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Design and Optimization of Numerical Methods for Solving Inverse Problems

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Abstract
. The purpose of inverse problems is to identify the unknown causes or parameters based on observable effects or measurements in a variety of scientific and technical domains. To arrive at precise and trustworthy solutions, numerical algorithms for inverse problems must be designed and optimised. The creation and optimisation of numerical algorithms specifically created for solving inverse issues are presented in detail in this abstract.The formulation of inverse issues and the mathematical models that explain the underlying processes are the primary topics of the first part of this work. We examine many inverse issues, such as ill-posed, parameter estimation, and linear and nonlinear ones. Prior information and regularisation methods must be used to increase the stability and uniqueness of the answers.The creation and application of numerical algorithms for the solution of inverse problems is the focus of the second component. We study in depth a number of iterative techniques, including the conjugate gradient method, Levenberg-Marquardt algorithm, and Gauss-Newton method. There is also discussion of sophisticated methods such variational methods, Bayesian inference, and approaches based on optimisation.The third consideration focuses on optimising numerical techniques to raise their effectiveness and precision. To hasten convergence and lower computational costs, methods like adaptive mesh refinement, parallel processing, and model reduction are examined. Additionally, methods for handling noisy or missing data are looked at, as well as methods for choosing the right regularisation settings.

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Introduction

A very effective quantum many-body theory that is frequently used to model finite and periodic systems is density functional theory (DFT) [1]. Due to the accessibility of approximation exchange-correlation functionals used in the direct problem to calculate the ground-state electronic density, DFT is effective. In contrast, retrieving the correct exchange-correlation potential from a given electronic density is the goal of the Kohn-Sham (KS) DFT inverse issue. The inverse problem is referred to as density-to-potential inversion in this tutorial because it largely focuses on the ground-state form of KS DFT.The forward and inverse problems use the identical equations, but because the input and output variables differ greatly, they call for different approaches to solving them. The course focuses on the numerical techniques needed to resolve the density-to-potential inversion problem inside DFT as a result [2].

The study of inverse issues related to distributed parameter systems and their numerical approximation with the finite element method are the main topics of this work. With regard to inverse identification and optimum control problems, we specifically discuss the estimation of convergence rates. In [3] many practical applications, inverse problems show nonlinearity and ill-posedness, making it difficult to solve them numerically. These issues also typically have nonlinear parameter-to-observation mappings that are not invertible. As a result, we look into issues that have the following broad formulation:

$\min \mathrm{F(u)} + \mathrm{fiG(q)};\ \text{subject to}\ \mathrm{l\_(q,u)} = \mathrm{g}\ \text{in}\ H^{-1},$ ……..(1)

The goal is to identify the unknown parameters or controls related to the underlying distributed parameter system using observable data, often in the form of measurements or partial information. To do this, we discretize the issue and create a numerical approximation using mathematical models and the finite element approach. The discretization produces an equation system that can be iteratively solved using the right algorithms and optimisation methods.We examine the inverse identification and optimum control problem's convergence rates in order to gauge the precision and effectiveness of the numerical solution. Estimates of convergence offer important insights into how the numerical approximation behaves as discretization parameters like mesh size or time step are improved.

I. Inverse Method and Direct method

Although the Kohn-Sham (KS) equations are used in both the direct and inverse problems of density functional theory (DFT) [4], they display substantial differences that call for different techniques and convergence criteria. In this section, we give a brief summary of the numerical techniques that are frequently employed to address the direct DFT problem. Then, we go into great length to explain several inverse-problem techniques. For the sake of simplicity, we only explore one-dimensional systems in our examples, but the provided formulas can also be used to model multidimensional systems [5], which will speed up future research. Additionally, we concentrate on spin-compensated systems and typically skip the spin index from formulae.

$$\varepsilon_j \underline{\phi_j}\,(\mathbf{r}) = \left[-\frac{\Delta}{2} + v_{\mathrm{KS}}\,([\underline{n}], \mathbf{r})\right] \underline{\phi_j}\,(\mathbf{r}), \quad \ldots\ldots(1)$$

