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Surrogate-Assisted Reliability, Optimization, and Parameter Back-Analysis in Geotechnical Engineering: A State-of-the-Art Synthesis

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Abstract

Surrogate metamodeling in geomechanics has reached a critical structural turning point. While legacy approximation frameworks built upon static, linearizing response surfaces historically optimized computational workflows, their structural failure is evident when navigating the high-dimensional parameter spaces, severe multi-physics couplings, and localized non-linear failure envelopes typical of real-world infrastructure assets. A highly rigorous, state-of-the-art critical synthesis is delivered in this paper, breaking away from redundant historical tracking to chart the 2024–2026 data-driven frontier. A definitive, comparative taxonomy of six core metamodel variants is established: Polynomial Response Surfaces (PRSM), Radial Basis Functions (RBF), Kriging (KSM), Artificial Neural Networks (ANN), Support Vector Regression (SVR), and Moving Least Squares (MLSM). Crucially, the limitations of traditional frameworks are exposed, and the paradigm shift toward sequential active learning loops, multi-fidelity information fusion, and Physics-Informed Neural Networks (PINNs) is decoded. The operational execution of these advanced hybrid architectures is dissected across three core pillars: low-probability geotechnical reliability analysis under spatial variability (Random Fields), generative multi-objective design optimization, and real-time parameter inverse back-analysis for digital twin deployment. Finally, current structural bottlenecks — including curse-of-dimensionality limits, numerical noise filtering, and automated hyper-parameter tuning (AutoML) — are critically cross-examined. By bridging the gap between historical

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foundational mechanics and modern intelligent computing, a definitive strategic roadmap is provided for resilient and predictive geotechnical engineering.

Keywords: Metamodeling lineage; Data-driven geotechnics; Physics-Informed Machine Learning (PINN); Active learning schemes; Real-time parameter inversion; Multi-fidelity co-kriging.

1. Introduction

The integration of surrogate modeling—or metamodeling—in civil engineering traces its roots back to the structural optimization breakthroughs of the late 20th century. Originally conceptualized to resolve highly non-linear multidisciplinary design constraints, these mathematical approximations have evolved into an indispensable core paradigm within contemporary data-driven geomechanics [1, 2]. In geotechnical engineering, boundary value problems are inherently complex, governed by severe material anisotropy, spatial variability of soil strata, and intricate hydro-mechanical couplings. When high-fidelity numerical models, such as advanced Finite Element Methods (FEM), are embedded into iterative stochastic frameworks like Monte Carlo Simulations (MCS), the computational footprint quickly becomes prohibitive. To bypass this bottleneck, surrogate models construct a computationally lightweight, mathematically elegant mapping between high-dimensional soil input parameters and structural response vectors [3, 4].

However, a critical rift has emerged between historical implementation strategies and modern infrastructural demands. Early literature relied extensively on explicit Polynomial Response Surface Methodologies (PRSM) and static Design of Experiments (DoE) [5, 6]. While these pioneering approaches laid the groundwork for approximation theory, recent literature (2024–2026) demonstrates that legacy static frameworks struggle significantly when mapping localized, highly non-linear failure envelopes typical of progressive slope failures or deep mechanized tunneling [7, 8]. This limitation has driven an innovative paradigm shift. Instead of treating the surrogate as a passive, purely statistical data-fitting tool, contemporary frameworks leverage dynamic, data-enabled architectures. Classic Kriging (KSM) and Support

Vector Regression (SVR) are now being hybridized with Deep Learning topologies and Physics-Informed Neural Networks (PINNs) [9].

To clearly understand this evolution, Table 1 establishes a critical comparison between the historical baseline methods and emerging modern solutions.

Table 1: Methodological shift in geotechnical surrogate modeling paradigms

Dimension	Historical Baseline (Legacy)	Modern Framework (2024–2026)
Sampling Philosophy	Static, space-filling DoE (LHS, Orthogonal Arrays)	Sequential, active learning (Adaptive refinement at limit states)
Mathematical Nature	Purely data-driven / statistical (Black-box interpolation)	Physics-informed / Hybrid (Governed by constitutive laws & PDEs)
Dimensionality Capacity	Low-dimensional spaces (Suffers from curse of dim.)	High-dimensional, multi-scale Big Data structures

This transition from static to adaptive learning has radically redefined the operational execution of three major pillars in geomechanics:

- (i) Geotechnical Reliability Analysis: Traditional first-order methods (FORM) fail under highly non-linear limit state functions [10, 11]. Modern adaptive surrogates resolve this by executing active learning loops that intelligently sample data points exclusively near the failure boundary, providing MCS-level accuracy for low-failure-probability infrastructures with a fraction of the cost [12].
- (ii) Geotechnical Design Optimization: Early optimization relied on single-objective, rigid functions [13]. Recent state-of-the-art applications utilize multi-fidelity surrogates coupled with heuristic evolutionary algorithms, enabling real-time cost-safety optimization under strict regulatory uncertainties.
- (iii) Inverse Parameter Back-Analysis: Classical back-analysis suffered from ill-posed mathematical conditions due to sparse field data. Modern frameworks combine real-time field monitoring instrumentation (e.g., automated inclinometer arrays) with high-speed proxy models to execute real-time inverse calibration of constitutive soil parameters, unlocking the true potential of the geotechnical observational method.

Despite the rapid expansion of this field, existing review papers exhibit significant redundancy, frequently replicating the structure, mathematical expressions, and conclusions of early reviews without critically analyzing recent structural breakthroughs. This paper directly addresses this gap. Rather than providing a purely historical chronicle or an isolated look at machine learning, this manuscript offers an independent, current, and balanced synthesis that critically bridges foundational metamodeling with the 2024–2026 data-enabled frontier. The manuscript is organized as follows: Section 2 formalizes the mathematical continuity from legacy formulations to modern active learning schemes; Section 3 analyzes explicit comparative applications in reliability, optimization, and real-time inversion; and Section 4 synthesizes

current computational bottlenecks, explicitly charting the deployment of physics-informed surrogates for digital twins in underground engineering.

2. Surrogate model approach

2.1 The basic principles of the surrogate model approach

The operational architecture of surrogate metamodeling in geomechanics relies on constructing a mathematically continuous, high-fidelity approximation that maps a high-dimensional input vector to its corresponding structural or behavioral response. While specific boundary conditions and material models vary across different geotechnical scenarios, the unified objective is to substitute a computationally expensive numerical simulator (e.g., non-linear FEM/FDM) with an analytical proxy $\hat{y}(X)$ that executes almost instantaneously.

Formally, let $X = [x_1, x_2, \dots, x_n]^T \in \mathbb{R}^n$ represent the vector of n independent geotechnical design variables or uncertain parameters (such as friction angle ϕ , cohesion c , or Young's modulus E). The feasible domain Ω is bounded by explicit hyper-rectangular constraints defined by lower and upper operational limits:

$$\Omega = \prod_{i=1}^n [x_i, L, x_i, U] \quad (1)$$

The fundamental implementation workflow is systematically executed through a three-stage mathematical paradigm:

(1) Spatial Discretization and Design of Experiments (DoE): The continuous high-dimensional space Ω is sampled using advanced space-filling experimental designs to select a finite sequence of m initial trial points. The design matrix X is formulated as:

$$X = [X^{(1)}, X^{(2)}, \dots, X^{(m)}]^T \in \mathbb{R}^{m \times n} \quad (2)$$

Historically, orthogonal arrays and uniform test designs were utilized to secure deterministic spacing [5, 6]. In modern data-driven geotechnics, these have been largely superseded by stochastic space-filling algorithms, primarily optimized Latin Hypercube Sampling (LHS) or Sobol' sequences, which maximize the minimum distance between sample points to prevent data clustering in uninformative sub-regions [3].

(2) High-Fidelity Numerical Evaluation: Each discrete experimental coordinate $X^{(i)}$ is processed through the true deterministic or stochastic geotechnical solver $\mathcal{M}(x)$ (e.g., a complex elastoplastic finite element mesh computing tunnel settlement or slope safety factors). This yields a corresponding vector of exact physical responses Y :

$$Y = [y^{(1)}, y^{(2)}, \dots, y^{(m)}]^T \in \mathbb{R}^m \text{ where } y^{(i)} = \mathcal{M}(X^{(i)}) \quad (3)$$

(3) Metamodel Synthesis: Utilizing the paired dataset $D = \{X, Y\}$, an analytical surrogate model is trained to yield an efficient function approximation $\hat{y}(X)$ such that:

$$y = \hat{y}(X) + \varepsilon(X) \quad (4)$$

where $\varepsilon(X)$ denotes the total residual error framework, encapsulating both the epistemic approximation bias and numerical solver noise.

