SOME RECENT DEVELOPMENTS AND OPEN PROBLEMS IN SOLUTION METHODS FOR MATHEMATICAL INVERSE PROBLEMS

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Abstract. *The area of mathematical inverse problems is quite broad and involves the qualitative and quantitative analysis of a wide variety of physical models. Applications include, for example, the problem of inverse heat conduction, image reconstruction, tomography, the inverse scattering problem, and the determination of unknown coefficients or boundary parameters appearing in partial differential equation models of physical phenomena.*

We will survey some recent developments in the area of regularization methods for mathematical inverse problems and indicate where further contributions are needed. We will discuss methods for which a primary goal is to avoid the oversmoothing of solutions that typically occurs when classical regularization schemes (such as Tikhonov regularization) are used. Oversmoothing is particularly troublesome in imaging and tomographic applications, where it is of high priority to recover sharp or fine features of solutions. We will also explore the trend to design localized regularization methods which complement the qualitative nature of a particular inverse problem (as opposed to the application of a generic regularization method such as Tikhonov's method). Local regularization methods tend to be more attractive in terms of numerical costs and implementation, but a number of open questions remain in their theoretical analysis. Finally, we will discuss current work in the area of iterative solution methods, regularization schemes which have been successfully applied to a number of important nonlinear inverse problems.

Key-words: *mathematical inverse problems, regularization methods, iterative regularization, local regularization methods, inverse heat conduction, imaging.*

1. INTRODUCTION

The purpose of this paper is to survey some recent developments in the area of regularization methods for mathematical inverse problems. In undertaking this task it is difficult to avoid a certain amount of mathematical rigor. Nevertheless, because one goal of the paper is to try to explain some newer developments in mathematical regularization theory to an audience which may not have the needed background courses in operator theory or functional analysis, we will wherever possible try to use more formal (less rigorous) explanations and to supplement the mathematical concepts below with examples. We will also take a few short-cuts in some definitions and statements of the theory in order to keep notation simplified and the level of mathematical exposition within reach of a more general audience. We do this with apologies to those readers wishing a more careful mathematical treatment of these topics (and who will recognize fairly quickly the short-cuts we have taken) and strongly encourage these readers to explore the references given at the end of the paper.

Mathematically, an *inverse problem* is often expressed as the problem of finding $\bar{u}$ (a function, typically) which solves the *operator equation*

$$\mathcal{A}(u) = f \tag{1}$$

where f is an "idealized" data function. (Usually we require $\bar{u} \in X$, a real Banach or real Hilbert space, and we take f belonging to a real Hilbert space Y.) The operator $\mathcal{A}$ may be linear or nonlinear, depending on the application; below we will give explicit definitions of $\mathcal{A}$ in the case of several important examples. If the data f is not in the range of $\mathcal{A}$ there is no possibility of a solution of (1), so typically we generalize the inverse problem and instead seek a solution $\bar{u}$ of the output least squares problem

$$J(\bar{u}) = \min_{u} J(u) \tag{2}$$

where

$$J(u) \stackrel{def}{=} \|\mathcal{A}(u) - f\|_{Y}^{2}, \tag{3}$$

for $\mathcal{A}$ the operator in (1) and for $\|\cdot\|_Y$ the norm used to measure data functions (i.e., the norm on the Hilbert space Y). For the latter, a common situation is where Y indicates the space of square-integrable functions on a given domain Ω; in this case, the norm $\|\cdot\|_Y$ is defined via

$$\|\mathcal{A}(u) - f\|_{Y}^{2} = \int_{\Omega} |\mathcal{A}(u)(\mathbf{x}) - f(\mathbf{x})|^{\mathbf{2}}\, \mathbf{dx}. \tag{4}$$

It can be the case that there are many solutions of the output least squares problem; in this case, uniqueness can often be restored by seeking a minimum norm solution $\bar{u}$ of the least squares problem (see, e.g., [20, 28]).

An inverse problem is generally *ill-posed* in the sense that $\bar{u}$ does not depend continuously on f; what this means in a practical setting is that whenever we only have in hand an imprecise measurement f^{δ} of the data (instead of the idealized f – in fact, this is the normal situation due the usual presence of measurement error or computer round-off error), then one cannot rely upon the solution $\bar{u}^{\delta}$ obtained by solving (1) (or (2)) using the perturbed data f^δ in place of f. That is, we generally have $\bar{u}^\delta$ far from $\bar{u}$ even if f^δ is close to f. Typically the presence of data error leads to highly oscillatory solutions, and this can only be avoided if a stabilization procedure or *regularization method* is used.

In what follows we give two examples of *linear* inverse problems, followed by one example of a *nonlinear* inverse problem; in each case we define the associated operator $\mathcal{A}$ and we indicate what kind of finite-dimensional equations arise when discretization methods are applied to enable computer-based solution of each inverse problem.

Example 1. The inverse heat conduction problem (IHCP).
The inverse heat conduction problem (IHCP), or sideways heat equation, is typically stated as the problem of using *internal* temperature or temperature-flux measurements to determine the unknown heat or heat flux source which is being applied at the *surface* of a solid. Temperature measurements are collected at various internal spatial locations and monitored over the course of time, the final goal of which is to reconstruct a time-varying function representing the temperature history on the surface of the solid. The IHCP occurs in numerous applied settings, for example, in the determination of the temperature profile of the surface of a space vehicle during its re-entry into the earth's atmosphere [8].

As one example of the IHCP, consider the problem of recovering a heat source $u = u(t)$ at the boundary $x = 0$ of an insulated semi-infinite bar on the non-negative x-axis. If u is known, the governing partial differential equation (for zero initial heat distribution) is

$$\begin{aligned} w_t(t,x) &= w_{xx}(t,x), \quad 0 < x < \infty,\ 0 < t < T, \\ w(t,0) &= u(t), \quad 0 < t < T, \\ w(0,x) &= 0, \quad 0 < x < \infty. \end{aligned}$$