Finding the ground-state electronic density by resolving the KS equations is the direct DFT problem. For this purpose, self-consistent field (SCF) iteration schemes, such as the well-known Hohenberg-Kohn-Sham approach, are frequently used in numerical methods. The KS equations are iteratively solved in SCF using an initial estimate of the electronic density until self-consistency is reached. The density is often compared between iterations until a predetermined tolerance is met as part of the convergence criteria.

$$\underline{n}\,(\mathbf{r}) = 2\sum_{j=1}^{N} |\underline{\phi_j}\,(\mathbf{r})|^2, \quad \ldots\ldots(2)$$

To recover the exchange-correlation potential from a given electronic density is the goal of the DFT inverse problem. To meet this challenge, a number of inverse-problem techniques have been created. One of these is the linear response approach, which updates the potential by linearizing

and solving the KS equations repeatedly until the necessary precision is attained. The optimization-based method [7] is an alternative strategy that formulates an optimisation problem to reduce the difference between the calculated and given densities by modifying the potential. This optimisation problem is frequently solved using iterative methods like gradient descent or conjugate gradient methods.

The orbitals[6] are commonly chosen in the density functional theory (DFT) inverse problem so that the set of lowest possible eigenvalues is formed by the related eigenvalues. The Kohn-Sham (KS) equations are effectively met by making this decision. The KS equations can be recast as follows for the inverse problem:

$$\varepsilon_j \underline{\phi_j(\mathbf{r})} = \left[-\frac{\Delta}{2} + v_{KS}\ ([n], \mathbf{r}) \right] \underline{\phi_j(\mathbf{r})}, \quad \text{..... (3)}$$

$$n(\mathbf{r}) = 2 \sum_{j=1}^{N} \underline{|\phi_j(\mathbf{r})|^2}, \quad \text{..... (4)}$$

$$v_{KS}([n], \mathbf{r}) = v_{ext}(\mathbf{r}) + v_H([n], \mathbf{r}) + \underline{v_{xc}([n], \mathbf{r})}, \quad \text{..... (5)}$$

The KS potential [7] demonstrates density dependence in the setting of the density functional theory (DFT) inverse issue, which results in a nonlinear eigenvalue problem. Equation 4 represents a linear eigenvalue issue, in comparison. Equation 5 illustrates how the definition of the density leads to the nonlinearity in the inverse issue. The eigenvalue problem in the inverse problem cannot be solved using the mixing strategies that are frequently used in numerical approaches for the direct problem because of the subtle difference in nonlinearity.

Numerous [8] [9] numerical techniques for resolving the Kohn-Sham (KS) equations can be divided into three basic categories: plane waves and grid approaches, localised atomic-(like) orbitals, and atomic sphere techniques. As in the Octopus time-dependent density functional theory (TDDFT) code, we apply the finite difference grid method for our calculations. The finite difference method has the advantage of being able to capture crisp features that could be difficult to get using other conventional basis sets for electronic structures. The finite difference formulation of density functional theory (DFT), which is essential for resolving the direct problem and also pertinent to several techniques used in the inverse problem, is briefly described in this section.

The grid-based [11]discretization of the domain of interest and finite difference approximations of derivatives are the foundations of the finite difference approach. The differential operators found in the KS equations can be represented simply using this method. The differential equations are transformed into a set of algebraic equations that can be solved numerically by discretizing the spatial coordinates. The finite difference method's grid-based design makes it possible to tackle systems with intricate geometries and distinct features, giving it an edge over alternative basis sets in some situations [10].

$$\frac{1}{h^2}\begin{bmatrix} \frac{15}{4} & -\frac{77}{6} & \frac{107}{6} & -13 & \frac{61}{12} & -\frac{5}{6} & 0 \\ \frac{5}{6} & -\frac{5}{4} & -\frac{1}{3} & \frac{7}{6} & -\frac{1}{2} & \frac{1}{12} & 0 \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & 0 & 0 \\ 0 & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & 0 \\ 0 & 0 & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ 0 & \frac{1}{12} & -\frac{1}{2} & \frac{7}{6} & -\frac{1}{3} & -\frac{5}{4} & \frac{5}{6} \\ 0 & -\frac{5}{6} & \frac{61}{12} & -13 & \frac{107}{6} & -\frac{77}{6} & \frac{15}{4} \end{bmatrix},$$

