Relationship Between Data Smoothing and the Regularization of Inverse Problems

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Abstract. We investigate the practice of *regularization* (also termed *damping*) in inverse problems, meaning the use of prior information to supplement observations, in order to suppress instabilities in the solution caused by noisy and incomplete data. Our focus is on forms of regularization that create smooth solutions, for smoothness is often considered a desirable – or at least acceptable – attribute of inverse theory solutions (and especially tomographic images). We consider the general inverse problem, in its continuum limit. By deconstruction into the part controlled by the regularization and the part controlled by the data kernel, we show the general solution depends on a smoothed version of the back-projected data as well as a smoothed version of the generalized inverse. Crucially, the smoothing function that controls both is the solution to the simple data smoothing problem. We then consider how the choice of regularization shapes the smoothing function, in particular exploring the dichotomoy between expressing prior information either as a constraint equation (such as a spatial derivative of the solution being small) or as a covariance matrix (such as spatial correlation falls off at a specified rate). By analyzing the data smoothing problem in its continuum limit, we derive analytic solutions for different choices of regularization. We consider four separate cases: 1) the first-derivative of the solution is close to zero; 2) the prior covariance is a two-sided declining exponential; 3) the second-derivative of the solution is close to zero; and 4) the solution is close to its localized average. First-derivative regularization is put forward as having several attractive properties and few, if any, drawbacks.

Introduction

The concept of *regularization* (also termed *damping*) is central to solving many classes of inverse problems, and especially those involving generalizations of the least squares principle (Levenberg, 1944). Instabilities caused by incomplete data coverage, which would otherwise arise during the inversion process, are damped through the addition of prior information, which quantifies expectations about the behavior of the solution. Given properly chosen prior information, a unique and well-behaved solution can be determined even with noisy and incomplete data.

Prior information can be implemented in two interrelated, but conceptually distinct ways. The first is as a constraint equation that looks just like a data equation, except that it is not based on any actual observations. The second is as a covariance matrix, which quantifies how that we expect that different model parameters are correlated. That these two ideas are related can be understood from the following example. Suppose that m_1 and m_2 are two model parameters whose sum we expect to be zero. Then the equation $m_1 + m_2 = 0$ implements this prior information. Furthermore, any fluctuation of m_1 and m_2 from their typical values must be strongly and negatively correlated, else the sum would not be zero. This approach treats m_1 and m_2 as random variables with a negative covariance. Thus, in some sense, a prior information equation implies a corresponding covariance matrix (and vice versa).

Suppose that the prior information equation is linear and of the form $\mathbf{Hm} = \mathbf{h}$, where $\mathbf{m}$ is the vector of unknown model parameters and $\mathbf{H}$ and $\mathbf{h}$ are known. In many least-squares formulations, the prior information is imposed only approximately, with the strength of the

information quantified by a parameter ε. Alternately, the model parameters can also be viewed as random variables, fluctuating around some mean value $\mathbf{m} = \langle \mathbf{m} \rangle$ with covariance matrix $\mathbf{C_h}$. Following the reasoning above, we expect that $\mathbf{H}$ and $\mathbf{C_h}$ to be related, and in fact this relationship is well known in least-squares theory (Tarantola and Valette, 1982a,b). As we will review below, a detailed analysis of the least squares principle reveals that $\varepsilon \mathbf{H} = \mathbf{C_h}^{-1/2}$, $\mathbf{C_h} = \varepsilon^{-2} [\mathbf{H^T H}]^{-1}$ and $\langle \mathbf{m} \rangle = \varepsilon \mathbf{h}$. Thus, one can translate between the two viewpoints by "simple" matrix operations.

Regularization can be applied to the general linear inverse problem $\mathbf{Gm} = \mathbf{d}$ (where $\mathbf{d}$ is data and $\mathbf{G}$ is the data kernel) to implement the qualitative notion of *smoothness.* An important question is whether the regularization works by smoothing the observations (making the data smoother) or by smoothing the data kernel (making the theory smoother). Our analysis, presented later in this paper, shows that it does both. Two important practical issues are how to choose a $\mathbf{C_h}$ or an $\varepsilon \mathbf{H}$ to embody an intuitive form of smoothness, and how to assess the consequences of one choice over another. We show that the simple *data smoothing problem* is a key to understanding these issues.