The *direct problem* associated with this model is that of determining w when u is known, while the *inverse problem,* (of interest in this paper) is the problem of using data, or information about w, to recover the "true" value $\bar{u}$ of the boundary function. Suppose that data is collected at the spatial location $x = 1$ (i.e., unperturbed measurements are given by $f(t) \equiv w(t,1) \in \mathbb{R}$ for $0 < t < T$). Then it may be shown that the unknown source $\bar{u}$ is the solution of an equation of the form (1), i.e., $\bar{u}$ solves

$$\mathcal{A}(u)(t) = f(t), \quad t \in [0,T], \tag{5}$$

where $\mathcal{A}$ is the (bounded linear) operator given by

$$\mathcal{A}(u)(t) = \int_0^t k(t,t')u(t')\,dt', \quad t \in [0,T], \tag{6}$$

with the kernel k of convolution type, namely, $k(t,s) = \kappa(t-s)$ where

$$\kappa(t) = \frac{1}{2\sqrt{\pi}\,t^{3/2}}e^{-1/4t}, \quad t \in [0,T].$$

In this example, the operator equation is of the form of a first-kind integral equation of *Volterra* (or *causal*) type [10], with $\mathcal{A}$ in (6) a *Volterra operator.* By causal we mean that the original problem has the property that, given $t_0 \in (0,T)$, the solution u on the interval $[0,t_0)$ is determined only from the values of f on that same interval; i.e., the solution only depends on information from the past.

Given "suitable" data f, there is a unique solution of (5). However, most measured data f^δ is not sufficiently smooth to guarantee such a result.

Discretization of the IHCP:
To solve this inverse problem in an applied setting, one discretizes (5) and implements a computer-based solution strategy. One such discretization is a collocation approach, as defined in the following. Let $N \geq 1$ be a fixed integer and define $\Delta t = T/N$, $t_i = i\Delta t$, $i = 1, \ldots, N$. We seek a piecewise constant solution u^N (with discontinuities in u^N occurring only at t_i, $i = 1, \ldots, N$) for which the following N conditions hold:

$$\mathcal{A}(u^N)(t_i) = f^\delta(t_i), \quad i = 1, \ldots, N.$$

This leads to a matrix equation

$$\mathbf{A}\mathbf{u}^N = \mathbf{f}^\delta \tag{7}$$

where $\mathbf{A}$ is $N \times N$, nonsingular, and lower triangular (due to the causal nature of the original operator $\mathcal{A}$), $\mathbf{f}^\delta \in \mathbb{R}^N$ with $\mathbf{f}^\delta = (f^\delta(t_1), \ldots, f^\delta(t_N))^\top$, and the entries in $\mathbf{u}^N = (u_1, \ldots, u_N)^\top$ corresponding to the values of the piecewise constant approximate solution u^N at the gridpoints t_i, $i = 1, \ldots, N$. (We note that in fact $\mathbf{A}$ and $\mathbf{f}^\delta$ also depend on N, but we simplify by only using N in the notation for $\mathbf{u}^N$ and u^N.) For more details on this approximation see, for example, [42, 44].

An unregularized solution of the discretized IHCP is $\mathbf{u}^N = \mathbf{A}^{-1}\mathbf{f}^\delta$. However, because the original IHCP is severely ill-posed the matrix $\mathbf{A}$ is badly ill-conditioned, meaning that small errors occurring in the entries in $\mathbf{f}^\delta$ lead to dramatic (and unacceptable) errors appearing in the components of $\mathbf{u}^N$. Thus some sort of regularization/stabilization method is needed for solution of either the infinite-dimensional or (discretized) finite-dimensional problem.

Example 2: Atmospheric imaging and image reconstruction [29]**.**
When a ground-based telescope is used to take an astronomical image, serious blurring can occur due to the scattering of light waves through the atmosphere (due to atmospheric turbulances). A simple model of this image blurring can be written as (1), i.e., as

$$\mathcal{A}(u)(x,y) = f(x,y), \quad (x,y) \in \Omega, \tag{8}$$

where $u = u(x,y)$ represents the gray-values of the true image at the two-dimensional location $(x,y) \in \Omega$, $f = f(x,y)$ denotes the gray-values of the observed image (the "data", as collected using the telescope), Ω is the (x,y)-region of the image, and the process of blurring or scattering is described via the (bounded, linear) operator $\mathcal{A}$,

$$\mathcal{A}(u)(x,y) = \int_\Omega k(x-x', y-y')\, u(x',y')\, d(x',y'), \quad (x,y) \in \Omega. \tag{9}$$

The kernel k is known as a point spread function and is generally assumed to be given; see [29] for a description of the manner in which k may be determined in actual imaging applications.

The reconstruction of the true image is an inverse problem; the task is to use the data f (or more likely, a perturbation f^δ of f) and the model equation (8) to recover an approximation of the true image $\bar{u}$. We note that, like the first example above, equation (8) is a first-kind linear integral equation but, in contrast to the IHCP, the operator $\mathcal{A}$ in (9) is no longer of Volterra or causal type.

Discretization of the image reconstruction problem:
A collocation approach may also be used to define discretizing equations for the image reconstruction problem. The resulting matrix equation in this case is also of the form (7) where now the matrix $\mathbf{A}$ is no longer lower-triangular (because the operator $\mathcal{A}$ is not of Volterra type). In fact, the 2-dimensional nature of the image reconstruction problem gives that the matrix $\mathbf{A}$ is an $N \times N$ block matrix, with each block itself an $N \times N$ matrix. The fact that the kernel k appearing in $\mathcal{A}$ in (9) is of convolution type means that $\mathbf{A}$ has additional structure in that each of its N^2 blocks is a Toeplitz matrix (i.e., the entries are unchanged along diagonals of the matrix) and the overall block matrix is block-Toeplitz (the blocks on each block-diagonal of the entire matrix are identical). See [29] for a complete description of this construction for an alternate approach (the midpoint method) that is nevertheless quite similar to collocation. In [29], it is noted that quite commonly N ranges from 256 to 1024 and more; for $N = 256$ this means that the matrix $\mathbf{A}$ is quite large at 65536×65536. Thus great care must be taken in developing computational regularization strategies to solve the discrete image reconstruction problem in order to ensure that the scale of the problem does not lead to unmanageable computational costs.