The mathematical deployment of Eq. (4) diverges into three specialized computational frameworks depending on the target engineering objective:

A. Multi-Objective and Constrained Optimization

For single-objective geotechnical optimizations, $\hat{y}(X)$ represents the exact proxy of the cost or safety function. In multi-objective design spaces (e.g., minimizing deep excavation cost while simultaneously minimizing structural wall deflection), a distinct, independent surrogate model must be constructed for each individual objective vector [14]. When the system is governed by complex, highly non-linear constraints, handling them independently via traditional methods often degrades algorithmic stability [15]. To circumvent this, contemporary optimization frameworks employ dynamic penalty function formulations, unifying the non-linear constraints directly into a modified objective function:

$$F(X) = \hat{y}(X) + \sum_{j=1}^k \lambda_j \max(0, g_j(X))^2 \quad (5)$$

where $g_j(X) \leq 0$ denotes the j -th structural constraint equation, and λ_j represents a dynamically scaled penalty multiplier [16]. To maximize global convergence and eliminate localized stagnation, modern frameworks do not rely solely on static training; they deploy active learning loops. Historical trial data points drive sequential infill criteria (e.g., Expected Improvement or Upper Confidence Bound), injectively adding new high-fidelity samples into region clusters near the predicted global optimum, thereby boosting local accuracy.

B. Geotechnical Reliability Analysis

Within probabilistic geomechanics, Eq. (4) is formulated directly as the structural limit state function $G(X) = \hat{y}(X)$, where $G(X) \leq 0$ defines the failure envelope. Traditional reliability computations, such as the First-Order Second-Moment method (FOSM), assume a linear approximation at the design center point [17]. However, under severe soil non-linearity, these legacy methods exhibit massive divergence. By substituting the implicit limit state with the hyper-speed proxy $\hat{y}(X)$, crude Monte Carlo Simulations (MCS) can evaluate billions of stochastic samples within seconds, yielding stable and mathematically rigorous failure probabilities (P_f) even within ultra-low probability regimes [18]:

$$P_f = \int_{G(X) \leq 0} f_X(X) dX \approx \frac{1}{N_{mcs}} \sum_{k=1}^{N_{mcs}} I[\hat{y}(X^{(k)}) \leq 0] \quad (6)$$

where $f_X(X)$ is the joint probability density function, and $I[\cdot]$ is an indicator function.

C. Parameter Inverse Back-Analysis

In inverse geomechanics, laboratory testing fails to capture macro-scale geological formations, necessitating real-time field-calibration. After constructing the rapid forward surrogate $\hat{y}(X)$ to predict field instrumentation responses (e.g., inclinometer displacements or pore-water pressure fields), the parameter inversion is cast as a mathematical optimization problem. The target constitutive soil parameters are back-calculated by minimizing the objective function formulated as the weighted sum of squared residuals (WSSR) between the field observations and proxy predictions:

$$X^* = \arg \min_{X \in \Omega} \sum_{i=1}^{N_{obs}} \omega_i \left[y_{obs}^{(i)} - \hat{y}^{(i)}(X) \right]^2 \quad (7)$$

where $y_{obs}^{(i)}$ is the real-time measured geotechnical deformation at sensor location i , and ω_i represents the observational instrumentation reliability weight. Because $\hat{y}(X)$ evaluates instantly, optimization algorithms can iteratively calibrate material profiles in real-time, executing the geotechnical observational method dynamically during active construction phases.

2.2 Types of surrogate models

The structural taxonomy of geomechanical metamodeling encompasses a diverse spectrum of mathematical approximation structures. Historically, these frameworks functioned as static mathematical interpolators. However, recent developments between 2024 and 2026 have shifted the paradigm toward physics-guided, adaptive-scale, and multi-fidelity formulations capable of mapping highly non-linear geotechnical responses.

(1) Polynomial Response Surface Methodology (PRSM)

The PRSM surrogate architecture maps the non-linear relationship between high-dimensional geotechnical input vectors and structural objective responses through multi-variable polynomial expansions. Representing the traditional baseline, a complete quadratic response surface is mathematically formalized as:

$$\hat{y}(X) = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j \quad (8)$$

where β_0 , β_i , β_{ii} , and β_{ij} represent the unknown regression coefficients to be calibrated; x_i denotes the i -th independent design variable; $\hat{y}(X)$ is the predicted system response; and k represents the total spatial dimensionality of the input parameters.

When the cardinality of the high-fidelity training dataset m strictly exceeds the number of unknown polynomial coefficients, these parameters are explicitly resolved using ordinary least-squares (OLS) estimation. While Eq. (2) performs adequately in low-dimensional spaces ($k \leq 3$), it suffers severely from the curse of dimensionality. The total number of parameters to be estimated escalates exponentially according to the formulation $2k + 1 + k(k-1)/2$.

To mitigate computational decline, legacy frameworks omitted the cross-product terms (β_{ij}). However, recent critical studies confirm that removing cross-terms introduces severe epistemic bias when modeling highly non-linear geotechnical configurations, such as progressive slope failures or deep anisotropic tunnel stability [19, 7]. Consequently, contemporary data-driven geotechnics has largely transitioned from classical PRSM toward Sparse Polynomial Chaos Expansions (PCE), which dynamically retain only the most influential interactive terms [20].

(2) Radial Basis Function (RBF)

The RBF network functions as a discrete, multi-variable deterministic interpolation framework. The predicted response is governed directly by the spatial Euclidean distance computed

between the unobserved coordinate vector and the historical training nodes. The global RBF topology is built through the linear superposition of localized kernel responses:

$$\hat{y}(X) = \sum_{i=1}^m \lambda_i \Psi(\|X - X^{(i)}\|) \quad (9)$$

where λ_i represents the deterministic weight coefficient corresponding to the i -th experimental trial point; $\|X - X^{(i)}\|$ denotes the explicit Euclidean norm between the target evaluation vector x and the sample node $X^{(i)}$; m is the total volume of sample points; and Ψ represents the characteristic radial basis kernel function.

The operational generalization capability of the RBF model depends on selecting an appropriate kernel architecture (e.g., multiquadric, Gaussian, or cubic) and calibrating its shape parameter. Traditional applications treated these parameters as global constants, leading to severe localized smoothing or numerical instability. To resolve this structural bottleneck, recent literature has introduced Adaptive-Scale Localized RBF networks [8, 21]. These modern formulations dynamically tune the localized shape parameters based on dense regional sampling data, vastly improving localized gradient capture across complex, sharp material interfaces in stratified rock and soil formations.

(3) Kriging Surrogate Model (KSM)

The KSM framework, rooted in spatial geostatistics, operates as a localized, minimum-variance unbiased estimator. It decomposes the target black-box function into a deterministic global trend and a localized stochastic fluctuation component. The localized prediction at an unobserved position is formulated through linear weighting of known experimental points:

$$\hat{y}(X) = \sum_{i=1}^m \lambda_i y^{(i)} = \lambda^T Y \quad (10)$$

where $\lambda = [\lambda_1, \lambda_2, \dots, \lambda_m]^T$ represents the vector of optimized Kriging weights, and $y^{(i)}$ denotes the exact high-fidelity response value extracted from numerical solvers [22, 23].

To ensure unbiased estimation under minimum variance criteria, the expected value of the estimator must equal the true response, forcing the sum of weights to equal unity while minimizing the mean squared error estimation variance:

$$E[\hat{y}(X) - y(X)] = 0 \quad (11)$$

$$Var[\hat{y}(X) - y(X)] = E[(\lambda^T Y - y(X))^2] - 2\lambda^T \gamma + \gamma_0 \quad (12)$$

where γ represents the spatial correlation vector between the training points and the target prediction coordinate, and γ_0 is the process variance. Incorporating the Lagrange multiplier $\emptyset$ to resolve this constrained optimization problem yields the system of equations that defines the Kriging weights:

$$\begin{bmatrix} R & 1 \\ 1^T & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \emptyset \end{bmatrix} = \begin{bmatrix} \gamma \\ 1 \end{bmatrix} \quad (13)$$

where R represents the symmetric spatial correlation matrix capturing dependencies between all pairs of historical training points. Modern implementations favor the Gaussian exponential correlation kernel:

$$R(X^{(i)}, X^{(j)}) = \exp \left[- \sum_{l=1}^k \theta_l |x_l^{(i)} - x_l^{(j)}| p_l \right] \quad (14)$$

where θ_l and p_l represent the hyper-parameters governing the correlation range and smoothness along the l -th spatial dimension.

While optimizing these hyper-parameters via Maximum Likelihood Estimation (MLE) enhances model robustness [24], standard single-fidelity Kriging exhibits severe performance drops when handling noisy or sparse geotechnical datasets. To bridge this gap, state-of-the-art literature has advanced toward Deep Multi-Fidelity Co-Kriging (MFK) [12, 25]. MFK architectures integrate massive volumes of low-fidelity numerical data (e.g., coarse-mesh FEM) with a highly sparse selection of high-fidelity data (e.g., fine-mesh elastoplastic FEM and actual field tests), filtering out numerical noise while significantly reducing computational costs.