Similar to the Octopus TDDFT code [14], we solve the KS equations using the finite difference grid technique. Sharp features can be captured using this method, which may be difficult with conventional electronic-structure basis sets. We give a general overview of the finite difference DFT formulation, which is crucial for resolving the direct problem and has application to particular techniques used to solve the inverse problem.

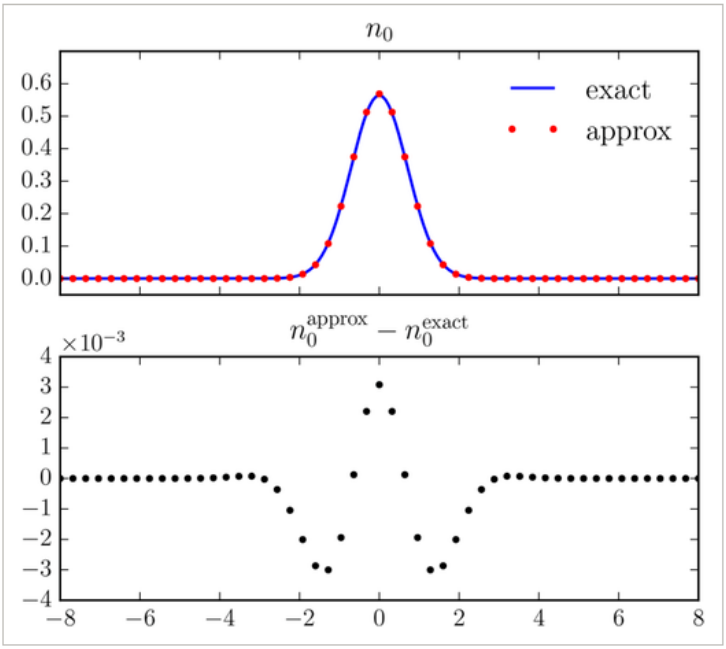

Figure 1: Density of the harmonic oscillator in comparison to an approximation using numbers

A typical [16]density functional theory (DFT) computation for an interacting system requires numerous eigenvalue solutions inside the context of the self-consistent field (SCF) approach, in contrast to the previous example of a noninteracting system, which only required solving a single eigenvalue problem.

II. Inverse-problem methods

We discuss existing density-to-potential algorithms in this context and describe two new inversion techniques. These techniques are defined in terms of the finite-difference method, and it might be essential to make some modifications to algorithms created for basis-set techniques.

1. Two electrons, one and two: One-orbital formula

The review covers well-known density-to-potential methods and discusses the benefits and drawbacks of each. In addition, we present two fresh inversion approaches that add to the arsenal of methods already available for dealing with the DFT inverse problem. Notably, the finite-difference method is used in all of the examples, enabling the explicit treatment of spatial derivatives and making it easier to include sharp features in the potential.

Although the algorithms given here are mostly developed in the context of the finite-difference approach, certain adjustments could be necessary when switching from basis-set methods. The finite-difference framework's algorithms are compatible and effective thanks to these improvements.Numerous [15] numerical techniques are available for the DFT inverse problem, each with advantages and drawbacks of their own. We offer two innovative inversion techniques and give a thorough analysis of density-to-potential procedures. The presentation is based on the finite-difference approach, however algorithms created for basis-set methods may need some minor adaptations.

$$v_{KS}([n],\mathbf{r})=\frac{\Delta\phi_0(\mathbf{r})}{2\phi_0(\mathbf{r})}=\frac{\Delta\sqrt{n_0(\mathbf{r})}}{2\sqrt{n_0(\mathbf{r})}} \quad \text{..... (6)}$$

By setting the energy to zero and solving for the potential in terms of the ground state density, represented as n0, it is possible to derive the KS potential from Equation 1. This strategy is appropriate because the potential can only be calculated up to a constant. In the scenarios of a single electron or two electrons with opposing spins occupying the same orbital, the resulting formula is precise. The bosonic potential or one-electron potential are typical names for it.