Example 3: A parameter estimation problem.
Perhaps the most common way in which a *nonlinear* inverse problem arises is when one wishes to determine an unknown (physical) coefficient appearing in an ordinary or partial differential model, using data related to the solution of the model equation. We illustrate some features of the parameter estimation problem with the use of a particularly simple example from [68] (with additional development from [28]) before turning to a more complicated example below. Suppose we are observing a population of animals that propagates at the known rate of $g(t)$ per year, but we do not know the death rate u (assumed constant) for these animals. We let $w(t)$ denote the population at time t, where $w(0) = W$, with $W > 0$ known. Then a simple growth model is

$$w'(t) + uw(t) = g(t), \quad 0 < t < T, \tag{10}$$
$$w(0) = W, \tag{11}$$

where our goal is to use observations of the size of the population at any given time to recover the constant death rate u. An application of the variation of constants formula gives us an explicit expression for the solution w of (10)–(11), given any constant value of u; i.e., we may write $w(t) = e^{-ut}\left[W + \int_0^t e^{-us} g(s)\, ds\right]$, whenever u is given. If the data function $f = f(t)$ corresponds to measurements of $w = w(t)$, the inverse problem problem is then to solve

$$\mathcal{A}(u)(t) = f(t), \quad 0 \le t < T, \tag{12}$$

for $\bar{u}$, where

$$\mathcal{A}(u)(t) = e^{-ut}\left[W + \int_0^t e^{-us} g(s)\, ds\right], \quad 0 \le t < T. \tag{13}$$

It is clear that the operator $\mathcal{A}$ is nonlinear in u and that the parameter estimation problem becomes a nonlinear inverse problem. Is is also obvious that if we are seeking a constant-valued solution $\bar{u}$ of (12)–(13), then the inverse problem is severely overdetermined because (12) must hold for all $t \in [0,1]$ with the single constant $\bar{u}$. To handle this, an output least squares approach is typically used instead so that we seek a constant-valued $\bar{u}$ minimizing

$$J(u) = \int_0^T |\mathcal{A}u(t) - f(t)|^2\, dt \tag{14}$$

over all feasible constants in $\mathbb{R}$. With perturbed data f^δ, we replace f by f^δ in (14).

More complicated parameter estimation problems occur, for instance, when one wishes to determine variable coefficients representing unknown physical parameters appearing in partial differential equations. For example, suppose we wish to model heat conduction in a semi-infinite bar on the nonnegative x-axis but the bar's thermal properties are unknown to us. Suppose we know the heat distribution $g(t)$ at the boundary $x = 0$ and we know that the initial temperature of the bar is 0. The model equations for the temperature $w = w(t, x)$ are then

$$\begin{aligned} w_t(t,x) &= (u(x) w_x(t,x))_x, \quad 0 < x < \infty,\ 0 < t < T, && (15)\\ w(t,0) &= g(t), \quad 0 < t < T, && (16)\\ w(0,x) &= 0, \quad 0 < x < \infty, && (17) \end{aligned}$$

where $u = u(x)$ is the unknown spatially-varying parameter representing the heat conductivity. If we are able to observe the internal temperature of the bar at location $x = 1$, our data $f(t)$ would correspond to "ideal" observations of $w(t,1)$. Using measured values f^δ of the data f, the inverse problem is to approximate the "true" conductivity $\bar{u} = \bar{u}(x)$. It would be difficult to write an explicit representation of $\mathcal{A}$ in this case, and in fact we usually avoid even attempting to define $\mathcal{A}$ explicitly in nonlinear inverse problems; instead we take the output least squares approach of finding $\bar{u}$ solving

$$\min_u J(u), \tag{18}$$

where now

$$\begin{aligned} J(u) &\stackrel{\text{def}}{=} \|w(\cdot,1) - f^\delta\|_Y^2 && (19)\\ &= \int_0^T \left(w(t,1) - f^\delta(t)\right)^2 dt \end{aligned}$$

where $w = w(t, x; u)$ solves (15)–(17) for a given value of u. An iterative solution method (e.g., a gradient-based method) for this optimization problem would thus require solving the equations (15)–(17) for $w(\cdot, 1)$ every time that a new value of u is iteratively supplied by the procedure.

Obviously, for nonlinear inverse problems, questions of existence and uniqueness of solutions are of great importance.

Discretization of the parameter estimation problem:
Discretization of a parameter identification problem usually amounts to performing a minimization of a discrete form $\mathbf{J}^N$ of the functional J in (18)–(19) over a set of finite-dimensional representations $\mathbf{u}^N$ of the unknown function u. The discretization of J is usually accomplished via a suitable discretization (finite difference or finite element techniques, etc.) of the partial differential equation system (15)–(17). The discrete output least squares problem is then to find $\bar{\mathbf{u}}^N$ solving

$$\min_{\mathbf{u}^N} \mathbf{J}^N(\mathbf{u}^N), \tag{20}$$

for

$$\mathbf{J}^N(\mathbf{u}^N) = \|\mathbf{w}^N - \mathbf{f}^\delta\|^2 \tag{21}$$

where $\mathbf{f}^\delta$ is a discretization of the measured data f^δ, $\mathbf{w}^N = \mathbf{w}^N(\mathbf{u}^N)$ is the solution of the *discretized* partial differential equation system (15)–(17) for a given value of $\mathbf{u}^N$, and $\|\cdot\|$ denotes the usual Euclidean norm. See [4, 5, 6, 7, 43, 50, 51] for numerous examples of discretizations of parameter estimation problems and for some theory regarding their validity as approximations.

2. STABILIZED SOLUTION OF THE MATHEMATICAL INVERSE PROBLEM

Inverse problems, whether stated in the form of (1) or (2), are typically ill-posed problems in the sense that solutions $\bar{u}$, when they exist, need not be unique and need not depend continuously on data f. The question of existence and uniqueness of solutions is a very important one, but beyond the scope of this paper. In what follows we assume the existence of a unique solution $\bar{u}$ and focus on the issue of continuous dependence on data, which is also known as the issue of *stability*.

To discuss stability issues, we will assume as earlier that our "ideal" data is given by f but that we are only able to obtain observed or measured data f^δ, where $\|f - f^\delta\|_Y \leq \delta$ for some $\delta > 0$ small. In the absence of regularization a solution $\bar{u}^\delta$ of either (1) or (2) with f^δ used in place of f, can generally be a very bad approximation of $\bar{u}$. A regularization method should give us an alternate method of constructing an approximate solution for which we are guaranteed the convergence of the regularized solution to $\bar{u}$ as the noise level δ converges to zero. That is, for suitably small δ, the regularized approximation should do a "reasonable" job of estimating $\bar{u}$.