(4) Artificial Neural Network (ANN)

The ANN surrogate represents a non-parametric, parallel-distributed computational architecture inspired by biological neural processing systems. Its primary strength lies in its universal approximation capacity, enabling it to map highly non-linear, multi-scale geotechnical data without requiring an explicit mathematical formulation of the target function.

The fundamental feedforward processing mechanism within a single neuron maps input vectors X to an output y through the following mathematical transformation:

$$y = f \left(\sum_{j=1}^n \omega_{ij} x_j + \theta_i \right) \quad (15)$$

where x_j denotes the incoming signal from the j -th neuron of the preceding layer; ω_{ij} represents the synapse weight matrix; θ_i is the activation bias or threshold parameter; and f denotes the non-linear activation function (such as the hyperbolic tangent, Sigmoid, or modern Rectified Linear Unit, ReLU).

In traditional geotechnical applications, network training relied almost exclusively on standard Back-Propagation (BP) algorithms utilizing gradient descent to minimize output mean squared errors. However, recent critical evaluations highlight that classical shallow BP networks suffer from severe overfitting, vanishing gradients, and poor generalization when trained on sparse, highly uncertain soil parameters. To overcome this limitation, contemporary deep learning frameworks have shifted from purely data-driven ANNs to Physics-Informed Neural Networks (PINNs) [9, 26]. By embedding governing differential equations, boundary conditions, and geomechanical conservation laws directly into the loss function of Eq. (9), PINNs ensure that predictions remain physically consistent even under sparse or incomplete data regimes.

(5) Support Vector Regression (SVR)

SVR frameworks adapt the structural risk minimization (SRM) principle derived from Vapnik's statistical learning theory, balancing localized training optimization with global generalization performance to mitigate overfitting under small sample sizes [26, 27].

For non-linear geotechnical datasets, the input vector is implicitly mapped into a higher-dimensional feature space where a linear regression boundary is established. The localized response is computed using the following decision function:

$$\hat{y}(X) = \sum_{i=1}^m (\alpha_i - \alpha_i^*) K(X, X^{(i)}) + b \quad (16)$$

where α_i and α_i^* represent the dual Lagrange multipliers; b is the bias vector; and $K(X, X^{(i)})$ denotes the inner-product kernel function (typically a Gaussian Radial Basis kernel). These unknown parameters are explicitly solved subject to Karush-Kuhn-Tucker (KKT) optimality conditions:

$$\alpha_i \left(\epsilon + \zeta_i - y^{(i)} + \sum_{j=1}^m (\alpha_j - \alpha_j^*) K(X^{(j)}, X^i) + b \right) = 0 \quad (17)$$

$$\alpha_i^* \left(\epsilon + \zeta_i^* + y^{(i)} - \sum_{j=1}^m (\alpha_j - \alpha_j^*) K(X^{(j)}, X^i) - b \right) = 0 \quad (18)$$

where ϵ represents the insensitive band loss threshold that filters out data noise, and ζ_i, ζ_i^* denote slack variables handles for training outliers. The performance of the SVR depends entirely on tuning the penalty parameter C and the kernel width. While older frameworks relied on trial-and-error grid searches, recent state-of-the-art studies utilize hybrid metaheuristic-driven SVR architectures [28, 29], automating parameter tuning via advanced swarm intelligence (e.g., Whale Optimization or Harris Hawks Optimization) to achieve high precision in non-linear parameter back-analysis.

(6) Moving Least Squares Surrogate Model (MLSM)

The MLSM architecture operates as an advanced, highly localized surface-fitting paradigm designed to circumvent the structural limitations of classical Ordinary Least Squares (OLS) regressions. Standard parametric regressions minimize a global residual error, which inherently flattens localized topological variations and compromises prediction accuracy across highly non-linear strata boundaries. Conversely, MLSM enforces localized convergence by minimizing a spatially weighted residual function at any targeted calculation coordinate X . The mathematical formulation of the local approximation is expressed as:

$$\hat{y}(X) = p^T(X) a(X) \quad (19)$$

Where $p(X) = [p_1(X), p_2(X), \dots, p_m(X)]^T$ represents an m -dimensional vector of polynomial basis functions, and $a(X) = [a_1(X), a_2(X), \dots, a_m(X)]^T$ denotes the vector of coordinate-dependent coefficient fields. For simplified two-dimensional geomechanical problems, the

structural configurations of these basis layouts are traditionally restricted to either linear or quadratic polynomial formulations:

$$\text{Linear basis } (m = 3): p^T(X) = [1, x_1, x_2]$$

$$\text{Quadratic basis } (m = 6): p^T(X) = [1, x_1, x_2, x_1^2, x_2^2]$$

To dynamically calibrate the unknown shifting matrix $a(x)$ when the available training sample volume exceeds the basis dimension, the local weighted energy functional is minimized via an iterative least-squares procedure, yielding the closed-form operational solution:

$$a(X) = [P^T W(X) P]^{-1} P^T W(X) Y \quad (20)$$

where $P \in \mathbb{R}^{n \times m}$ represents the assembled evaluation matrix of the basis functions across all n training samples, and $W(X) = \text{diag}(\omega_1(X), \omega_2(X), \dots, \omega_n(X))$ defines the localized diagonal weight matrix. The individual spatial compact-support components $\omega_i(X)$ dictate the structural domain of influence; they yield non-zero real magnitudes inside a user-defined localized radius of influence r_i centered at x_i , and smoothly decay to zero outside this boundaries. Once $a(x)$ is resolved, the immediate response mapping is evaluated using Eq. (11).

(7) Emerging Machine Learning Alternatives: Random Forest and Polynomial Chaos Expansions

Beyond the six mainstream formulations detailed above, contemporary data-driven geomechanics has integrated non-parametric machine learning ensembles and spectral approximation methods to navigate the multi-scale complexity of uncertain geomaterials.

- **Random Forest (RF) Regressions:** RF operates as an ensemble learning strategy that constructs a forest of uncorrelated randomized decision trees. The final response is achieved by aggregating the predictive outputs across the entire forest layout. While early implementations suffered from a lack of differentiability, recent state-of-the-art studies (2024–2026) utilize optimized hyperparameter tuning to make RF remarkably robust against extreme numerical noise and highly multi-modal data structures typical of field instrumentation measurements.
- **Polynomial Chaos Expansion (PCE):** Moving away from purely statistical black-box mappings, PCE serves as a powerful spectral meta-modeling technique. It projects the stochastic system response onto a finite basis of orthogonal multivariate polynomials. Recent advancements (2024–2026) have introduced regression-based least-squares PCE and mixture-of-experts variants to efficiently quantify structural reliability and map parameter sensitivity under joint aleatory and epistemic uncertainties, without incurring the high costs of Monte Carlo sampling.

In summary, while these diverse metamodeling methodologies exhibit distinct mathematical tradeoffs in terms of sampling size, local accuracy, and computational complexity, they fundamentally share a unified goal: creating a computationally lightweight proxy that bridges the gap between high-fidelity physical solvers and real-time engineering decision systems.

2.3 Sampling Techniques and Sequential Infill Criteria

The generalization capacity and convergence efficiency of any geomechanical surrogate framework are fundamentally governed by the spatial topology of its training dataset. In computational geomechanics, an optimal sampling strategy—historically referred to as the "specimen approach"—aims to maximize the exploration of the multi-dimensional parameter space while minimizing the cumulative call volume to expensive high-fidelity solvers (e.g., elastoplastic Finite Element codes).