The equation determining the KS potential [17] can be explicitly solved by setting the energy to zero, resulting in a formula that directly connects the potential to the ground state density. For systems with one electron or two electrons occupying the same space with opposite spins, this connection is perfect.

$$v(x)=\frac{x^2}{2}[\Theta(x-4)-\Theta(x+4)]-x[\delta(x-4)+\delta(x+4)]+[\delta'(x-4)-\delta'(x+4)]/2, \quad \text{..... (7)}$$

Approximations of the potential values close to the boundaries can sometimes be obtained when the density is artificially set to zero at the boundaries. By applying the boundary requirements, discontinuous behaviour was introduced, which is where these approximations come from. The potential, however, is accurate everywhere, including at and near the boundaries, as it fulfils the Dirac delta and Heaviside functions when the approximate boundary requirements are not imposed.

We explore the ground state density of a particle-in-a-box system to demonstrate the idea of smoothing.

$$n_0^{\text{exact}}(x)=\frac{2}{L}\sin^2\left(\frac{\pi x}{L}\right) \quad \text{..... (8)}$$

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Correspond to

$$v(x)=\begin{cases}0 & \text{if } 0<x<L\\ \infty & \text{otherwise}\end{cases}. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(9)$$

We can use a small bit of weighted noise produced by the common normal distribution to add a small amount of noise to the precise ground-state density. This is how the procedure might be summed up:

$$n_0^{\text{noise}}=n_0^{\text{exact}}\left[1+\mathrm{N}\left(0,1\times10^{-10}\right)\right], \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$

In contrast to the potential obtained without any scaling prior to smoothing, Figure 2 clearly shows that the potential generated by applying logarithmic scaling before fitting exhibits much increased accuracy in the asymptotic area.

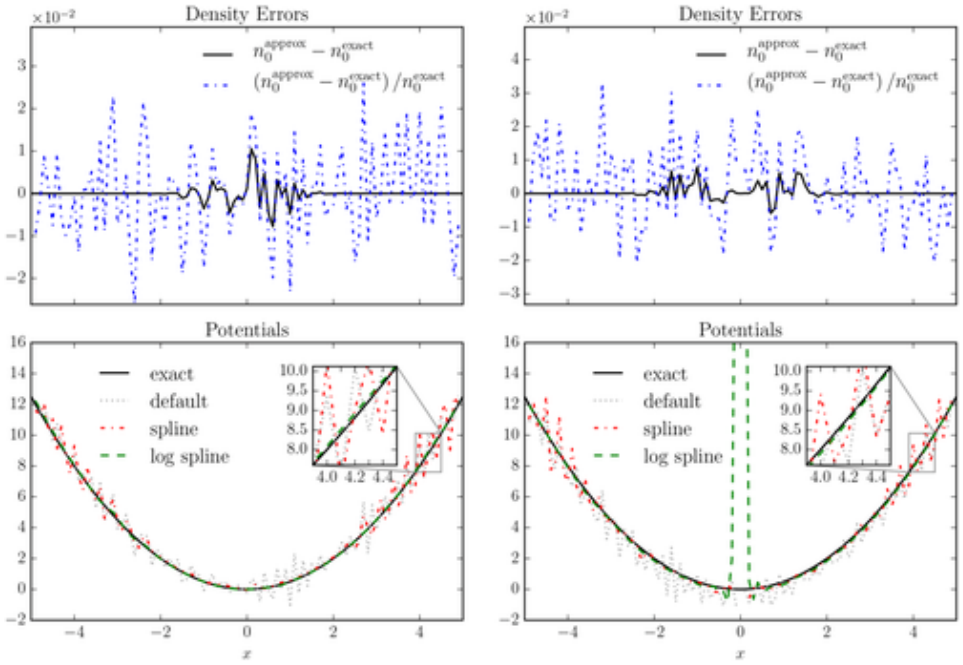

Figure 2: Weighted randomly distributed noise contaminates the harmonic oscillator's density.