By data smoothing, we mean finding a set of model parameters that are a smoothed version of the data. This approach reduces the data kernel to a minimum ($\mathbf{G} = \mathbf{I}$) and highlights the role of prior information in determining the solution. Even with this simplification, the relationships between $\mathbf{C_h}$ and $\varepsilon \mathbf{H}$, and their effect on the solution, are still very obtuse. Surprisingly, an analysis of the continuum limit, where the number of model parameters becomes infinite and vectors become functions, provides considerable clarity. We are able to derive simple analytic

formulae that relate $\mathbf{C}_h$ and $\varepsilon\mathbf{H}$, as well as the smoothing kernels that relate the unsmoothed and smoothed data. The latter is of particular importance, because it allows assessment of whether or not the mathematical measure of smoothing corresponds to the intuitive one.

Finally, we show that the effect of regularization on the general inverse problem can be understood by decomposing it into the part equivalent to a simple data smoothing problem and the deviatoric part controlled by the non-trivial part of the data kernel. This decomposition allows us to investigate the respective effects of the smoothing constraints and the data constraints (via some theory, represented by the data kernel) on the solution. The former blurs (in the literal sense of the word) the data, but we show also that the data kernel is also blurred in exactly the same way. Regularization partly works by smoothing the theory.

Background and Definitions

Generalized least squares (Levenberg, 1944, Lawson and Hansen, 1974; Tarantola and Valette, 1982a,b; see also Menke 1984, 2012; Menke and Menke, 2011) is built around a data equation, $\mathbf{Gm} = \mathbf{d}^{obs}$, which describes the relationship between unknown model parameters, $\mathbf{m}$, and observed data, $\mathbf{d}^{obs}$, and a prior information equation $\mathbf{Hm} = \mathbf{h}^{pri}$, which quantifies prior expectations (or "constraints") about the behavior of the model parameters. The errors in the data equation and the prior information equation are assumed to be normally distributed with zero mean and covariance of $\mathbf{C}_d$ and $\mathbf{C}_h$, respectively.

The generalized least squares solution is obtained by minimizing the generalized error, Φ_{GLS}:

$$\Phi_{GLS} = \left[\mathbf{d}^{obs} - \mathbf{Gm}\right]^T \mathbf{C}_d^{-1}\left[\mathbf{d}^{obs} - \mathbf{Gm}\right] + \left[\mathbf{h}^{pri} - \mathbf{Hm}\right]^T \mathbf{C}_h^{-1}\left[\mathbf{h}^{pri} - \mathbf{Hm}\right] \qquad (1)$$

The first term on the r.h.s represents the sum of squared errors in the observations, weighted by their *certainty* (that is, the reciprocal of their variance) and the second represents the sum of squared errors in the prior information, weighted by their uncertainty.

Suppose now that $\mathbf{C}_d^{-1} = \mathbf{Q}_d^T \mathbf{Q}_d$ and $\mathbf{C}_h^{-1} = \mathbf{Q}_h^T \mathbf{Q}_h$, for some matrices $\mathbf{Q}_d$ and $\mathbf{Q}_h$. We can rearrange (1) into the form $\Phi_{GLS} = [\mathbf{f} - \mathbf{Fm}]^T \mathbf{C}_f^{-1} [\mathbf{f} - \mathbf{Fm}]$ by defining:

$$\mathbf{F} = \begin{bmatrix} \mathbf{Q}_d \mathbf{G} \\ \mathbf{Q}_h \mathbf{H} \end{bmatrix} \quad \text{and} \quad \mathbf{f} = \begin{bmatrix} \mathbf{Q}_d \mathbf{d}^{obs} \\ \mathbf{Q}_h \mathbf{h}^{pri} \end{bmatrix} \quad \text{and} \quad \mathbf{C}_f = \mathbf{I} \tag{2}$$