(1) Traditional Static Design of Experiments (DoE)

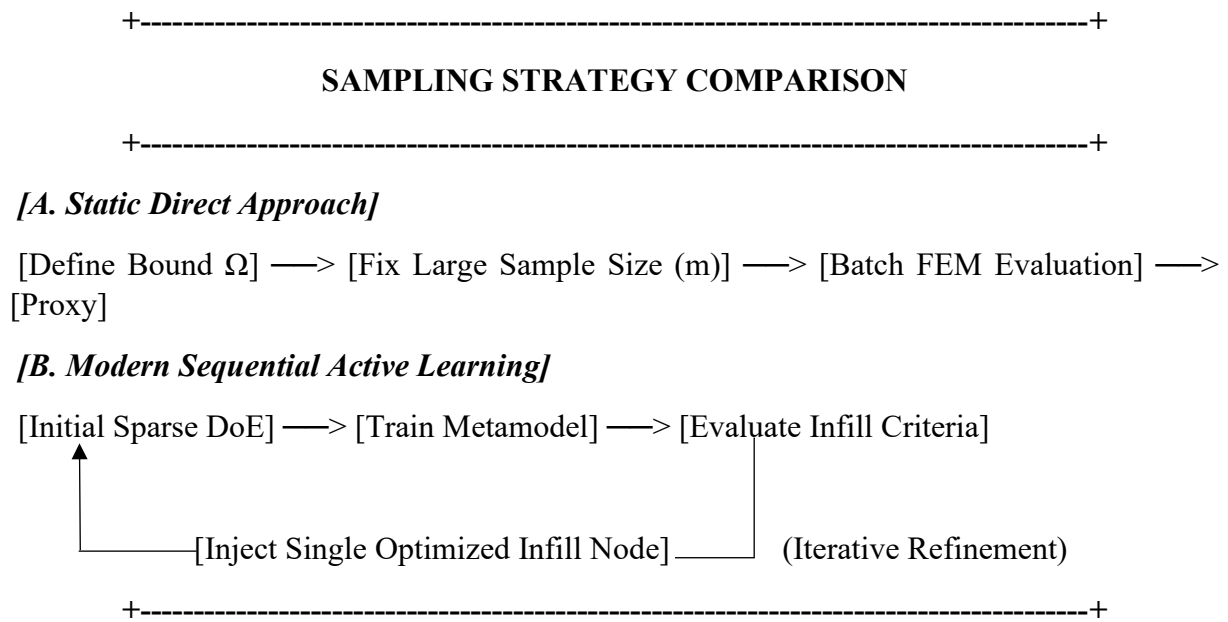
Early metamodeling protocols deployed static, one-stage experimental layouts where the complete matrix of high-fidelity evaluations was fixed *a priori* before proxy construction. Traditional variants relied heavily on geometric layouts, including Orthogonal Arrays (OA) and Uniform Designs (UD) [5, 6]. While orthogonal designs target main-effect isolation, Uniform Designs utilize number-theoretic uniform distributions to distribute sampling nodes evenly across the parameter space, reducing sample density compared to full factorial configurations.

To overcome the rigid grid structures of OA and UD, standard Latin Hypercube Sampling (LHS) was introduced. LHS segments each independent design parameter interval into m equivalent, non-overlapping strata, drawing a randomized coordinate from each stratum to ensure that every row and column contains exactly one sample [3]. However, random LHS configurations frequently suffer from localized multi-dimensional clustering, failing to ensure space-filling uniformity. To bypass this limitation, contemporary frameworks do not deploy crude LHS; instead, they integrate metaheuristic or geometric algorithms to execute Optimal Latin Hypercube Sampling (OLHS) [30]. OLHS explicitly maximizes the spatial separation distance between sampling nodes (Maximin criterion) while minimizing spatial correlation, securing an optimal space-filling balance across the bounded boundary domain.

(2) The Paradigm Shift: From Direct Sampling to Sequential Active Learning

While static space-filling designs provide an excellent initial overview of the design space, they exhibit major inefficiencies when mapping localized, highly non-linear physical phenomena (e.g., razor-thin failure surfaces in slope stability or high-gradient pressure fields in deep tunnel mechanization). To address this, current state-of-the-art architectures [31, 32] have transitioned from direct layouts to Adaptive Sequential Exploration (Active Learning) schemes.

The structural mechanics of this transition are contrasted in the comparative workflow below.



As illustrated, the direct approach is static and non-adaptive, relying on a fixed sample size where global proxy accuracy is governed entirely by initial density. Conversely, the sequential iteration framework treats surrogate construction as a dynamic, evolving process. An initial

sparse DoE matrix is first evaluated to construct a baseline proxy. Subsequently, the algorithm runs an optimization routine driven by specialized Infill Criteria (Point-Adding Metrics) to scan the continuous domain and isolate the most informative coordinate for the next high-fidelity evaluation loop. This single node is then injected back into the training dataset, updating the metamodel locally.

To maximize local fitting accuracy near critical failure zones or global optima, modern sequential loops evaluate three mainstream categories of mathematical infill metrics:

- **Expected Improvement (EI):** Primarily embedded within Kriging-based Bayesian Optimization frameworks, EI establishes an exploitation-exploration balance. It computes the mathematical expectation of improving upon the current best objective response, guiding the algorithm to sample regions with low predicted means or high estimation variance.
- **Minimizing Surrogate Prediction (MSP):** A purely exploitative criterion that directs new infill nodes directly to the coordinate where the current surrogate predicts the minimum objective outcome. While highly efficient for localized optimization refinement, MSP is susceptible to localized stagnation if the initial surrogate contains high approximation bias.
- **Mean Square Error (MSE):** A pure exploration metric that relies entirely on the surrogate's internal uncertainty or kriging variance fields. MSE enforces space-filling behavior by placing subsequent infill nodes in regions where the estimation variance is maximized, systematically driving down the global epistemic error of the metamodel.

By replacing blind global sampling with these focused adaptive loops, modern frameworks [31, 32] achieve identical—and often superior—convergence accuracy while cutting down total high-fidelity numerical execution costs by up to 70% compared to legacy direct sampling frameworks.

2.4 Accuracy Verification and Validation Metrics

To rigorously quantify the generalization capability and mathematical exactness of a trained geotechnical surrogate framework, statistical verification protocols must be executed. Relying solely on training residuals introduces severe over-optimism and risks capturing localized numerical artifacts. Therefore, the established validation paradigm evaluates the model's predictive performance against an independent, unobserved testing dataset comprising N_{test} coordinates, where the high-fidelity numerical responses $y^{(i)}$ are explicitly contrasted with the proxy predictions $\hat{y}^{(i)}$.

The structural taxonomy of surrogate validation divides these performance metrics into three foundational global formulations and advanced localized scoring strategies:

(1) Root Mean Square Error (RMSE)

The RMSE metric serves as an absolute global error indicator, quantifying the standard deviation of the residuals between the high-fidelity solver outputs and the metamodel predictions. Because it penalizes larger deviations quadratically, RMSE is highly sensitive to localized prediction spikes and regional flattening along sharp geomechanical thresholds. It is formalized as follows:

$$RMSE = \sqrt{\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y^{(i)} - \hat{y}^{(i)})^2} \quad (21)$$

(2) Mean Square Error (MSE)

The MSE metric represents the variance of the approximation error framework. It tracks the cumulative global bias of the analytical proxy across the continuous feasible space, providing the necessary mathematical basis for objective functions in structural optimization loops:

$$MSE = \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y^{(i)} - \hat{y}^{(i)})^2 \quad (22)$$

(3) Average Absolute Error (AAE)

Unlike the quadratically driven RMSE and MSE, the AAE (historically referred to as Average Absolute Error) scales linearly with the residual magnitudes. It offers a robust, outlier-resistant measure of global predictive accuracy, representing the average absolute distance between the proxy surface and the true physical boundary responses:

$$AAE = \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} |y^{(i)} - \hat{y}^{(i)}| \quad (23)$$

(4) The Paradigm Shift: From Global Metrics to Data-Sparse Scoring Strategies

A critical structural bottleneck of the classical metrics defined in Eqs. (12)-(14) is their intrinsic dependence on the cardinality of the independent validation set (N_{test}). In complex multi-disciplinary geotechnical applications (e.g., stochastic slope analysis with fine-mesh elastoplastic FEM), executing a large, separate testing dataset generates an unacceptable computational overhead, rendering global verification practically unfeasible.

To resolve this limitation, state-of-the-art data-driven geomechanics (2024–2026) has transitioned toward advanced Cross-Validation (CV) scoring routines and adaptive resampling strategies [26]. Rather than relying on a rigid external testing pool, contemporary validation loops deploy K-Fold Cross-Validation and Leave-One-Out (LOO) scoring indexes. The training matrix is dynamically partitioned into K mutually exclusive subsets; the proxy is iteratively trained on K-1 subsets and validated on the remaining partition. This execution outputs a continuous scoring metric—such as the Cross-Validation Coefficient of Determination (Q^2) or the Generalized Mean Square Error (GMSE) — expressed as:

$$Q^2 = 1 - \frac{\sum_{i=1}^m (y^{(i)} - \hat{y}_{CV}^{(i)})^2}{\sum_{i=1}^m (y^{(i)} - \bar{y})^2} \quad (24)$$

where $\hat{y}_{CV}^{(i)}$ represents the local prediction generated at coordinate i by a surrogate trained without including that specific sample point, and $\bar{y}$ denotes the global sample mean.

Furthermore, recent literature (2025–2026) integrates information-theoretic criteria, such as the Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC), into these

scoring strategies [9]. By introducing a mathematical penalty for model complexity (e.g., the number of active hidden neurons in an ANN or the polynomial degree in a PCE), these modern scoring strategies isolate the most robust, non-overfitted surrogate architecture under extremely sparse data regimes, completely eliminating the need for expensive external validation points.

