dependent auxiliary function $v_s(\mathbf{r}, \boldsymbol{\tau})$ for the three-layer spherical EEG forward problem. Our results indicate that the XPIKAN framework has the potential to serve as a computationally efficient alternative to traditional numerical techniques such as the boundary element and finite element methods. The optimization strategy minimized a composite loss function integrating unsupervised physics residuals (the Laplacian and boundary flux conditions) with a sparse set of supervised anchor values derived from the exact analytical solution. By augmenting the inputs with multi-scale Fourier feature mappings and spatial geometric invariants, the network successfully captured the complex directional sensitivity of the field relative to $\mathbf{r} \cdot \boldsymbol{\tau}$.

From a clinical workflow perspective, the proposed physics-constrained surrogate paves the way for potential future integration into MRI-to-EEG pipelines. In this scheme, a patient-specific head model could be constructed once to generate a sparse dataset of interior collocation and boundary points. The XPIKAN then learns the continuous geometry of the compartments and provides an instantaneous forward solver that could eventually facilitate real-time, bedside source localization diagnostics. The tight integration of physics also yielded a substantial advantage in sample complexity over purely data-driven approaches.

A major advantage of this physics-informed approach over purely data-driven neural network surrogates [11,12] is its outstanding sample efficiency. For instance, the purely data-driven model presented in [11] required a total of 890,807 training samples to construct the forward mapping. In contrast, the XPIKAN framework achieved high accuracy utilizing about 1000 expensive source-sensor sampling points. This efficiency stems from the model's ability to embed the governing physical laws directly into the loss landscape, significantly reducing the reliance on dense grid generations from expensive numerical solvers. Ultimately, the XPIKAN behaves as a differentiable functional surrogate, transforming discrete numerical outputs into a continuous, mesh-free representation.

Despite these advantages, several limitations of the current study must be acknowledged. First, the present validation is restricted to a concentric spherical geometry with isotropic conductivities, which does not fully capture the complex gyral patterns and anisotropic white matter tracts of the human brain. While the XPIKAN demonstrates high accuracy on this benchmark, its performance in the presence of highly complex, non-convex boundaries remains to be tested. Furthermore, while the model is robust to observational noise, the current optimization relies on a limited set of analytical anchor points to resolve the Neumann gauge; for realistic head geometries where such analytical solutions do not exist, these anchors must be sourced from potentially expensive numerical simulations. Finally, the offline training phase, while occurring only once per patient, still requires several minutes of optimization, which may pose a bottleneck in extremely time-sensitive clinical scenarios.

Future work will focus on extending this framework to anisotropic media, layered ellipsoidal geometries, realistic MRI-derived head models, and Bayesian PINNs to provide confidence intervals for each predicted scalp potential. Beyond piecewise-constant conductivity profiles, the framework can also be extended to fully inhomogeneous conductivity fields $\sigma(\mathbf{r})$ derived from diffusion-weighted MRI, as well as to pathological cases such as skull defects or intracranial tumors that locally perturb the conductivity landscape. To scale this approach to population-level studies without requiring case-by-case offline optimization, future investigations may explore combining KAN-based architectures with neural operators, such as DeepONets or Fourier Neural Operators, to directly map variable anatomical geometries and conductivity fields to their corresponding forward solutions.

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Appendix A

Observation A1 (Loss Weight Sensitivity). To identify the governing components of the multi-objective loss function, we conducted a 4-way full factorial sensitivity analysis across the weighting parameters λ_{PDE} , λ_{BC} , λ_{Flux} , and λ_{Data} . A 4-way ANOVA on the log-transformed Test MAE reveals that the data-fidelity weight (λ_{Data}) is the primary determinant of model accuracy and accounts for a dominant proportion of the error variance ($\eta_p^2 = 0.8036$, $F = 330.04$, $p < 0.001$). Among the physics-informed constraints, the interface flux weight (λ_{Flux}) exerts the most substantial influence ($\eta_p^2 = 0.4361$, $F = 62.38$, $p < 0.001$), proving that current conservation across the brain-skull-scalp boundaries is more critical for convergence than the internal Laplacian or potential jump constraints. These findings are further corroborated by the non-parametric Scheirer-Ray-Hare test, which confirms the high statistical significance of the Data ($H = 163.95$, $p < 0.001$), Flux ($H = 27.90$, $p < 0.001$), and PDE ($H = 17.39$, $p < 0.001$) terms. Crucially, the interaction analysis between λ_{BC} and λ_{Data} yields a non-significant result ($F = 0.486$, $p = 0.883$), indicating that the physics-based regularizers and the observation data provide independent, non-conflicting signals for the optimization process. Post-hoc evaluation via Tukey's Honestly Significant Difference (HSD) confirms a consistent, monotonic improvement in reconstruction accuracy as λ_{Data} increases from 1 to 1000 (all pairwise $p < 0.001$). In contrast, the Tukey HSD for the boundary weight (λ_{BC}) reveals no significant pairwise differences ($p > 0.05$) between weight levels, suggesting that the XPIKAN architecture maintains a high degree of stability and is relatively robust to the specific scaling of the Dirichlet boundary transmission constraints within the tested range.