III. Example of inversion Method

More realistic cases in practical DFT inversions contain interacting densities, and Equation 4 is used to separate the exchange-correlation potential from the retrieved KS potential. Unless otherwise stated, we use the one-orbital approximation as the first assumption for the unknown potential throughout our examples. In Appendix B, the gradients used for the PDE-constrained optimisations are listed. Table 1 lists the abbreviations used in this section to distinguish between the various inversion techniques covered.To demonstrate the inversion techniques, we use well-known noninteracting quantum systems. We may concentrate on the numerical features of each inversion approach because the recovered KS potentials for these systems match the known external potentials. Interacting densities and Equation 4's extraction of the exchange-correlation

potential from the recovered KS potential are necessary for realistic DFT inversions. The one-orbital approximation is frequently used in the examples as the initial estimation of the potential, and Table 1 lists the abbreviations used to distinguish between the various inversion techniques.

Table 1: DFT inversion technique using labels

Method used a Inversion	Lables
Constraint Optimization (PDF)	PDF
Wu & Yang	WY
Constraint Variation	CV
Van LeeuwanBaerends	vLB

We use scaling, several finite difference approximations, and the DCBC approach in the PDE and CV routines of the examples supplied. Our decision-making is influenced by our familiarity with these methods and the way they are currently implemented in our code. The vLB and WY techniques can also be altered to include comparable features, guaranteeing that all implementations show comparable error patterns in asymptotic regions. To permit easier comparisons and to emphasise differences, the mistake patterns in the examples have been purposefully changed.

1. Harmonic potential inversion

In our first inversion example, we assume a non-interacting system with six electrons that is subjected to a harmonic potential. The target density is created by taking into account the system's lowest three orbitals.

$$\phi_0(x)=\pi^{-1/4}e^{-\frac{x^2}{2}}, \quad \text{(11)}$$

$$\phi_1(x)=\frac{\sqrt{2}x}{\pi^{1/4}}e^{-\frac{x^2}{2}}, \text{ and} \quad \text{(12)}$$

$$\phi_2(x)=\frac{(2x^2-1)}{\sqrt{2}\pi^{1/4}}e^{-\frac{x^2}{2}}, \quad \text{(13)}$$

In this illustration, the target density is created by taking into account the lowest three doubly occupied orbitals of a noninteracting system, as stated in Equation 1. We study the inversion of this density using a variety of techniques, and Figure 3 shows the related recovered potentials. We also plot the discrepancies between the recovered potentials and the precise potential because the potential is only unique up to a constant. A stronger potential recovery is indicated by larger constant differences.