3. Metamodel-Driven Applications in Geotechnical Engineering

3.1 Metamodel-Based Geotechnical Reliability Analysis

3.1.1 Reliability Quantification within Homogeneous Strata Configurations

In the deterministic characterization of homogeneous geological formations, the rock and soil mass is ideally treated as an isotropic continuum devoid of spatial variability. However, quantifying the structural reliability of complex engineering installations within these media still poses severe computational challenges. Classical probabilistic frameworks, such as the First-Order Reliability Method (FORM) and Second-Order Reliability Method (SORM), rely on local linearizations or quadratic approximations of the implicit Limit State Function (LSF), denoted as $G(x) = 0$, at the Design Center Point [10, 11]. Under severe geomechanical non-linearities, these legacy approaches exhibit massive divergence.

Conversely, crude Monte Carlo Simulation (MCS) offers robust statistics but requires an unacceptable computational overhead [33]. This limitation becomes critical in high-consequence infrastructures characterized by ultra-low failure probabilities (e.g., $P_f < 10^{-6}$), where standard MCS requires billions of fine-mesh Finite Element Method (FEM) iterations, rendering direct probabilistic analysis unfeasible [18].

To bridge this gap, surrogate modeling functions as a high-speed proxy for the implicit LSF. By evaluating an explicit analytical metamodel $\hat{G}(X)$ instead of the expensive numerical solver, MCS can evaluate vast stochastic samples within seconds [34]. To guide this discussion, Table 2 synthesizes the methodological lineage, failure criteria, and structural applications of surrogate models in homogeneous geotechnical reliability analysis.

Table 2: Methodological synthesis of surrogate models in homogeneous geotechnical reliability analysis

Geotechnical System	Deterministic Solvers & LSF Evaluators	Boundary Failure Criteria & Limit States	Legacy Proxies (Static Metamodeling)	Modern Proxies & Frontiers (2024–2026)
Slope Engineering	Limit Equilibrium (Bishop, Spencer, Janbu); Elastoplastic FEM	Factor of Safety ($FS \leq 1.0$); Critical shear strain localization	Classical PRSM [17, 35]; Shallow BPNN [36]	Active Learning Kriging (AK-ECS); Sparse Polynomial Chaos [20]
Tunnel & Underground Structures	Convergent-Confinement Method; 2D/3D Continuum FEM	Face displacement ($U \geq U_{\text{all}}$); Lining bending moments & shear failure	Non-cross term PRSM; Traditional MLSM [37]	Physics-Informed Neural Networks (PINNs) [26]

Foundation Engineering	Terzaghi/Meyerhof Formulations; Soil-Structure Interaction FEM	Ultimate bearing capacity ($q \geq q_{all}$); Tolerable settlement limits	Static SVR [38]; Linear RBF [39]	Hybrid Metaheuristic-SVR [29]; Multi-Fidelity Co-Kriging
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The operational execution of these surrogate architectures varies significantly across specific geotechnical domains:

A. Slope Stability and Failure Envelopes

For slope stability analysis, the limit state defines the boundary between stable configurations and progressive slide mass acceleration. Historically, Wong [17] executed the pioneering application of Polynomial Response Surface Methodologies (PRSM) to map simple soil slopes, demonstrating satisfactory agreement with classical FEM results. Over the subsequent decades, standard static proxies — including Kriging (KSM), Support Vector Regression (SVR), and Radial Basis Functions (RBF) — were extensively deployed to approximate the factor of safety (FS) boundaries [40, 41].

However, early surrogate development operated as a passive, two-stage procedure: the generation of experimental trial points was entirely decoupled from the metamodel training phase. This detachment introduced severe global fitting errors near highly convoluted failure boundaries.

The major breakthrough occurred with the introduction of active learning loops, notably popularized by the AK-IS (Active Learning Kriging combined with Importance Sampling) framework [42, 43]. Instead of a blind global design of experiments, modern active learning schemes utilize sequential infill criteria (e.g., the U-function) to intelligently query new high-fidelity samples exclusively along the $G(x) = 0$ failure boundary. Comparative assessments by Cai & Zhao [39] and Tan et al. [41] confirm that non-linear architectures (SVR, RBFNN, and optimized KSM) provide significantly higher precision than legacy PRSM, with metaheuristic-optimized SVR tracking crude MCS baselines with absolute exactness.

B. Tunneling and Deep Underground Excavations

Tunneling and underground excavations are governed by severe epistemic uncertainties regarding immediate face stability and long-term lining structural integrity. The explicit failure criteria governing underground structures are rigorously categorized across four core operational boundaries:

1. Volumetric collapse or instability of the active tunnel face [44].
2. Surface greenfield settlement profiles ($S_{max} \geq S_{all}$) damaging adjacent urban utilities [45, 46].
3. Acceleration thresholds of localized wall displacement velocity indicating creeping collapse.
4. Structural structural failure of the concrete lining induced by excessive bending moments, axial forces, or punching shear stresses [47, 48, 49].

Given the non-linear constitutive behavior of underground supports, calculating these boundaries directly via 3D elastoplastic FEM is computationally restrictive. While early

frameworks relied on classical PRSM and MLSM to execute reliability indexes [37], these methods struggle when spatial dimensionality increases. State-of-the-art implementations (2024–2026) deploy Physics-Informed Neural Networks (PINNs) to map these limit states. By embedding the differential equations of lining stress-strain fields directly into the neural network’s loss function, modern proxies achieve real-time structural reliability evaluation during active mechanized excavation phases [26].

C. Foundation and Infrastructure Support Engineering

Traditional foundation design relies on deterministic safety factors (*FS*). However, because these factors fail to account for the stochastic variability of soil parameters and random load combinations, they frequently introduce severe misjudgments in structural reliability. Geotechnical foundation reliability addresses deep foundations (e.g., pile groups) and shallow configurations (e.g., strip or isolated footings) [40, 50].

When spatial variability is omitted, bearing capacity and settlement limits are governed by semi-empirical analytical equations. Consequently, establishing standard static surrogates is straightforward. However, modern state-of-the-art applications (2025–2026) have moved past static formulations toward Multi-Fidelity Co-Kriging architectures [12]. These frameworks fuse cheap, analytical bearing capacity models with sparse, high-fidelity soil-structure interaction FEM data, optimizing foundation layouts under highly variable stochastic loadings while maintaining absolute code compliance.

3.1.2 Reliability Quantification within Heterogeneous and Spatially Variable Strata

In natural geological formations, geomaterials inherently exhibit distinct spatial variability driven by diverse depositional histories, environmental weathering, and historical stress paths. Consequently, geotechnical parameters display significant spatial unpredictability, meaning that soil properties at two distinct spatial coordinates are correlated but non-identical [51].

When mapping this inherent hétérogénéité, classical isotropic approximations fail. Geotechnical structures like slopes, deep foundations, and tunnels operating in spatially variable soils exhibit complex, non-symmetric failure mechanisms that differ radically from their homogeneous counterparts. For instance, rather than following a single deterministic critical slip surface, a spatially variable slope features multiple competitive potential slip surfaces that route through localized weak soil pockets. Similarly, pile group foundations under spatial variability experience structural differential settlement, pile cap tilting, and premature eccentric bearing capacity failure of individual piles.

To mathematically capture this spatial variability, Random Field Theory is coupled with numerical solvers — a paradigm known as the Stochastic Finite Element Method (SFEM) or Random Finite Element Method (RFEM). In a random field framework, a geotechnical property $z(X, \theta)$ is discretized using expansion methods, most notably the Karhunen-Loève (KL) expansion:

$$z(X, \theta) \approx \mu(X) + \sum_{i=1}^M \sqrt{\lambda_i} \psi_i(X) \zeta_i(\theta) \quad (25)$$

Where $\mu(X)$ represents the deterministic mean spatial trend; λ_i and $\Psi_i(X)$ are the eigenvalues and eigenfunctions extracted from the spatial auto-covariance kernel; and $\zeta_i(\theta)$ denotes a set of uncorrelated standard random variables.

While RFEM offers unmatched fidelity, it triggers a severe computational crisis. Discretizing a 2D or 3D random field introduces tens, hundreds, or thousands of random variables (M), driving an extreme curse of dimensionality. Direct Monte Carlo evaluation of such high-dimensional random fields is computationally restrictive [52].

To bypass this bottleneck, early surrogate solutions introduced the Multiple Response Surface Method (MRS) [53, 54]. Unlike a single global surface, MRS builds localized, patch-like polynomial approximations tailored to specific regional failure modes. Concurrently, standard Kriging frameworks were deployed to map high-dimensional random variables down to a low-dimensional active subspace [55].