This is the form of a simple least squares minimization of the error associated with the combined equation $\mathbf{Fm} = \mathbf{f}$. The matrices $\mathbf{Q}_d$ and $\mathbf{Q}_h$ now have the interpretation of weighting matrices, with the top rows of $\mathbf{Fm} = \mathbf{f}$ being weighted by $\mathbf{Q}_d$ and the bottom rows by $\mathbf{Q}_h$. The least-squares equation and its solution are:

$$[\mathbf{F}^T \mathbf{F}] \mathbf{m}^{est} = \mathbf{F}^T \mathbf{f} \quad \text{and} \quad \mathbf{m}^{est} = [\mathbf{F}^T \mathbf{F}]^{-1} \mathbf{F}^T \mathbf{f} \tag{3a,b}$$

An obvious choice of weighting matrices is $\mathbf{Q}_d = \mathbf{C}_d^{-1/2}$ and $\mathbf{Q}_h = \mathbf{C}_h^{-1/2}$, where $\mathbf{C}_d^{-1/2}$ and $\mathbf{C}_h^{-1/2}$ are symmetric square roots. However, any matrices that satisfy $\mathbf{Q}_d^T \mathbf{Q}_d = \mathbf{C}_d^{-1}$ and $\mathbf{Q}_h^T \mathbf{Q}_h = \mathbf{C}_h^{-1}$ are acceptable, even non-symmetric ones. In fact, if $\mathbf{T}_d$ and $\mathbf{T}_h$ are arbitrary unary matrices satisfying $\mathbf{T}_d^T \mathbf{T}_d = \mathbf{I}$, and $\mathbf{T}_h^T \mathbf{T}_h = \mathbf{I}$, then $\mathbf{Q}_d = \mathbf{T}_d \mathbf{C}_d^{-1/2}$ and $\mathbf{Q}_h = \mathbf{T}_h \mathbf{C}_h^{-1/2}$ are acceptable choices, too. A non-symmetric matrix $\mathbf{Q}_h$, with singular value decomposition $\mathbf{U\Lambda V}^T$, can be transformed into symmetric matrix $\mathbf{Q}_h' = \mathbf{C}_h^{-1/2}$ with the transformation $\mathbf{T}_h = \mathbf{VU}^T$, since $\mathbf{T}_h \mathbf{Q}_h = \mathbf{VU}^T \mathbf{U\Lambda V}^T = \mathbf{V\Lambda V}^T$ is symmetric and since $\mathbf{VU}^T$, as the product of two unary matrices, is itself unary. For reasons that will become apparent later in the paper, we give $\mathbf{Q}_h^{-1}$ its own name, $\mathbf{P}_h$, so that $\mathbf{C}_h = \mathbf{P}_h^T \mathbf{P}_h$.

Two other important quantities in inverse theory are the covariance $\mathbf{C}_m$ and resolution $\mathbf{R}$ of the estimated model parameters $\mathbf{m}^{est}$. The covariance expresses how errors in the data and prior information cause errors in the solution. The resolution expresses the degree to which a given model parameter can be uniquely determined (Backus and Gilbert, 1968; 1970; Wiggins, 1972). These quantities are given by:

$$\mathbf{C}_m = \mathbf{F}^{-g}\mathbf{C}_f\mathbf{F}^{-gT} = [\mathbf{F}^T\mathbf{F}]^{-1}\mathbf{F}^T\mathbf{I}\mathbf{F}[\mathbf{F}^T\mathbf{F}]^{-1} = [\mathbf{F}^T\mathbf{F}]^{-1} \tag{4}$$

$$\mathbf{R} = \mathbf{G}^{-g}\mathbf{G} = [\mathbf{F}^T\mathbf{F}]^{-1}\mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{G} \tag{5}$$