Among the many different regularization methods, perhaps the classic and most familiar is the method of *Tikhonov regularization.* We briefly review some of the features of Tikhonov regularization below, and then turn to a second general class of regularization methods, *iterative regularization methods.*

2.1. Tikhonov regularization.

Tikhonov regularization takes the output least squares formulation (2) of the inverse problem and adds a stabilizing term to the least squares functional J. More precisely, given measured data f^δ and a selection of a parameter $\alpha > 0$, Tikhonov regularization prescribes a solution $\bar{u}^\delta_\alpha$ of the new problem

$$\min_u J^\delta_\alpha(u), \tag{22}$$

for

$$J^\delta_\alpha(u) \stackrel{def}{=} \|\mathcal{A}(u) - f^\delta\|^2_Y + \alpha\|\mathcal{L}u\|^2; \tag{23}$$

here $\mathcal{L}$ is an operator used for stabilization (i.e., $\mathcal{L}$ is the identity, a differentiation operator, etc.), and $\|\cdot\|$ is the norm on the range space for $\mathcal{L}$. The idea of Tikhonov regularization is to penalize large values or large oscillations in potential solutions, while still asking that the matching of the model output $\mathcal{A}(u)$ to measured data f^δ occur to some degree. The parameter α, known as the *Tikhonov regularization parameter*, serves to coordinate the trade-off which is to occur between accuracy of the model-fitting and the achievement of stability through the penalty term.

Numerous methods exist in the literature for determining the Tikhonov parameter α given noisy data f^δ and an estimate of the noise level δ. In one approach, the Morozov discrepancy principle, the idea is to fix $\tau \geq 1$ and choose $\alpha = \alpha(\delta)$ so that

$$\|\mathcal{A}u^\delta_{\alpha(\delta)} - f^\delta\|^2_Y = \tau\delta^2. \tag{24}$$

The theory of Tikhonov regularization for *linear* inverse problems (i.e., with $\mathcal{A}$ a bounded linear operator) is very well developed, as is a theory for Tikhonov regularization coupled with the Morozov discrepancy principle. In the linear case these combined results guarantee the existence of a unique parameter $\alpha = \alpha(\delta)$ satisfying the discrepancy principle (24); further, if the Tikhonov problem (22)–(23) is then solved for $\bar{u}^\delta_{\alpha(\delta)}$ using this parameter, we have that $\bar{u}^\delta_{\alpha(\delta)}$ converges to the "true" solution $\bar{u}$ as $\delta \to 0$. It should be noted that convergence rates for Tikhonov regularization using the Morozov discrepancy principle are not optimal, and that other principles may be better suited for practical use [20].

Over the last 15 years, the theory of Tikhonov regularization has been systematically extended to nonlinear problems as well, although it can by no means be considered as complete; see, for example, [20, 63, 64, 65, 66], and the references therein (see also the references in [25]).

One problem with Tikhonov regularization that has been well-documented in the literature is the problem of over-smoothing. This disadvantage of Tikhonov regularization can be described in the following way:

> *If the "true" solution $\bar{u}$ has discontinuities or corners (or other rough features), Tikhonov regularization tends to produce an overly smooth approximation which can lead to the loss of such sharp features.*

In applications such as the imaging example of this paper, over-smoothing means that detailed information in images can be lost entirely due to the regularization process.

In either the linear or nonlinear case, practical implementation of Tikhonov regularization usually takes one of two approaches, which we discuss in more detail below:

- *Approach #1*: Solve the infinite-dimensional Tikhonov problem (22)–(23) directly, via either an (infinite-dimensional) minimization procedure or a direct solution of the necessary conditions (operator equations) associated with the minimization; afterward, a discretization method is implemented in order to allow solution by computer. Or,

- *Approach #2*: Discretize the operator $\mathcal{A}$ and data f^δ first, then apply the method Tikhonov regularization directly to the discretized inverse problem.

Approach #1 ("Regularize, then discretize"): We first consider the case of Approach #1 for the example of the IHCP. If we consider the necessary conditions for the minimization of the Tikhonov functional J_α^δ in (23) for the linear case, we have (formally) that $\bar{u}_\alpha^\delta$ solves

$$(\mathcal{A}^\star \mathcal{A} + \alpha \mathcal{L}^\star \mathcal{L})u = \mathcal{A}^\star f^\delta, \tag{25}$$

where $\mathcal{A}^\star$ and $\mathcal{L}^\star$ are the adjoint operators associated with the operators $\mathcal{A}$, $\mathcal{L}$, respectively. For the IHCP and for $\mathcal{L}$ the identity operator, equation (25) becomes the integral equation

$$\int_t^T \int_0^s k(s,t)k(s,t')u(t')\,dt'\,ds + \alpha\, u(t) = \int_t^T k(s,t) f^\delta(s)\,ds, \quad t \in [0,T]. \tag{26}$$

This is a *second-kind* integral equation in u, a well-posed (with respect to stability) integral equation whenever the Tikhonov regularization parameter α is positive; however, the outer integration from t to T on both sides of equation (26) means that the equation is *non-causal*. Thus a strong disadvantage of Tikhonov regularization for a Volterra problem such as the IHCP is that a causal problem is converted into a non-causal problem. For a causal problem, only data values from the *past and present* are needed, meaning that solution methods can potentially be determined in real-time as t progresses over the interval $[0,T]$; for a non-causal problem such as (26), real-time solution methods are not possible because we must have past, present, and all *future* values of the data in hand before we may determine the value of the regularized solution at any given time t. This leads to nontrivial increases in costs of implementation.

From the above discussion we see a second disadvantage of Tikhonov regularization:

> *Tikhonov regularization may destroy special structure (causality, for example) inherent in the original inverse problem.*

An alternative that stays within the framework of Approach #1 is to avoid the necessary conditions (26) entirely, and instead find solutions by applying an iterative optimization method (such as Newton's method, the method of steepest descent, etc.) directly to (22)–(23). We will postpone discussion of this approach until Section 2.2, where iterative-based methods are considered in more detail; for now we simply note that the above disadvantage associated with Tikhonov regularization is not always remedied by turning to an iterative approach.