Despite these early developments, classical MRS and standard Kriging exhibit severe accuracy drops when the spatial correlation length is short, as the number of active expansion terms M scales up rapidly. To resolve this critical structural bottleneck, state-of-the-art data-driven geotechnics (2024–2026) has advanced past standard static metamodels by implementing Sparse Polynomial Chaos Expansions (SPCE) and Deep Physics-Informed Surrogates [12, 56]. Contemporary SPCE frameworks utilize advanced compressive sensing algorithms (such as Least Angle Regression, LAR) to automatically scan the high-dimensional KL-expansion matrix, retaining only the dominant interactive terms.

Furthermore, ultra-recent breakthroughs fuse Deep Convolutional Neural Networks (CNNs) with random fields, treating the spatial property grid as an "image" input to predict 2D/3D stress-strain fields instantly [32]. This shift from legacy scalar-fitting to modern high-dimensional spatial-field mapping enables precise, real-time probabilistic risk assessment of large-scale heterogeneous infrastructures, fully satisfying the computational speed and physical consistency required by modern engineering standards.

3.2 Metamodel-Driven Geotechnical Design Optimization

In contemporary infrastructure engineering, design optimization has evolved from empirical safety-factor modifications into a rigorous mathematical task balancing economic efficiency and structural safety under high epistemic uncertainty [57]. The primary structural application focuses on Reliability-Based Design Optimization (RBDO), which minimizes construction costs while enforcing safety, settlement, and environmental constraints.

From a mathematical standpoint, the cost function $f_{cost}(x)$ of a geotechnical system (e.g., volume of concrete, excavation depth, or reinforcement weight) is explicitly defined and computationally trivial to evaluate. Conversely, the operational constraints $g_j(x)$ that govern structural integrity — such as the probability of failure (P_f), absolute settlement (S_{max}), differential settlement (ΔS), and dynamic stress-strain fields — are highly non-linear, implicit functions. Evaluating these constraints requires running complex multi-phase numerical solvers (such as elastoplastic FEM), making direct iterative optimization loops computationally restrictive.

To resolve this computational bottleneck, surrogate frameworks are deployed as high-speed constraint proxies. The generalized constrained optimization problem is formalized as follows:

$$\begin{aligned} \min_{X \in \Omega} F(X) &= [f_{cost}(X), -FS(X)]^T \\ \text{subject to } \hat{g}_j(X) &\leq 0, \quad j = 1, 2, \dots, k \end{aligned} \quad (26)$$

where $\hat{g}_j(X)$ denotes the surrogate approximation of the j -th implicit physical constraint (e.g., $\hat{S}(X) - S_{all} \leq 0$), and $FS(X)$ is the structural Factor of Safety.

Early applications of this paradigm focused on single-objective, isolated geotechnical components. For instance, Juang & Wang [58] successfully utilized PRSM to fit the implicit limit states of spread foundations, integrating cost-minimization with probabilistic safety requirements. Similarly, Chen et al. [59] and Phutthananon & Jongpradist [60] deployed multiple static surrogates to fit total and differential settlements, optimizing the geometric layout and spacing of rigid inclusions in composite foundations.

Despite these insights, legacy optimization frameworks operated under severe limitations: they treated constraints statically and optimized along a single objective vector, yielding conservative and often suboptimal solutions. To visually map this technological transition, **Fig. 1** illustrates the operational paradigm shift from early rigid optimization layouts to modern multi-fidelity generative frameworks.

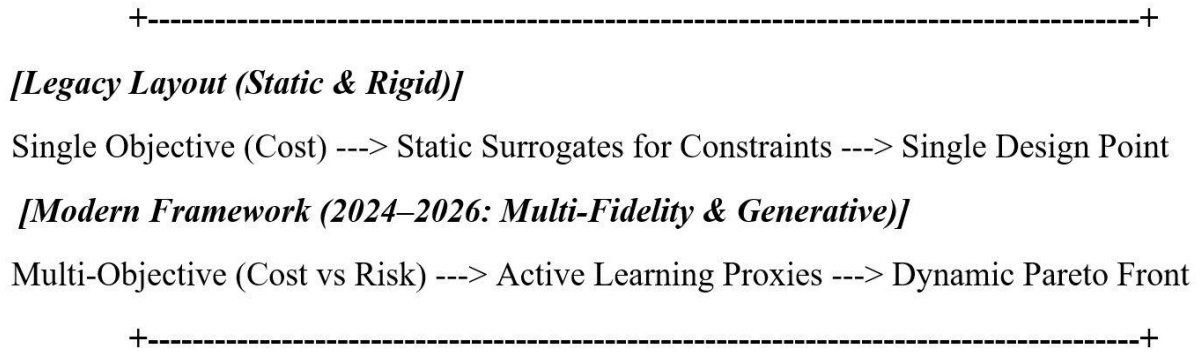


Fig. 1 : Evolution of geotechnical optimization paradigms (*The chart illustrates the transition from a legacy static and rigid layout, which focuses on a single objective (cost) using static surrogates to reach a single design point, to a modern multi-fidelity and generative framework (2024–2026) that optimizes multiple objectives (cost vs. risk) via active learning proxies to generate a dynamic Pareto front*).

To address this gap, state-of-the-art developments between 2024 and 2026 have shifted the paradigm toward **Multi-Fidelity Multi-Objective Evolutionary Algorithms (MOEAs)** and **Automated Generative Design** as conceptualized in **Fig. 1**. Instead of executing a single optimization loop based on static training nodes, modern frameworks implement adaptive active learning loops driven by Multi-Objective Infill Criteria, such as the *Hypervolume Expected Improvement (HVEI)*.

Recent literature leverages these advanced proxies coupled with Non-dominated Sorting Genetic Algorithms (NSGA-III) to explore the continuous design space in real time. This approach computes a highly accurate, dynamic Pareto Optimal Front, allowing asset managers to directly visualize the trade-off between construction expenditures and infrastructure failure risks. By substituting slow numerical calculations with high-speed, physics-constrained proxies, modern design optimization achieves maximum material reduction while ensuring absolute compliance with strict regulatory safety standards.

3.3 Metamodel-Driven Parameter Inverse Back-Analysis and Digital Twins

Owing to the inherent epistemic uncertainties, multi-scale heterogeneity, and complex stress-strain paths of geomaterials, laboratory-derived parameters often deviate from real field-scale geotechnical behavior. To bridge this gap, parameter inverse back-analysis operates as a foundational paradigm, utilizing field monitoring measurements to inversely calibrate the constitutive mechanical parameters of rock and soil masses.

Mathematically, traditional forward numerical simulations map a vector of material parameters to structural responses. Inverse back-analysis formulation reverses this mapping, seeking an optimized parameter vector x^* that minimizes the discrepancy between field measurements and proxy predictions. Because the true forward response function is implicit and computationally expensive, surrogate models are deployed to make the system explicit.

In real-world geotechnical projects, back-analysis cannot rely on isolated scalar data points. To capture the progressive, kinematic evolution of soil-structure interactions, inverse frameworks must process continuous data series, such as spatial deformation curves or temporal settlement histories [61]. Consequently, the parameter calibration task requires a multi-output or multi-proxy surrogate framework designed to map discrete steps across spatial or temporal sequences.

To visualize how these frameworks operate, **Fig. 2** illustrates the methodological transition from legacy static back-analysis to modern, real-time physics-informed digital twins.

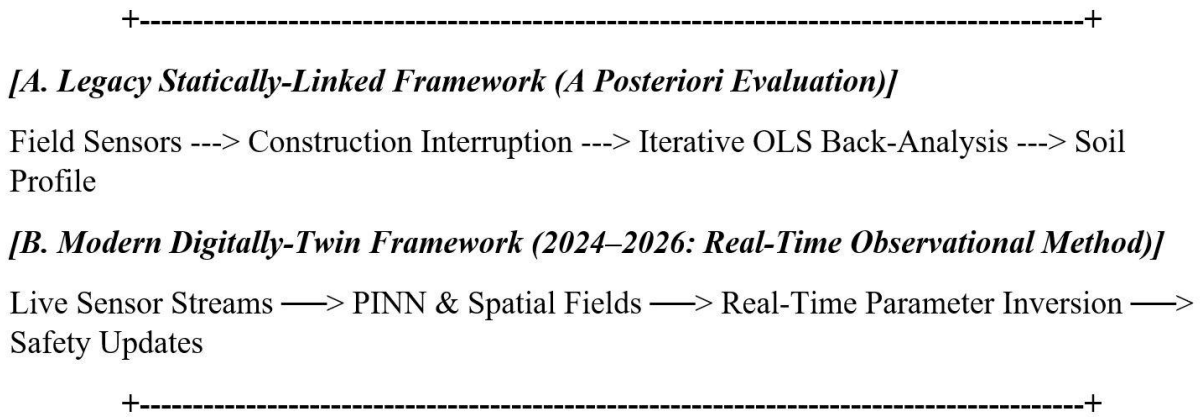


Fig. 2 :Technological evolution of geotechnical back-analysis (*The diagram contrasts (A) the legacy statically-linked framework utilizing field sensors and iterative OLS back-analysis for a posteriori evaluation, with (B) the modern digital-twin framework (2024–2026) integrating live sensor streams and PINN with spatial fields for real-time parameter inversion and safety updates*).