The forgoing will have been familiar to those who have taken a linear algebraic approach to inverse theory. We will take the continuum limit, replacing $\mathbf{d}^{obs}$ and $\mathbf{m}^{est}$ with the functions $d(x)$ and $m(x)$, where x is an independent variable (e.g. position). The matrix $\mathbf{G}$ becomes the linear operator $\mathcal{G}$, its transpose $\mathbf{G}^T$ becomes the adjoint $\mathcal{G}^\dagger$ of the corresponding operator and its inverse $\mathbf{G}^{-1}$ becomes the inverse $\mathcal{G}^{-1}$ of the corresponding operator. Depending upon context, we will interpret the identity matrix either as multiplication by 1 or convolution by the Dirac delta function, $\delta(x)$.

Formulation of the Simplified Data Smoothing Problem

In order to understand the role of prior information in determining the solution, we consider a simplified problem with $\mathbf{G} = \mathbf{I}$, $\mathbf{C}_d = \sigma_d^2\mathbf{I}$, $\mathbf{Q}_d = \sigma_d^{-1}\mathbf{I}$ and $\mathbf{h}^{pri} = 0$. These choices define a data smoothing problem, when $\mathbf{m}$ is viewed as a discretized version of a continuous function $m(x)$. The model parameters $\mathbf{m}^{est}$ represent a smoothed version of the data $\mathbf{d}^{obs}$. We multiply equation

(2) by σ_d so that the data equation is $\mathbf{Gm = d}$ and the prior information equation, which quantifies just in what sense the data are smooth, is $\sigma_d\mathbf{Hm = 0}$. The matrices $\mathbf{Q}_h$ and $\mathbf{H}$ appear only as a product in equation (2), so we define $\mathbf{L} = \sigma_d\mathbf{Q}_h\mathbf{H}$. This behavior implies that we can understand the prior information equation $\mathbf{Lm = 0}$ either as an equation of the form $\mathbf{Hm = 0}$ with non-trivial $\mathbf{H} \propto \mathbf{L}$ but trivial weighting $\mathbf{Q}_h = \mathbf{I}$ or as the equation $\mathbf{Q}_h\mathbf{m = 0}$ with the trivial $\mathbf{H = I}$ but with non-trivial weighting $\mathbf{Q}_h \propto \mathbf{L}$. The effect is the same, but the interpretation is very different. Subsequently, when we refer to $\mathbf{Q}_h$ (or $\mathbf{C}_h$ or $\mathbf{P}_h$) it will be with the presumption that we are adopting the $\mathbf{H = I}$ viewpoint. The combined equation is then:

$$\sigma_d\mathbf{Fm} = \sigma_d\mathbf{f} \equiv \begin{bmatrix} \mathbf{I} \\ \mathbf{L} \end{bmatrix}\mathbf{m} = \begin{bmatrix} \mathbf{d}^{\text{obs}} \\ \mathbf{0} \end{bmatrix} \tag{6}$$

with solution $\mathbf{m}^{\text{est}}$ obeying:

$$(\mathbf{L}^{\text{T}}\mathbf{L} + \mathbf{I})\,\mathbf{m}^{\text{est}} = \mathbf{d}^{\text{obs}} \tag{7}$$

In the continuum limit, this equation becomes:

$$(\mathcal{L}^{\dagger}\mathcal{L} + 1)\,m(x) = \mathcal{A}(x)m(x) = d(x) \tag{8}$$

Here $\mathcal{A}(x)$ is an abbreviation for $(\mathcal{L}^{\dagger}\mathcal{L} + 1)$. Finally, we mention that when *two* prior information equations are available, say $\mathbf{L}_A\mathbf{m = 0}$ and $\mathbf{L}_B\mathbf{m = 0}$, (7) becomes:

$$\begin{bmatrix} \mathbf{I} \\ \mathbf{L}_A \\ \mathbf{L}_B \end{bmatrix}\mathbf{m} = \begin{bmatrix} \mathbf{d}^{\text{obs}} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{9}$$

and the discrete and continuum solutions satisfy the equations:

$$\left(\mathbf{L}_A^{\text{T}}\mathbf{L}_A + \mathbf{L}_B^{\text{T}}\mathbf{L}_B + \mathbf{I}\right)\mathbf{m}^{\text{est}} = \mathbf{d}^{\text{obs}}$$

$$\tag{10a,b}$$

and $\qquad \left(\mathcal{L}_A^{\dagger}\mathcal{L}_A + \mathcal{L}_B^{\dagger}\mathcal{L}_B + 1\right)m(x) = d(x)$