Approach #2 ("Discretize, then regularize"): We now consider the case of Approach #2 above for the example of the IHCP. Standard discretizations of (5), (6), lead to an equation of the form (7), where we recall that the $N \times N$ matrix $\mathbf{A}$ is lower-triangular. If we now apply Tikhonov regularization directly to the discrete system (7), we solve the finite-dimensional minimization problem

$$\min_{\mathbf{u} \in \mathbb{R}^N} \left\{ \|\mathbf{A}\mathbf{u} - \mathbf{f}^\delta\|^2 + \alpha \|\mathbf{u}\|^2 \right\}$$

where we have again used the identity for the regularization operator, and where $\|\cdot\|$ denotes the usual Euclidean norm. Now taking the approach of solving the necessary conditions associated with the minimization problem, these conditions reduce to the matrix equation for the discrete Tikhonov solution $\mathbf{u}_\alpha^{N,\delta}$,

$$(\mathbf{A}^T\mathbf{A} + \alpha\,\mathbf{I})\mathbf{u} = \mathbf{A}^T\mathbf{f}^\delta, \tag{27}$$

where $\mathbf{I}$ is the $N \times N$ identity matrix. Even when we "discretize before regularizing", we see evidence of how Tikhonov regularization may destroy special structure in problems. The matrix $\mathbf{A}$ in the discrete IHCP (7) is lower-triangular allowing for *sequential* solution techniques, while the governing matrix $(\mathbf{A}^T\mathbf{A} + \alpha\,\mathbf{I})$ in (27) is a *full* matrix requiring far more expensive solution techniques.

We now turn to a second common form of regularization for inverse problems, namely, iterative regularization.

2.2 Iterative regularization.

Tikhonov regularization may not always be an attractive alternative for nonlinear inverse problems. One of the difficulties in the nonlinear case is that the functional J_α^δ in (23) is no longer strictly convex (in contrast to the linear case), leading to the possibility of multiple local minima. In addition, it is generally not computationally feasible to find any of the minima of (23) in the nonlinear case (see [20, 25] and the references therein). These difficulties make an alternative class of regularization methods, iterative regularization methods, extremely attractive for nonlinear problems. We should mention that iterative regularization methods can also be very competitive methods for linear inverse problems.

In iterative regularization, one picks an initial guess u_0 (a function, if we have not yet discretized the inverse problem) for the unknown solution $\bar{u}$, and then one iteratively constructs updated approximations via a scheme like

$$u_{n+1} = U_n(u_n; f^\delta), \quad n = 0, 1, \ldots,$$

where f^δ is the usual measured data and U_n is determined by the particular iterative process. For even the best iterative methods one does not want to let the iteration parameter n to get too large because this may cause the noise in f^δ to be amplified to the point where the results are no longer reliable. The regularization parameter associated with iterative regularization is thus the (f^δ, δ)-dependent *stopping point* of the iterative sequence, and an important part of the mathematical theory is in the development of *stopping criteria* for terminating the iteration. (Alternatively, one may implement regularization via a coordination of the iterative scheme with some other form of regularization, such as the process of applying a gradient-like iterative procedure directly to the minimization of a Tikhonov functional.)

As with Tikhonov regularization, practical implementation of an iterative process usually takes one of two approaches depending on whether one approaches the iterative minimization of the *infinite-dimensional* problem (2)–(3) first (prior to any discretizations), or whether one discretizes first, leading to a finite dimensional problem of the form (20)–(21) (which one then solves using a finite-dimensional iterative minimization procedure).

Approach #1 ("Implement the infinite-dimensional iteration procedure first, then discretize"): As an example of iterative regularization for the fully infinite-dimensional problem, we consider an application of Newton's Method to the inverse problem as stated in output least squares formulation (2)–(3); here and for the remainder of the section, we assume that $\mathcal{A}$ is continuously differentiable.

With noisy data, problem (2)–(3) becomes

$$\min_u \|\mathcal{A}(u) - f^\delta\|_Y^2,$$

and the Newton iteration applied to this infinite-dimensional problem is (formally) defined as

$$u_{n+1} = u_n - \mathcal{A}'(u_n)^{-1}(\mathcal{A}(u_n) - f^\delta), \quad n = 0, 1, \ldots, \tag{28}$$

where $\mathcal{A}^{-1}$ need not be defined everywhere [25]. For this approach, one must determine at each step n of the iteration

$$\mathcal{A}(u_n) \text{ and } \mathcal{A}'(u_n)^{-1}(\mathcal{A}(u_n) - f^\delta),$$

where the latter is found via solution of

$$\mathcal{A}'(u_n)z = \mathcal{A}(u_n) - f^\delta, \tag{29}$$

given the most recent iterate u_n. It is in the solution of (29) and the determination of $\mathcal{A}(u_n)$ that a discretization is desirable; in parameter estimation problems, often $\mathcal{A}(u_n)$ is approximated using a finite difference or finite element scheme applied to a system of model equations. In fact, however, Newton's method (in this its unmodified form) is usually not used for ill-posed problems because equation (29) is generally equivalent to a linear ill-posed problem [20, 25]; thus discretization of (29) would typically have to be combined with yet another regularization method.

An alternative approach to the minimization of (2) might be through a modified Newton method, or via a descent method such as the method of steepest descent or the method of conjugate gradients. Descent methods have become quite popular in the last fifteen years for solution of the IHCP, a linear inverse problem, and for nonlinear extensions of the IHCP. If the minimization procedure is formulated *prior* to the discretization of the original inverse problem, the result is an iteration which requires solving both the original partial differential equation and an *adjoint* partial differential equation at each step of the iterative minimization process (see, for example, [2, 3]); this approach to regularization of the IHCP is often referred to as the "adjoint method" in the applications literature because the abstract adjoint operator $\mathcal{A}^\star$ is used in the formulation of the adjoint partial differential equation. (We note that the adjoint partial differential equation is solved backwards in time so that, as with Tikhonov regularization, the property of causality of the original IHCP is destroyed under this type of regularization.) Discretization is applied to the original and adjoint partial differential equations, and thus discretization is applied *after* the infinite-dimensional iterative descent method structure (which defines the adjoint equation) is in place.

Another popular iterative regularization scheme for nonlinear inverse problems is Landweber's iteration, which arises from converting the necessary conditions for minimizing (2) into a fixed point iteration. Landweber's iteration takes the form

$$u_{n+1} = u_n - \mathcal{A}'(u_n)^\star(\mathcal{A}(u_n) - f^\delta), \quad n = 0, 1, \ldots, \tag{30}$$

starting from an initial guess u_0. Note the similarity to the Newton method in (28) above, with one fundamental difference: for Landweber one need not compute the *inverse* of $\mathcal{A}'(u_n)$. For more discussion on this and numerous other iterative regularization schemes, see [20, 25].