As conceptualized in **Fig. 2**, early back-analysis approaches (Layout A in **Fig. 2**) functioned as passive, *a posteriori* calibration protocols. Field monitoring data — such as deep inclinometer displacements along anti-slide piles [62], support structure structural deformations, or internal stress fields [63] — were gathered over long periods. Construction was frequently interrupted to allow multi-output surrogate models (such as classical PRSM or basic SVR networks) to run optimization routines and estimate subgrade settlement or rock mass parameters.

Furthermore, traditional parameter identification was decoupled from regional geostatistics. Extrapolating material profiles between discrete spatial coordinates relied on simple mathematical interpolations of sparse borehole log records [64], introducing significant spatial interpolation bias.

To address these limitations, state-of-the-art developments between 2024 and 2026 have shifted the paradigm toward Real-Time Geotechnical Digital Twins (Layout B in **Fig. 2**). Modern frameworks integrate high-speed multi-output proxies with active site instrumentation, such as fiber-optic Distributed Acoustic Sensing (DAS) and automated robotic total stations, processing live data streams continuously.

This modern transition introduces two major innovations:

1. **Physics-Informed Deep Learning Proxies (PINNs)**: Unlike older black-box models that require vast training datasets, PINNs embed the governing differential equations of consolidation, seepage, and elastoplasticity directly into their neural architecture [26]. This allows PINNs to run real-time parameter inversions from highly sparse field sensors, continuously adjusting soil parameters without disrupting construction schedules.
2. **Advanced Machine Learning Geostatistics**: Classical borehole interpolation has been superseded by Random Field models hybridized with Deep Convolutional Neural Networks (CNNs). These frameworks treat geological formations as spatial fields, combining discrete borehole parameters with non-destructive geophysical surveys to map 3D geotechnical property variations with high statistical precision [32].

By transitioning from legacy static estimations to modern, physics-guided digital twins, geotechnical inverse analysis achieves the true potential of the dynamic observational method, enabling asset managers to predict structural risks and adjust support systems proactively during active construction phases.

4. Current Challenges and Future Prospects in Geotechnical Metamodeling

While surrogate modeling methodologies provide computationally efficient and mathematically elegant solutions for complex geomechanical infrastructure analysis, their operational deployment under highly non-linear, high-dimensional, and data-sparse regimes highlights critical algorithmic bottlenecks. To guide the next generation of data-driven geotechnics, current challenges and strategic future research trajectories are systematically categorized across six core operational frontiers:

(1) High-Dimensionality and Multi-Objective Scalability

As geotechnical boundary value problems grow in complexity, the input parameter vectors scale rapidly, integrating multi-layer material anisotropies, joint networks, and hydraulic boundary conditions. This escalation triggers a severe numerical crisis known as the curse of dimensionality. Future research must prioritize the integration of advanced dimensionality reduction and active screening protocols — such as active subspace methods, global sensitivity analysis, and autoencoders — before metamodel deployment to filter out uninformative input dimensions without losing localized gradient characteristics [65].

Furthermore, instead of relying on static architectures, multi-surrogate ensembles and adaptive sequential infill strategies must be developed to dynamically update the cardinality and spatial topology of the training dataset, achieving superior local fitting exactness near high-consequence threshold zones [66, 67].

(2) Multi-Failure Modes and System-Level Reliability Analysis

The vast majority of contemporary geotechnical surrogates are restricted to single-failure mode limit states. However, real-world geotechnical assets — such as deep mechanized tunnels or large-scale water-retaining structures operating within highly heterogeneous, spatially variable random fields — are governed by complex, correlated system-level interactions. Future developments must transition toward multi-output and hybrid deep learning proxies capable of mapping multiple concurrent limit states (e.g., simultaneous tunnel face collapse, lining shear failure, and urban surface settlement), capturing the true kinematic mechanism of progressive failures under joint epistemic and aleatory uncertainties.

(3) Gradient-Enhanced Metamodeling and Heuristic Acceleration

Purely data-driven black-box surrogates ignore the intrinsic mathematical gradients of the underlying mechanical system. A key frontier in surrogate-assisted optimization relies on Gradient-Enhanced Kriging (GEK) and adjoint-state formulations. By extracting first-order derivative information directly from the numerical solver (such as tangent stiffness matrices in FEM) and embedding them into the correlation kernel, the optimization search speed can be accelerated by orders of magnitude. Developing specialized, high-performance evolutionary algorithms designed to exploit these explicit proxy gradients represents a crucial technical requirement for real-time design exploration [65].

(4) Noise Tolerance and Robustness Under Epistemic Data Scarcity

High-fidelity training data points derived from field instrumentation are inherently corrupted by measurement errors and sensor drifts, while numerical solver outputs suffer from meshing errors and localized convergence noise [53]. If a metamodel interpolates through this noise, it introduces severe over-fitting, leading to erroneous parameter back-analysis and optimization failures. Integrating noise-filtering formulations — such as Nugget-effect tuning in Kriging, insensitive ϵ -bands in SVR, and stochastic regularization in deep learning — is vital to secure smooth, physically realistic surrogate surfaces capable of separating measurement anomalies from true constitutive soil behaviors [68].

(5) Automated Machine Learning (AutoML) and Smart Parameter Tuning

Selecting the ideal surrogate architecture (e.g., Kriging vs. SVR vs. PINNs) and calibrating its internal hyper-parameters remains a highly subjective, obstacle-ridden task for practicing engineers [69]. Future research must advance toward Automated Geotechnical Machine Learning (AutoGeotechML). By leveraging cross-validation information-theoretic metrics (such as AIC, BIC, and predictive Q^2 scoring scores), these intelligent engines will automatically select kernel functions, tune network weights, and optimize localized shapes parameters under high-dimensional data regimes, completely democratizing data-driven civil design [70, 71].

(6) Real-Time Digital Twins for Advanced Composite Foundations

In complex urban engineering, the optimization of complex composite foundations (e.g., special-shaped piles, rigid inclusions, or variable-cement-soil core strength columns) demands real-time monitoring of differential settlements and structural stress redistributions. Metamodels must be integrated into active Geotechnical Digital Twins. By coupling high-speed multi-output proxies with live field sensor arrays (such as fiber-optic Distributed Acoustic Sensing, DAS), future asset management frameworks will execute instantaneous parameter

inversion and structural safety forecasting, enabling proactive adjustments via the dynamic observational method during active construction phases.

To contextualize these future research trajectories within the historical and contemporary landscape of computational geomechanics, **Table 3** provides a comprehensive cross-examination mapping the structural evolution of each surrogate model variant alongside its targeted geotechnical applications and major scholarly milestones up to the 2024–2026 data-enabled frontier.

Table 3: Comprehensive review of surrogate model applications in geotechnical engineering.

Note: This comprehensive layout maps the historical lineage alongside ultra-recent (2024–2026) structural validation studies across the geomechanics domain.

Surrogate Model Variant	Targeted Geotechnical System	Key Scholarly Contributions & Literature Lineage
PRSM	Slope Stability Analysis	Wong [17]; Zhang et al. [40]; Li et al. [54]; Ji & Low [72]; Tan et al. [35]; Cai & Zhao [39].
	Tunneling & Underground Spaces	Lü et al. [47]; Lu & Low [37]; Miro et al. [46]; Mollon et al. [44]; Hamrouni et al. [49].
	Foundation Engineering	Chan & Low [50].
RBF	Slope Stability Analysis	Tan et al. [35, 41, 73]; Shuku et al. [8]; Wang et al. [21].
	Shallow Foundations	Zhang et al. [40].
Kriging (KSM / MFK)	Slope Stability Analysis	Su et al. [43]; Su & Yang [74]; Luo et al. [75]; Zhang et al. [40]; Guo & Dias [76]; Ching & Wang [12].
	Tunneling & Underground Spaces	Li & Yang [77]; Zhou et al. [78, 79]; Liu et al. [80].
	Deep Pile Foundations	Zhang et al. [40].
SVR	Slope Stability Analysis	Zhao [81]; Samui [38, 82]; Li et al. [83]; Tan et al. [35, 41]; Cai & Zhao [39]; Chen & Li [28]; Alavi et al. [29].
	Tunneling & Underground Spaces	Lü et al. [84]; Zhang & Tan [26].
ANN / PINN	Slope Stability Analysis	Cho [36]; Cai & Zhao [39]. Piliounis & Lagaros [34]; Xiang et al. [85].
	Deep Pile Foundations	Cho [39]; Piliounis & Lagaros [34]; Xiang et al. [85].