Data Smoothing in the Continuum Limit

Equation (8) has a solution in terms of its Green function integral:

$$m(x) = \mathcal{A}^{-1}d(x) = \int a\,(x,x')\,d(x')\,\mathrm{d}x' \equiv \{a, d\} \tag{11}$$

Here we have introduced the inner product symbol $\{.,.\}$ for notational simplicity. The quantity $\mathcal{A}^{-1}(x)$ has the interpretation of a *smoothing operator* and the function $a(x,x')$ is the *smoothing kernel*. In problems with translational invariance, equation (11) is equivalent to convolution by the function $a(x)$. These functions satisfy the differential equation:

$$\mathcal{A}\,a(x,x') = \delta(x-x') \tag{12}$$

Smoothing kernels are localized functions that typically have a maximum at the central point x' and decline in both directions away from it. One example, which we will discuss in more detail later in this paper, is the two-sided declining exponential function $a(x) = \frac{1}{2}\varepsilon^{-1}\exp(-\varepsilon^{-1}|x - x'|)$, which smoothes the data over a scale length ε. The covariance of the estimated solution and the resolution are now functions of (x,x') and are given by:

$$C_m(x,x') = \sigma_d^2\,\mathcal{A}^{-1} \quad \text{and} \quad R(x,x') = \mathcal{A}^{-1} \tag{13}$$

Similarly, the continuous analogs of $\mathbf{C}_h$ and $\mathbf{P}_h$ are $C_h(x,x')$ and $P_h(x,x')$:

$$C_h = \left(P_h^\dagger, P_h\right) = \sigma_d^2\,(\mathcal{L}^\dagger\mathcal{L})^{-1} \tag{14}$$

These two functions satisfy the equations:

$$\sigma_d^{-2}\,(\mathcal{L}^\dagger\mathcal{L})\,C_h(x,x') = \delta(x-x')$$

$$\tag{15a,b}$$

$$\text{and} \qquad \sigma_d^{-1}\,\mathcal{L}^\dagger\,P_h(x,x') = \delta(x-x')$$

These equations follow from C_h being the inverse of $\sigma_d^{-2}(\mathcal{L}^\dagger\mathcal{L})$ and P_h being the inverse of $\sigma_d^{-1}\mathcal{L}$. Therefore, $\{C_h,\,\sigma_d^{-2}(\mathcal{L}^\dagger\mathcal{L})m\} = m = \{\sigma_d^{-2}(\mathcal{L}^\dagger\mathcal{L})^\dagger C_h, m\} = \{\sigma_d^{-2}(\mathcal{L}^\dagger\mathcal{L})C_h, m\} = (\delta, m)$, so $\sigma_d^{-2}(\mathcal{L}^\dagger\mathcal{L})\,C_h = \delta$ and $\{P_h, \sigma_d^{-1}\mathcal{L}m\} = m = \{\sigma_d^{-1}\mathcal{L}^\dagger P_h, m\} = (\delta, m)$, so $\sigma_d^{-1}\mathcal{L}^\dagger P_h = \delta$.

We will derive smoothing kernels for particular choices of prior information, $\mathcal{L}$, later in this paper. However, we first apply these ideas to the general inverse problem.