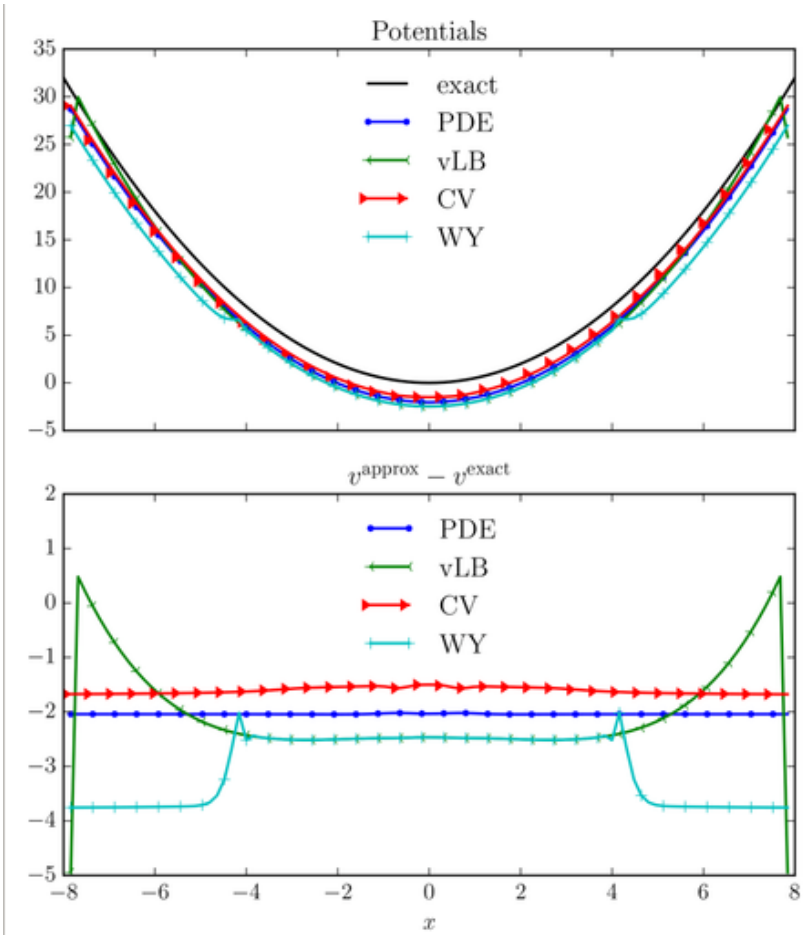

Figure 3: Recovered Potential for inversion density techniques

2. Morse potential inversion

We consider a non-interacting system made up of six electrons in the Morse potential for our second inversion example. When modelling diatomic molecules and performing molecular spectroscopy, the Morse potential is a frequently utilised potential function.

$$v(r)=D_e\left(1-e^{-a(r-r_e)}\right), \quad \text{..... (14)}$$

The non-interacting system with the Morse potential and the parameters a = 1/2, De = 10, and re = 3 is the subject of the second inversion example. Reference 19 has the analytical answers for the wave functions of this system, and Equation 1b uses these wave functions as input to create the target density.

The Morse potential governs a non-interacting system in the second inversion scenario. Figure 4 uses a grid with 51 evenly spaced points in the range of 1 to 9 to display the potentials that are recovered from the target density, which is created using analytical wave functions.