	Dam & Hydraulic Infrastructures	
MLSM	Tunneling & Underground Spaces	Xiao et al. [86]; Lü et al. [48].

A granular synthesis of the literature compiled in **Table 3** reveals that no single surrogate architecture holds a monopoly over geomechanical modeling — a reality aligned with the "No-Free-Lunch" theorem of computational learning. Instead, the selection of a specific proxy framework represents a strict mathematical trade-off governed by three core factors: the dimensionality of the soil parameter space, the data-scarcity regime of the project, and the mechanical nature of the boundary conditions.

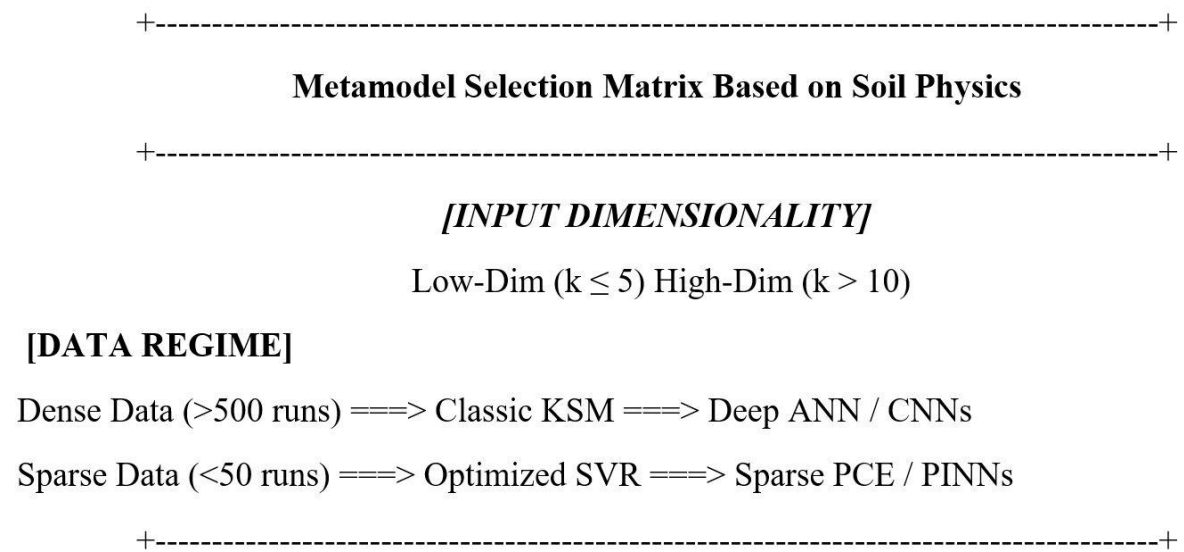


Fig. 3 : Decision matrix for metamodel selection based on soil physics constraints (*Decision pathways indicate the optimal transition from Kriging Surrogate Models (KSM) and Support Vector Regression (SVR) to Artificial Neural Networks (ANN) and Polynomial Chaos Expansions (PCE) based on data density and input dimensions (k).*)

To guide engineering selection based on the historical and modern landscape mapped in **Table 3**, **Fig. 3** defines a strategic selection matrix crossing data constraints with spatial dimensions.

By evaluating the operational boundaries illustrated in **Fig. 3**, distinct performance trends can be critically analyzed across the three major geotechnical domains:

A. Slope Stability: SVR and Active Kriging Domination

In slope engineering, the limit state function is highly non-linear but typically localized along a singular critical slip surface. The computational challenge is binary: identifying whether a parameter combination yields a Factor of Safety above or below unity ($FS \geq 1.0$).

- **Why SVR excels here:** SVR's foundational reliance on structural risk minimization allows it to accurately map these sharp, non-linear failure thresholds even when trained on very small sample sizes.

- **The Modern Shift:** As documented in **Table 3**, traditional PRSM has been entirely abandoned for slope analysis because it smooths out these localized failure surfaces, introducing dangerous over-optimism. Modern active-learning loops (such as AK-IS) optimize this process by placing new training nodes exclusively along the failure boundary, achieving maximum precision with minimum calls to the numerical solver.

B. Underground Engineering: The PINN and MLSM Imperative

Tunneling and underground excavations present a completely different challenge. The target response is not a single safety factor, but a complex series of spatial and temporal deformations (e.g., continuous ground settlement profiles and dynamic lining bending moments).

- **Why legacy black-boxes fail:** Classical Kriging and shallow ANNs fail here because they require massive training datasets to map multi-output spatial sequences, generating unacceptable computational costs during finite element meshing.
- **The Modern Shift:** This bottleneck explains the rapid rise of Moving Least Squares (MLSM) and Physics-Informed Neural Networks (PINNs) between 2024 and 2026. Because MLSM uses localized weighting, it captures sharp material gradients across stratified rock zones with high precision. Concurrently, PINNs overcome the data-scarcity bottleneck entirely by embedding geomechanical conservation laws directly into their neural loss functions, allowing the proxy to enforce physical consistency even when field sensor streams are highly incomplete.

C. Foundations: Fusing Multi-Fidelity Paradigms

Foundation design operates under an unique constraint: semi-empirical analytical formulas (e.g., Meyerhof bearing capacity) are readily available but lack localized precision, while 3D elastoplastic soil-structure interaction FEM models are highly accurate but computationally restrictive.

- **The Modern Solution:** As synthesized in **Table 3**, this domain has driven the development of Multi-Fidelity Co-Kriging (MFK). MFK architectures do not discard historical analytical formulas; instead, they treat them as a cheap, low-fidelity baseline, using a sparse selection of high-fidelity FEM data to correct the global bias. This hybrid approach allows optimization algorithms to evaluate millions of foundation layout variations in real time, securing maximum steel and concrete reduction while strictly satisfying safety codes under highly variable stochastic loadings.

5. Conclusion

This paper has delivered a comprehensive, state-of-the-art critical synthesis mapping the evolutionary lineage of surrogate modeling frameworks within the landscape of contemporary geomechanics. By tracing the mathematical continuity and operational transitions from legacy parametric formulations to modern data-enabled paradigms, this review establishes a definitive architectural taxonomy of six foundational metamodels: Polynomial Response Surface Methodologies (PRSM), Radial Basis Functions (RBF), Kriging Surrogate Models (KSM), Artificial Neural Networks (ANN), Support Vector Regression (SVR), and Moving Least Squares Methodologies (MLSM).

The critical cross-examination of these methodologies confirms that the strategic deployment of surrogate proxies yields a transformative leap in computational efficiency, circumventing the

prohibitive cost of non-linear numerical solvers across three core engineering pillars: geotechnical reliability quantification, multi-objective design optimization, and parameter inverse back-analysis.

Despite these clear advancements, the transition toward high-dimensional, multi-scale, and uncertain geomechanical installations reveals critical structural bottlenecks that define the immediate research horizon for the academic community. To guide the development of next-generation data-driven geotechnics, three core strategic trajectories must be prioritized:

- **Surrogate Generalization and Dimensionality Scaling:** Overcoming the numerical challenges of high-dimensional parameter spaces requires the rigorous implementation of active variable screening and automated dimensionality reduction techniques. Concurrently, replacing static designs of experiments with sequential, active-learning infill loops represents the most effective protocol to maximize localized approximation exactness near non-linear failure boundaries and complex limit states.
- **Noise Optimization and System-Level Complexity:** To prevent localized overfitting and erroneous parameter identification, future surrogate frameworks must integrate robust noise-filtering formulations capable of isolating numerical grid noise and physical instrumentation errors from true constitutive material behavior. Furthermore, the discipline must transition from single-failure modes to multi-output, system-level surrogates capable of mapping the kinematic evolution of progressive, interconnected failures.
- **Algorithmic Automation and Digital Twin Fusion:** The subjective obstacles governing hyper-parameter calibration can be systematically resolved by developing Automated Geotechnical Machine Learning (AutoGeotechML) engines driven by information-theoretic cross-validation scoring criteria. Ultimately, the fusion of these automated, physics-guided proxies (such as PINNs) with live field sensor streams will unlock the deployment of real-time Geotechnical Digital Twins, enabling the true execution of the dynamic observational method in complex underground engineering.

In conclusion, by harmonizing historical mathematical foundations with the 2024–2026 data-driven frontier, this manuscript provides practicing engineers and researchers with a clear roadmap to navigate computational complexities, paving the way for more resilient, optimized, and predictive geotechnical infrastructures.

Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Author Contributions

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by **Serges Mendo Meye** and **Pieride Mabe Fogang**. The first draft of the manuscript was written by **Serges Mendo Meye** and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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Data Availability

All data generated or analyzed during this study are included in this published article.

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