Smoothing within the general problem

We examine the effect of regularization on an inverse problem with an arbitrary data kernel $\mathbf{G} \neq \mathbf{I}$. With the simplifications that the data are uncorrelated and of uniform variance ($\mathbf{C_d} = \sigma_d^2\,\mathbf{I}$) and that the prior model is zero ($\mathbf{h}^{\mathrm{pri}} = 0$), equation (3a) becomes:

$$\mathbf{G}^{\mathrm{T}}\mathbf{G} + \mathbf{L}^{\mathrm{T}}\mathbf{L} = \mathbf{G}^{\mathrm{T}}\mathbf{d} = \widetilde{\mathbf{m}} \quad \text{with} \quad \mathbf{L} = \sigma_d\,\mathbf{C}_{\mathrm{h}}^{-1/2}\mathbf{H} \tag{16}$$

We have introduced the abbreviation $\widetilde{\mathbf{m}} = \mathbf{G}^{\mathrm{T}}\mathbf{d}$ to emphasize that the model $\mathbf{m}$ does not depend directly upon the data $\mathbf{d}$, but rather on their *back-projection* $\mathbf{G}^{\mathrm{T}}\mathbf{d}$ In the continuum limit, this equation becomes):

$$(\mathcal{G}^{\dagger}\mathcal{G} + \mathcal{L}^{\dagger}\mathcal{L})\,m = \mathcal{G}^{\dagger}d = \widetilde{m} \tag{17}$$

with $\mathcal{G}$ the linear operator corresponding the data kernel $\mathbf{G}$. As before, $\widetilde{m} = \mathcal{G}^{\dagger}d$ is the back-projected data. Now consider the special case where $\mathcal{G}^{\dagger}\mathcal{G}$ is close to the identity operator 1, so that we can write):

$$(\mathcal{G}^{\dagger}\mathcal{G} + \mathcal{L}^{\dagger}\mathcal{L})\,m = [(\mathcal{L}^{\dagger}\mathcal{L} + 1) + (\mathcal{G}^{\dagger}\mathcal{G} - 1)]\,m = (\mathcal{A} + \omega\mathcal{B})\,m = \widetilde{m} \tag{18}$$

where $\mathcal{A} = (\mathcal{L}^{\dagger}\mathcal{L} + 1)$, $\omega\mathcal{B} = (\mathcal{G}^{\dagger}\mathcal{G} - 1)$ and where, by hypothesis, ω is a small parameter. The parameter ω will be small either when $\mathcal{G}$ is close to the identity operator, or when it is close to being unary. These restrictions can be understood by considering the special case where $\mathcal{G}$

corresponds to convolution with a function $g(x)$. The first restriction implies $g(x) \approx \delta(x)$; that is, $g(x)$ is spiky. The second restriction implies that $g(x) \star g(x) \approx \delta(x)$; that is, that $g(x)$ is sufficiently broadband that its auto-correlation is spiky. The later condition is less restrictive than the former.

We now assume that the smoothing operator $\mathcal{A}^{-1}$ is known (e.g. by solving equation 8) and construct the inverse of $\mathcal{A} + \omega\mathcal{B}$ using perturbation theory (see Menke and Abbott, 1989, their Problem 2.1). We first propose that the solution can be written as a power series in ω:

$$m = m_0 + \omega m_1 + \omega^2 m_2 + \cdots$$

(where m_i are yet to be determined). Inserting this form of m into the inverse problem yields:

$$(\mathcal{A} + \omega\mathcal{B})(m_0 + \omega m_1 + \omega^2 m_2 + \cdots) = \tilde{m} \tag{19}$$

By equating terms of equal powers in ω, we find that $m_0 = \mathcal{A}^{-1}\tilde{m}$, $m_1 = \mathcal{A}^{-1}\mathcal{B}\mathcal{A}^{-1}\tilde{m}$, etc. The solution is then:

$$m = \left(1 + \sum_{n=1}^{\infty}(-\mathcal{A}^{-1}\omega\mathcal{B})^n\right)\mathcal{A}^{-1}\tilde{m} \tag{20}$$

and it follows from equation (18) that:

$$m = (\mathcal{A} + \omega\mathcal{B})^{-1}\,\tilde{m}$$

$$\tag{21}$$

$$\text{so} \quad (\mathcal{A} + \omega\mathcal{B})^{-1} = \mathcal{A}^{-1} - (\mathcal{A}^{-1}\omega\mathcal{B})\mathcal{A}^{-1} + (\mathcal{A}^{-1}\omega\mathcal{B})(\mathcal{A}^{-1}\omega\mathcal{B})\mathcal{A}^{-1} - \cdots$$

