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OPTIMIZATION METHODS IN INVERSE PROBLEMS – OPTIMIZATION APPROACHES FOR DETERMINING THE SOURCE FUNCTION

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Abstract: This paper explores optimization methods for solving inverse problems, specifically focusing on determining unknown source functions in parabolic partial differential equations. The study discusses problem formulation, regularization techniques, numerical optimization algorithms, parameterization strategies, and uncertainty quantification. Applications in heat conduction, geophysics, medical imaging, and environmental monitoring are examined. Emerging hybrid approaches combining classical optimization and machine learning are also highlighted. The methods presented ensure stable and physically meaningful reconstruction of sources in ill-posed problems.

Keywords: Inverse problems, optimization methods, source function identification, regularization, gradient-based algorithms, derivative-free optimization, numerical methods, machine learning, uncertainty quantification.

МЕТОДЫ ОПТИМИЗАЦИИ В ОБРАТНЫХ ЗАДАЧАХ – ОПТИМИЗАЦИОННЫЕ ПОДХОДЫ ДЛЯ ОПРЕДЕЛЕНИЯ ФУНКЦИИ ИСТОЧНИКА

Аннотация: В данной работе рассматриваются методы оптимизации для решения обратных задач, с особым вниманием к определению неизвестных функций источников в параболических уравнениях с частными производными. Обсуждаются формулировка задачи, методы регуляризации, численные алгоритмы оптимизации, стратегии параметризации и оценка неопределенности. Рассматриваются приложения в задачах теплопроводности, геофизики, медицинской визуализации и мониторинга окружающей среды. Также освещаются новые гибридные подходы, объединяющие классическую оптимизацию и машинное обучение. Представленные методы обеспечивают стабильное и физически корректное восстановление источников в некорректных задачах.

Ключевые слова: Обратные задачи, методы оптимизации, идентификация функции источника, регуляризация, градиентные алгоритмы, методы оптимизации без производных, численные методы, машинное обучение, оценка неопределенности.

Inverse problems play a central role in scientific and engineering disciplines, where the objective is to determine unknown causes or parameters from observed effects. A prominent example is the identification of a source function in parabolic partial differential equations, such as the heat equation. In such problems, optimization methods are essential for reconstructing unknown source terms from measured data. These problems are generally ill-posed, meaning small errors in measurement can result in large deviations in

the solution, necessitating robust and stable optimization approaches. The source function represents an unknown distribution of energy or matter that affects the system's evolution. To determine this function, one defines an objective function that quantifies the difference between observed data and model predictions. Typically, this is expressed as a least-squares functional, integrating the squared differences between observed and simulated states. Minimizing this functional approximates the true source distribution. However, direct minimization can amplify noise due to ill-posedness, leading to unphysical solutions.

Regularization methods are introduced to stabilize the solution. One widely used technique is Tikhonov regularization, which adds a penalty term to suppress large or irregular solutions. The regularized objective function is commonly written as $J(f) = \|u(f) - u\_obs\|^2 + \alpha\|Lf\|^2$, where $u(f)$ is the system solution for source function f, u_obs is observed data, L is a regularization operator, and α is the regularization parameter controlling the balance between data fidelity and smoothness. Choosing an appropriate α is critical and can be guided by methods such as the L-curve, generalized cross-validation, or discrepancy principle.

Numerical optimization techniques for solving the regularized inverse problem can be categorized into gradient-based and derivative-free methods. Gradient-based methods, such as steepest descent, conjugate gradient, and quasi-Newton algorithms, utilize the sensitivity of the objective function with respect to source parameters. Gradients are often calculated efficiently through adjoint equations, which provide derivatives with respect to high-dimensional source spaces. Derivative-free methods, including genetic algorithms, particle swarm optimization, and simulated annealing, are valuable when gradients are difficult to compute or when the objective function has multiple local minima. Although these methods explore the solution space more globally, they usually demand higher computational resources.

Parameterization of the source function is a critical step to reduce problem dimensionality and improve numerical stability. Representing the source using a finite-dimensional basis, such as piecewise constants, splines, or orthogonal polynomials, simplifies optimization and can incorporate prior knowledge about smoothness or localization. Bayesian frameworks further enhance the solution by allowing the inclusion of prior distributions on the source, facilitating uncertainty quantification and probabilistic interpretation. Optimization-based inverse methods have broad applications. In heat conduction problems, the aim may be to identify heat sources from boundary temperature measurements. In geophysics, subsurface properties are inferred from surface seismic data. In medical imaging, techniques like diffuse optical tomography reconstruct tissue absorption or scattering coefficients. Each application presents unique challenges, including incomplete data, measurement noise, and complex geometries, necessitating careful adaptation of optimization strategies.