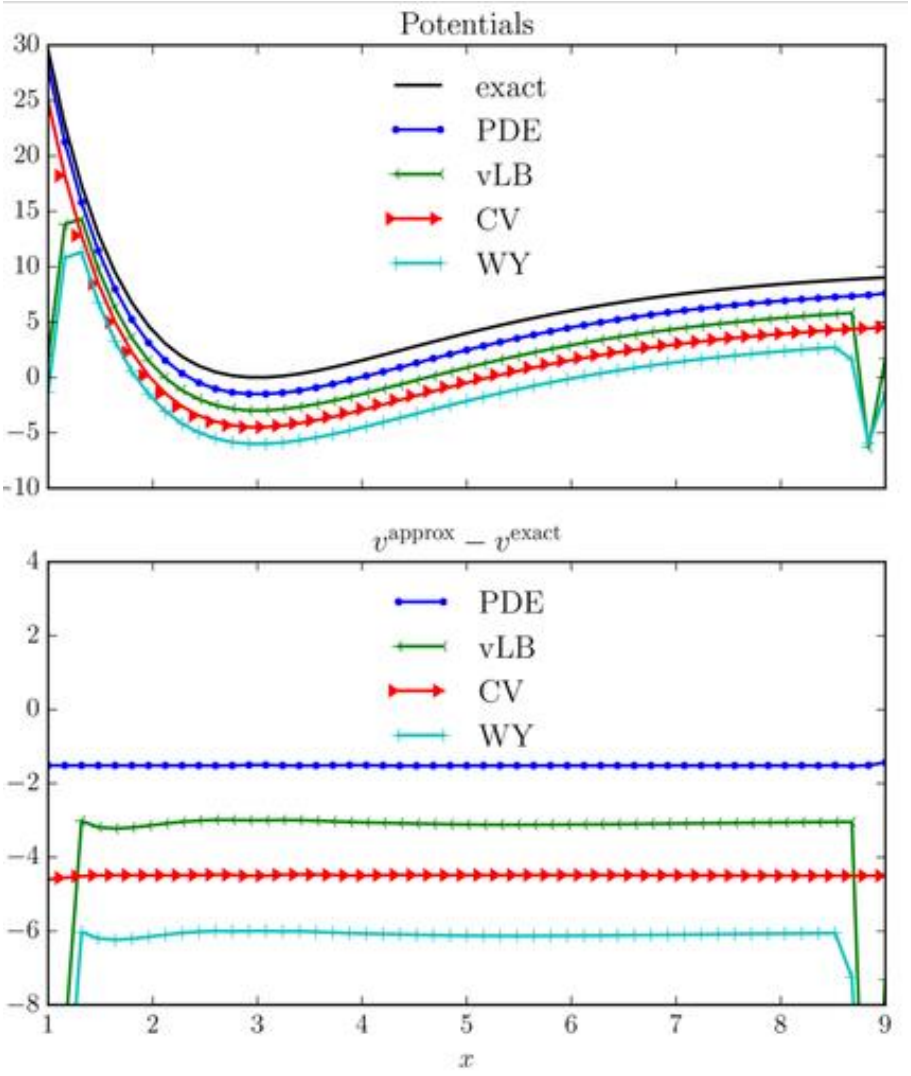

Figure 4:Potentials that are recovered from the target density

This inversion illustration demonstrates different mathematical difficulties. The precise representation of the kinetic energy operator on the selected grid is a major problem. In this case, the Laplacian is approximated by a fourth-order approximation in the PDE and CV methods and by a second-order approximation in the other methods. The WY and vLB potentials oscillate as a result of this accuracy disparity because the inversion methods are able to account for the flaws in the Laplacian approximation, especially on a coarse grid.Additionally, the scaled PDE-constrained optimization's initial estimation of a one-orbital approximation for the real potential is insufficiently precise. As a result, the optimizer is unable to find the right potential and becomes stuck in a local minimum. The shallowness of the potential makes this situation worse by making the scaled density overly high close to the right boundary.

The inversion example illustrates the numerical difficulties involved in appropriately modelling the kinetic energy operator on a grid. The WY and vLB potentials oscillate due to the mismatch between the fourth-order and second-order Laplacian estimates. Additionally, the scaled PDE-

constrained optimization's ability to find the proper potential is hampered by using the one-orbital approximation as an initial guess, in part because right boundary.

IV. Conclusion

Numerous scientific and engineering applications depend heavily on the invention and optimisation of numerical methods for tackling inverse issues. Due to their intrinsic ill-posedness and nonlinearity, inverse problems, which are encountered while trying to recover unknown parameters or functions from observable data or measurements, sometimes provide difficult obstacles.In this paper, we have focused on the inverse problem of Kohn-Sham (KS) DFT and investigated the unique context of inverse problems in the field of density functional theory (DFT). The distinctions between the direct and inverse DFT problems have been examined, with an emphasis on the necessity of specific methods and convergence standards for each problem.The direct problem of the DFT has been studied using a variety of numerical techniques, including as the plane wave and grid methods, localised atomic orbitals, and atomic sphere techniques. We have also investigated the numerical techniques used to solve the DFT inverse problem, emphasising density-to-potential inversion procedures and presenting novel inversion techniques. Our study has demonstrated the importance of elements like scaling, finite difference approximations, and boundary conditions in obtaining precise and trustworthy answers to inverse issues. We have also seen how various decisions and approximations affect the inversion algorithms' accuracy and convergence behaviour.A thorough grasp of the underlying mathematical models, problem-specific restrictions, and the interaction between the forward and inverse processes are necessary for the creation and optimisation of numerical methods for addressing inverse issues. We can improve our capacity to precisely reconstruct unknown characteristics and make contributions to developments across a range of scientific and engineering disciplines by creating efficient numerical algorithms.

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