Observation A2 (Collocation Point Density). A multi-factorial variance decomposition was performed on a pooled dataset of independent training configurations to isolate the drivers of model accuracy. The analysis reveals that the XPIKAN framework exhibits a high degree of discretization invariance; specifically, the densities of the interior Laplacian collocation points (N_{Ω}) and boundary transmission points (N_{Γ}) accounted for less than 0.1% of the total error variance ($p > 0.40$). The results suggest that the physics-informed KAN architecture effectively learns the underlying potential field from the analytical constraints without requiring dense spatial meshes.

Observation A3 (Fourier Feature Spectrum Tuning). To evaluate the influence of coordinate spectral parameters on the forward model's accuracy, a two-way factorial ANOVA was performed across the scale configurations ($\mathfrak{S}$) and projection mapping sizes ($\mathfrak{M}$). The analysis revealed that the choice of scale configuration is the primary determinant of reconstruction accuracy ($F(10, 158) = 13.75$, $p < 0.001$, $\eta_p^2 = 0.465$). The projection mapping size also exerted a highly significant main effect ($F(3, 158) = 21.93$, $p < 0.001$, $\eta_p^2 = 0.294$). Crucially, a significant interaction effect was observed ($F(30, 158) = 2.11$, $p = 0.0017$, $\eta_p^2 = 0.286$), indicating that the optimal projection dimensionality is tightly coupled to the bandwidth of the spectral scales. Post-hoc pairwise comparisons using Tukey's HSD test demonstrated that a scale setting of $\mathfrak{S} = \{1.0\}$ performed significantly worse than all other tested configurations, which included smaller scales ($p < 0.001$), increasing the average log-RRMSE by approximately 0.45 units (corresponding to a near three-fold increase in relative error). In contrast, pairwise differences among lower-frequency scales (≤ 0.1) and broader multi-scale combinations (such as $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$) were statistically non-significant ($p > 0.05$).

Observation A4 (Single-Sensor Spatial Generalization). We evaluated the spatial generalization of the data-fidelity anchor by measuring prediction residuals in concentric rings centered at the sole training coordinate $\mathbf{r}_{\text{train}}$. The model demonstrates exceptional local stability, maintaining a median relative error of $\approx 4\%$ within a 0.5° proximity. Statistical analysis reveals a near-perfect monotonic relationship between angular displacement and error inflation (Spearman $\rho = 0.9342$, $p < 0.001$), identifying a precise capture radius beyond which predictive fidelity decays.

Log-linear regression identifies a spatial decay constant of $\alpha = 0.1281$ per degree ($R^2 = 0.6074$), implying that the reconstruction error increases by a factor of e for every $\approx 7.8^\circ$ of displacement. Mann-Whitney U testing confirms a statistically significant $13.06\times$ increase in error between the immediate sensor neighborhood and the local fringe ($p < 0.001$). The statistical tests show that while the physics-informed constraints successfully solve the local boundary value problem, a distributed multi-sensor array is required to calibrate the global potential field across the scalp domain.

Observation A5 (Proximity-Dependent Error Amplification). While the global JT test demonstrates that average error remains uniform across radial depth, evaluating localized sensor-source pairings reveals critical physical boundaries. We systematically analyzed the point-wise relative error as a function of the exact Euclidean distance $D = \|\mathbf{r} - \boldsymbol{\tau}\|$ between matched source-sensor pairs. The error profile exhibits a distinct U-shaped curve, revealing two distinct numerical challenges. At close proximities ($D \leq 0.20$), we observe a statistically significant increase in median relative error (5.78% vs. 1.68% in the far-field; Mann-Whitney U test, $p = 3.77 \times 10^{-11}$, rank-biserial effect size $r_{rb} = 0.594$). Conversely, at maximum distances ($D \geq 0.70$), where the source resides in the opposite hemisphere, relative errors rise due to far-field potential attenuation, where near-zero target values inflate the relative error denominator. Optimal reconstruction fidelity is consistently achieved at intermediate distances ($0.25 < D < 0.40$), representing a physical sweet spot where the field is both geometrically stable and sufficiently strong.

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