Computational efficiency is essential for large-scale inverse problems. Efficient solvers for the forward and adjoint problems, combined with scalable optimization algorithms, enable the practical resolution of high-dimensional source identification tasks. Parallel computing, reduced-order modeling, and surrogate-based optimization are

frequently employed to accelerate computations. Validation of reconstructed sources is crucial to ensure physical plausibility. Synthetic tests, cross-validation with independent measurements, and residual analysis help assess solution quality. Sensitivity analysis examines how errors in measurements or modeling assumptions propagate to the reconstructed source, informing experimental design and measurement placement.

Recently, hybrid methods combining classical optimization and machine learning have emerged. Neural networks and deep learning models can approximate the mapping from observations to sources, accelerating inversion. Integrating data-driven models with regularized optimization leverages prior knowledge and observed patterns, enhancing reconstruction accuracy. In summary, optimization methods offer a powerful framework for solving inverse problems and determining source functions in parabolic and other PDEs. Through objective function formulation, regularization, numerical optimization, parameterization, and uncertainty quantification, physically meaningful and stable solutions can be obtained despite ill-posedness. Continuous research in this field improves stability, accuracy, and computational efficiency, extending the application of inverse problem optimization across diverse scientific and engineering areas.

Building on the foundational concepts of optimization methods in inverse problems, the second part focuses on practical implementation strategies, advanced numerical techniques, and emerging trends. A key step in applying optimization is the formulation of the forward problem, which models the system behavior for a given source function. Accurate numerical solutions of the forward model, typically using finite difference, finite element, or spectral methods, are essential for reliable source reconstruction. Inaccuracies in the forward model propagate directly into the inverse solution, emphasizing the importance of discretization accuracy and computational stability.

Adjoint-based sensitivity analysis is a cornerstone of gradient-based optimization for high-dimensional source functions. The adjoint problem allows efficient calculation of derivatives of the objective function with respect to all source parameters simultaneously. This method significantly reduces computational cost compared to finite difference approximations and enables the use of advanced gradient-based algorithms such as limited-memory BFGS or nonlinear conjugate gradient methods. Incorporating constraints, such as non-negativity or physical bounds on the source function, can further improve solution realism and prevent unphysical artifacts.

Derivative-free global optimization methods complement gradient-based approaches when the objective function is non-smooth or contains multiple local minima. Techniques like genetic algorithms evolve a population of candidate solutions using selection, crossover, and mutation, gradually converging towards optimal solutions. Particle swarm optimization uses collective behavior principles, with agents exploring the search space while sharing information to guide convergence. Simulated annealing mimics thermodynamic cooling processes to escape local minima and approach global optima. These methods are particularly useful in complex inverse problems with irregular geometries or highly nonlinear forward models.

Regularization strategies continue to play a critical role in stabilizing inverse solutions. Beyond classical Tikhonov regularization, modern approaches such as total variation (TV) regularization encourage piecewise-smooth reconstructions, preserving sharp transitions in the source function. Sparsity-promoting regularization using L1 norms facilitates identification of localized sources in large domains. Adaptive regularization schemes, where the regularization parameter evolves during optimization, can enhance both accuracy and convergence.

Hybrid frameworks integrating optimization with machine learning are emerging as powerful tools. Neural networks trained on synthetic or historical datasets can approximate forward mappings or inverse mappings directly. Combining such models with physics-based regularization ensures adherence to governing equations while leveraging data patterns. Bayesian deep learning further enables quantification of uncertainties in reconstructed sources, providing confidence intervals and probabilistic estimates.

Applications of these advanced methods span multiple fields. In environmental engineering, pollutant source identification relies on inverse transport models and optimization to track contaminant origins. In medical imaging, algorithms reconstruct spatially varying parameters such as tissue perfusion or metabolic activity from non-invasive measurements. In structural health monitoring, inverse optimization detects defects or damage in materials by interpreting vibration or stress response data. Each application benefits from tailored regularization, parameterization, and optimization strategies.

Computational considerations remain central for large-scale inverse problems. Parallel processing, GPU acceleration, and efficient linear solvers enable handling of fine-resolution models with millions of unknowns. Model reduction techniques, such as proper orthogonal decomposition (POD) or reduced basis methods, allow significant speedup while retaining essential system dynamics. Surrogate models or meta-models can further approximate the forward problem, allowing rapid exploration of parameter space during optimization.

Validation, verification, and uncertainty analysis are critical for practical deployment. Synthetic case studies, benchmarking against known sources, and cross-validation using independent measurements ensure the reliability of reconstructed solutions. Sensitivity analysis identifies dominant parameters and informs measurement planning, reducing ambiguity in inverse reconstructions.

In conclusion, the practical implementation of optimization methods for inverse problems combines accurate forward modeling, robust numerical optimization, regularization, and emerging data-driven techniques. These methods enable stable and physically consistent reconstruction of source functions in complex, ill-posed problems. Ongoing research integrates advanced computational strategies, hybrid machine learning approaches, and uncertainty quantification, expanding the reach and reliability of inverse problem solutions in scientific and engineering applications.

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