In recent years much attention has been paid by the mathematical inverse problems community to careful formulation of iterative regularization methods for nonlinear problems, to the development of practical and usable stopping criteria, and to the development of a rigorous convergence/regularization theory. More will be said in Section 3.3 below about recent progress made in the theory of iterative regularization.

Approach #2 ("Discretize, then apply an iterative procedure"): Iterative methods are used quite commonly in parameter estimation problems (which are typically nonlinear inverse problems). In the cases which most often appear in the applied literature, discretization occurs *prior* to an application of an iterative method for solution of the inverse problem. That is, a discretization method is usually applied to the model equations in which the unknown parameters (which are typically also discretized) appear, and then a suitable iteration method is used to solve the inverse problem of determining the unknown parameters from data. With each different application, special care must be taken in defining and implementing (typically application-appropriate) discretizations and iterative schemes. For example, in [17] one seeks to determine certain coefficients (parameters representing thermal conductivity and heat capacity) appearing in a partial differential equation representing heat conduction. The approach is to first use a finite difference approximation for the model equations, or to discretize *first*, and to then implement a Levenberg-Marquardt procedure, now in the setting of the finite-dimensional (discretized) problem.

3. SOME RECENT DEVELOPMENTS AND NEW IDEAS IN MATHEMATICAL REGULARIZATION THEORY

The field of mathematical inverse problems has become quite broad in the last twenty years, with emphasis on general regularization theory as well as application-specific solution methods. For an overview of inverse problems, especially as they occur in a number of applications, we refer the reader to recent conference proceedings [13, 15, 16, 21, 22, 23, 24] from the years of 1990–2000. We point the reader in particular to the excellent volume [15] (which appeared in the year 2000) containing surveys of numerous types of solution methods for inverse problems. Each paper in that reference was selected, according to the editors, because it typified "a new or promising method that could have impact on a wide variety of inverse problems" [15].

Below we highlight three areas of new development in the area of mathematical regularization theory for inverse problems.

3.1. Regularization methods which do not oversmooth solutions.

As stated earlier, classical Tikhonov regularization tends to find smooth solutions, a disadvantage if one is seeking a solution which has discontinuities or sharp features; such a solution is typical in image reconstruction and signal processing applications. The difficulty with Tikhonov regularization lies in the presence of the penalizing term $\|\mathcal{L}u\|_Y^2$ in (23); commonly one sees a choice of $\mathcal{L}$ which gives

$$\|\mathcal{L}u\|_Y^2 = \int_\Omega |\nabla u(\mathbf{x})|^2 \, d\mathbf{x}$$

or

$$\|\mathcal{L}u\|_Y^2 = \int_\Omega | \triangle u(\mathbf{x})|^2 \, d\mathbf{x},$$

either of which necessarily limits the minimization in (22) to u in a class of smooth functions. Oversmoothing occurs less with $\mathcal{L}$ the identity operator, but often in this case the undesirable result is highly oscillatory solutions.

In recent years, several authors [1, 11, 12, 38, 39, 67] have proposed a generalization of Tikhonov regularization, often called *bounded variation regularization* or *bounded variation minimization*, for which the following optimization problem is formulated: for a given value of the regularization parameter β, find u_β^δ solving

$$\min_u J_\beta^\delta(u) \tag{31}$$

where

$$J_\beta^\delta(u) \stackrel{def}{=} \|A(u) - f^\delta\|_Y^2 + \beta\, G(u). \tag{32}$$

The penalty term in (32) is the bounded variation seminorm

$$\begin{aligned} G(u) &= \int_\Omega |\nabla u|(\mathbf{x}) \, d\mathbf{x} \\ &\stackrel{def}{=} \sup \left\{ \int_\Omega u(\mathbf{x}) \, \nabla . w(\mathbf{x}) \, d\mathbf{x} \, : \, w \in C_0^1(\Omega), |w| \leq 1 \right\}, \end{aligned}$$

and the minimization in (31) must occur over a suitable class of u (a class which permits "rougher" functions than allowed by Tikhonov regularization using the choices of $\mathcal{L}$ given above).

An excellent discussion of the advantages and disadvantages of bounded variation regularization may be found in [58]. On the positive side, bounded variation regularization does not lead to overly-smoothed solutions; discontinuities and sharp features can be captured by the process. Two disadvantages are that the regularization does not stabilize the problem in the bounded variation norm, and (of great importance to practical implementation) the penalty term in J^δ_β is not differentiable. The latter problem leads to nontrivial difficulties in that one may *not* use standard (differentiable) optimization packages to solve the minimization problem; as a result, numerical implementation is costly and slow speed of convergence is a factor. Thus, although the recent idea of bounded variation regularization appears to be an attractive way to solve inverse problems when solutions are not smooth, the method comes equipped with some distinct disadvantages that must be handled in some manner.

To obtain the same success in capturing sharp features of solutions as bounded variation regularization without some of the down sides of that method, different strategies have taken (for example) by Coleman, Dobson, Li, Liu, Santosa, and others, to deal directly with the nondifferentiable cost functional, applying either an affine scaling approach or a quadratic programming strategy (see the references in [19]). A different point of view has been taken by Vogel, Dobson, Oman, and others, in which J^δ_β in (32) is altered slightly in order to restore differentiability of the cost functional and thus to allow for implementation of effective *differentiable* computational methods (see, e.g., [1]). An improvement (which also unifies some of the previous ideas) has been found recently in [58]. We do not detail the formulation of this approach here because it is quite technical; nevertheless the results seem to be applicable to many problems of interest in applications.

We note that an alternative approach to the problem of finding "rough" solutions of inverse problems may also be found in some of the local regularization methods given in Section 3.2 below. These approaches take a more classical formulation, via classical Tikhonov regularization, but they allow the use of a *variable* Tikhonov regularization parameter. That is, instead of using α a constant in (22)–(23), these methods allow for α to vary with the spatial location $\mathbf{x}$, as $\mathbf{x}$ ranges over the domain Ω of the solution. This approach allows for more regularization (i.e., smoothness) in some regions of the solution and less regularization (i.e., roughness) in others. This certainly allows for one to find some sharp features of solutions, but does not presently allow for the recovery of discontinuities.

3.2. Localized regularization methods.

Another new development in the mathematical theory of regularization is that of localized regularization methods which have been primarily studied for linear inverse problems. The advantages of such methods are generally that special structures of the original inverse problem can often be preserved, leading to savings in implementation and computational costs. For example, while Tikhonov regularization destroys the causal nature of Volterra problems such as the IHCP (as discussed above), the local regularization methods developed in [14, 42, 44, 45, 46, 48, 49, 52, 53] do not have this problem. Local regularization of equation (1) is based on a decomposition of the operator $\mathcal{A}$ and the data f into "local" and "nonlocal" parts. Then regularization is applied to problem of inverting the local part of $\mathcal{A}$ only. Because space is limited, we will present only a brief idea of local regularization methods here; in particular, we will focus mainly on local regularization methods for a Volterra inverse problem such as the

IHCP.

We recall that the "true" solution $\bar{u}$ of the IHCP solves an equation of the form

$$\int_0^t k(t,s)u(s)\,ds = f(t), \quad t \in [0,T]. \tag{33}$$

To motivate the ideas of local regularization, we let $r > 0$ be a small fixed constant and assume that equation (33) actually holds on an extended domain $[0, T+r]$ (which can always be accomplished by simply decreasing the size of T slightly). Then $\bar{u}$ satisfies

$$\int_0^{t+\rho} k(t+\rho,s)u(s)\,ds = f(t+\rho), \quad t \in [0,T],\ \rho \in [0,r],$$

or, splitting the integral at t and making a change of integration variable,

$$\int_0^t k(t+\rho,s)u(s)\,ds + \int_0^\rho k(t+\rho,t+s)u(t+s)\,ds = f(t+\rho),\ \ t \in [0,T],\ \rho \in [0,r].$$

For each $t \in [0,T]$, the ρ variable serves to advance the equation slightly into the future. One way to consolidate this future information is to integrate both sides of the equation with respect to ρ, i.e.,

$$\begin{aligned} \int_0^t \int_0^r k(t+\rho,s)\,d\rho\,u(s)\,ds + \int_0^r \int_0^\rho k(t+\rho,t+s)u(t+s)\,ds\,d\rho& \\ = \int_0^r f(t+\rho)\,d\rho, \quad t \in [0,T]&, \end{aligned} \tag{34}$$

where we have made a change of order of integration in the first integral above. (It is worth remarking that a more general approach, not detailed here, is to integrate with respect to a Borel measure $\eta = \eta(\rho)$; this approach generates an entire class of local regularization methods [44].)

We note that the true solution $\bar{u}$ satisfies equation (34); when f is replaced by f^δ, a regularized form of this equation is needed and we obtain this new equation by replacing $u(t+s)$ by $u(t)$ in the second integral term. That is, for fixed t, it is as if u is (temporarily) assumed to be constant on the small *local* interval $[t, t+r]$; the length r of this local interval becomes the regularization parameter. The "local regularization equation" which results is given by

$$\int_0^t \tilde{k}(t,s;r)u(s)\,ds \,+\, a(t;r)\,u(t) = \tilde{f}^\delta(t;r), \quad t \in [0,T], \tag{35}$$

where

$$a(t;r) \;:=\; \int_0^r \int_0^\rho k(t+\rho,t+s)\,ds\,d\rho, \tag{36}$$

$$\tilde{k}(t,s;r) \;:=\; \int_0^r k(t+\rho,s)\,d\rho, \tag{37}$$

$$\tilde{f}^\delta(t;r) \;:=\; \int_0^r f^\delta(t+\rho)\,d\rho. \tag{38}$$

We may regularize further by adding penalty term to (35), i.e.,

$$\int_0^t \tilde{k}(t,s;r)u(s)\,ds \;+\; [a(t;r)+\alpha(t)]\,u(t) = \tilde{f}^\delta(t;r), \quad t \in [0,T], \tag{39}$$

where $\alpha = \alpha(t)$ is a nonnegative penalty *function.* The t-dependence of α allows for *variable* regularization, that is, more regularization at some locations t in the domain $[0,T]$ and less at other locations. See [52, 53] for more discussion on this additional regularization parameter and for some numerical examples involving variable regularization parameters.

A regularization theory for this method was developed in [44] (for convolution kernels) and [52] (for nonconvolution kernels) provided that the kernel k satisfies $k \in C^1$ with $k(t,t) \neq 0$ for $t \in [0, T+\bar{r}]$. Under these conditions, a choice of the regularization parameter $r = r(\delta)$ may be made which guarantees $r(\delta) \to 0$, and

$$u^\delta(\cdot; r(\delta)) \to \bar{u} \;\text{ as }\; \delta \to 0, \tag{40}$$

where u^δ solves equation (35) for the given value of $r(\delta)$. In the case of equation (39), a similar statement about convergence of the solution of that equation may be made, for a choice of $r = r(\delta)$ and $\alpha = \alpha(t,\delta)$.

Further convergence results (for more general kernels k) may be found in [14, 42, 44, 45, 46, 48, 49, 52, 53]; convergence results for discretizations of (35) and (39) may be found in [42] and [53]. We note also that a special case of this local regularization method has been successfully used in a number of practical applications, including over 30 years of use by practitioners solving the IHCP [8]. In the applications, this method is often known as "Beck's method" and is named after its developer, J. V. Beck. We note that the IHCP is a particularly difficult Volterra example from the standpoint of ill-posedness, and that none of the existing convergence theory on local regularization applies to the IHCP.

For the above example, the ideas of local regularization are used to transform an ill-posed first-kind Volterra equation into a well-posed second-kind Volterra equation, much like Tikhonov regularization was shown to do for the IHCP. In contrast to Tikhonov regularization, which requires *all* future values of the data in order to be able to construct an approximate solution at time t (i.e., the Tikhonov equation is very non-causal), the local regularization method only uses a *very small* amount of future information for each t. This means that implementation has the potential to be carried out in "near real-time". In fact, it can be shown that discretization of equations associated with Tikhonov regularization takes $\mathcal{O}(N^3)$ multiplies, while the local regularization method takes only $\mathcal{O}(\frac{1}{2}N^2)$ multiplies, a considerable savings in cost; both estimates of cost are for the general nonconvolution Volterra problem [47].

Local regularization can also be extended to problems like the image reconstruction problem. In this case the operator $\mathcal{A}$ is not of Volterra type and an alternate local approach (the description of which is too long for this paper) is used. In the non-Volterra case, an iterative solution method must be combined with the method of local regularization; if the number of iterations is small, then local regularization of non-Volterra problems can be a savings over standard Tikhonov regularization for such problems [47].

As stated earlier, another feature of local regularization is the capability for allowing variable regularization parameters. We have already seen how the additional regularization parameter α can vary with respect to the independent variable. In addition, the parameter r above could be variable instead of a fixed constant, allowing for more or less regularization at a given location in the domain. See [48, 52, 53] for a theory based on the use of variable regularization parameters, and for examples which illustrate how a regularization parameter may be selected using a *variable discrepancy principle*.

There remain a number of open questions and problems associated with the theory of local regularization. For the Volterra problem, there is a serious limitation on the types of kernels k for which a mathematical convergence/regularization theory may be proven. As indicated earlier, the kernel k associated with the IHCP does not fall within the class of such kernels. Numerical evidence in [60] indicates that stability may not in fact be present for a certain class of kernels, although lack of stability has not been actually proven. It is evident that more work is needed to modify local regularization methods so that a mathematical convergence/regularization theory may be developed for a large class of kernels k.

Another open problem concerns the development of a theory (perhaps involving a classical discrepancy principle) for the selection of local regularization parameters r and α. Although numerical examples exist for selection of such variable regularization parameters [52, 53] no theoretical results are available at the present time.

Finally, we note that the local regularization method presented here is by no means the only possibility for a localized regularization approach. For example, we mention the theory of mollification (see, e.g., [54, 55, 56, 57] and see [41] for shortcomings of this approach for general Volterra problems), and also the work on distributional approximations of Nashed and Scherzer in [58].

3.3. Progress on iterative regularizations methods for nonlinear inverse problems.

As indicated above, iterative methods for the solution of nonlinear inverse problems are typically in the form of

$$u_{n+1} = U_n(u_n; f), \quad n = 0, 1, \ldots, \tag{41}$$

in the case where one has "ideal" data f, and in the case of perturbed data f^δ (where $\|f - f^\delta\|_Y \le \delta$ for some $\delta > 0$), we have the iteration

$$u_{n+1}^\delta = U_n(u_n^\delta; f^\delta), \quad n = 0, 1, \ldots.$$

In both cases above, an initial guess u_0 must be supplied by the user, while U_n is provided by the particular iterative method and depends in large part on $\mathcal{A}$ and its properties. For a given iterative procedure, the mathematical theory of this iteration as a regularization method for an inverse problem usually entails the following:

(a) Determination of conditions on the operator $\mathcal{A}$ which guarantee convergence of u_n to $\bar{u}$ in the case where "ideal" data f is used in the iterative process;

(b) Definition of a *stopping criteria* for the iteration in the case of perturbed data f^δ; that is, given δ and f^δ, we only iterate for $n = 0, 1, \ldots \hat{n}$, where $\hat{n} = \hat{n}(\delta, f^\delta)$. For this selection of $\hat{n}$, the mathematical theory should show that $\hat{n}(\delta, f^\delta) \to \infty$ and

$$u^\delta_{\hat{n}(\delta, f^\delta)} \to \hat{u} \tag{42}$$

as $\delta \to 0$, i.e., that the iteration method with stopping criteria is a regularization method; and

(c) Determination of conditions on the operator $\mathcal{A}$ for which a *convergence rate* may be given for the convergence in (42).

In the excellent survey [25], Engl and Scherzer detail the progress made in (a)–(c) above for a number of important iteration methods which are of great practical use in nonlinear inverse problems appearing widely in applications. In particular, much development in the last few years has taken place in advancing the theory of Landweber iteration for nonlinear inverse problems. Convergence of the Landweber iteration was shown in [62] using the fact that the operator U_n for Landweber iteration can be written independent of n, i.e., $U_n = U$, where for ideal data,

$$U(u) = u - \mathcal{A}'(u)^\star(\mathcal{A}(u) - f).$$

This means that the iteration in (41) can be viewed as a fixed point iteration, for which fixed point theory may be used to derive weak convergence of the iteration depending on assumptions on U. In [31], a convergence theory was developed which makes use of structure of the operator $\mathcal{A}$ (rather than U); in fact, proofs of (a)–(c) may be found in that reference, with the stopping criteria in (b) developed using a discrepancy principle. The iteration is to be stopped after $\hat{n}$ steps where $\hat{n} = \hat{n}(\delta, f^\delta)$ satisfies the following

$$\|\mathcal{A}(u^\delta_{\hat{n}}) - f^\delta\| \le \tau\delta < \|\mathcal{A}(u^\delta_n) - f^\delta\|, \quad 0 \le n < \hat{n},$$

for τ a positive number depending on the properties of $\mathcal{A}$ [25, 31]. The convergence rate (in (c)) found in [31] requires conditions on $\mathcal{A}$ which are generally too restrictive for strongly smoothing operators; alternative convergence rate results (for more general operators) may be found in [18].

A theory for the iterative method of steepest descent and the method of minimal error (see [25]) has also been developed for nonlinear inverse problems. In [59, 61], parts (a) and (b) were proven, while in [59], convergence rates in (c) were proven.

We have limited our discussion here to progress made on the Landweber, steepest descent, and minimal error iterations. For a more complete discussion of these methods, and for progress made in the mathematical analysis of other iterations, such as Newton's Method, Modified and Inexact Newton Methods (Levenberg-Marquardt, Gauss-Newton, etc.), the reader is referred to [25].

One of the present shortcomings of the theory for iterative regularization is that conditions on $\mathcal{A}$ needed to prove (a)–(c) are difficult to verify in practice. These conditions have been analyzed for some particular applications [20, 25]. For example, one may find an analysis of certain assumptions needed for the Landweber theory in [30, 32, 35, 36, 37] (for inverse scattering problems), in [33] (for inverse potential problems), in [9, 31] (for parameter estimation in ordinary differential equations), in [40] (for parameter estimation in a hyperbolic partial differential equation), and in [34] (for the determination of a discontinuity in a conductivity in an elliptic equation), to name a few applications. Because of the importance of having precise statements of convergence such as (a)–(c) in *every* instance in which an iteration is applied, it is clear that more work is needed on the development of assumptions on $\mathcal{A}$ which may be proven for a wider set of applications, and for a larger class of iterative schemes that are commonly in use.

4. CONCLUSION

In this paper we have reviewed some of the new developments in the theory of mathematical regularization for inverse problems, indicating briefly where some of this theory currently falls short. Numerous open problems in these and other theoretical areas mean that there will be an rich source of research problems in the area of mathematical regularization theory for many years to come.

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