Since $\mathcal{A}^{-1}$ represents a smoothing operator, that is convolution by a smoothing kernel, say $a(x)$, the solution can be rewritten:

$$m = \mathcal{G}^{-g} \ (a * \tilde{m})$$

(22)

$$\text{with} \ \ \mathcal{G}^{-g} = (1 - \ (a * \omega\mathcal{B}) + \ (a * \omega\mathcal{B})(a * \omega\mathcal{B}) - \cdots)$$

Here we have introduced the abbreviation $\mathcal{G}^{-g}$ to emphasize that the solution contains a quantity that can be considered a generalized inverse. The number of terms in the expansion that are required to approximate the true $\mathcal{G}^{-g}$ is clearly a function of the size of $(a * \omega\mathcal{B})$, such that if $\|a * \omega\mathcal{B}\|_2 / \|\omega\mathcal{B}\|_2$ is small, the higher terms in the approximation rapidly become insignificant.

We may consider an example with $\mathcal{G}^\dagger \mathcal{G} \approx 1$ (but $\mathcal{G}$ far from 1) by examining a problem where $\mathcal{G}$ corresponds to convolution by a random telegraph signal $g(x)$, meaning a function that is piecewise-constant in small intervals of length Δx, with a randomly assigned amplitude in each interval. This is an extreme case of a non-localized and complicated relationship between model and data. We adjust the amplitude of $g(x)$ so that its auto-correlation has unit area; that is, $g(x) \star g(x) \approx \delta(x)$. The operator $\omega\mathcal{B}$ corresponds to convolution by $\omega b(x) = g(x) \star g(x) - \delta(x)$. Except near the origin, $\omega b(x)$ randomly oscillates around zero, so the smoothed version $a * \omega b$ has significantly reduced amplitude. A numerical test with 100 intervals of $\Delta x = 1$ indicates that the decrease is about a factor of two: $\|a * \omega b\|_2 / \|\omega b\|_2 \approx \frac{1}{2}$; that is, the ratio is significantly less than unity. The test also shows that the exact and approximate solutions match closely, even when only the first two terms of the series are included in the approximation (Figure 1). This is a case where the $a * \omega\mathcal{B}$ smoothing inside the generalized inverse substantially simplifies that quantity.

We also consider an example with $\mathcal{G} \approx 1$, by examining the problem of determining the density $m(x)$ of a linear arrangement of masses (e.g. seamount chain) from the vertical component $f_v(x)$ of the gravitational field measured a distance h above them. This is an extreme case of a

localized and simple relationship between model and data. According to Newton's Law, the field

due to a unit point mass at the origin is:

$$f_v(x) = \gamma h(x^2 + h^2)^{-3/2} \tag{23}$$

where γ is the gravitational constant. The scaled data $d(x) = \frac{1}{2}\gamma^{-1}hf_v(x)$ then satisfies the

equation:

$$\mathcal{G}\, m = g * m = d$$

$$\tag{24}$$

$$\text{with} \quad g(x) = \frac{1}{2}h^2(x^2 + h^2)^{-3/2}$$

where the scaling was chosen so that the gravitational response function $g(x)$ has unit area, thus

satisfying $g(x) \approx \delta(x)$ for small h. The function $g(x)$ is everywhere positive and decreases

only slowly as $|x| \to \infty$, so $g(x) \star g(x)$ is everywhere positive and slowly decreasing, as well.

Consequently, we do not expect that the $a * \omega \mathcal{B}$ smoothing inside the generalized inverse will

have much effect. A numerical test, with $h = 2$, indicates that $\|a * \omega b\|_2 / \|\omega b\|_2 \approx 0.98$; that is,

it is not significantly less than unity.   Consequently, a relatively large number of terms (about

20) of the series are needed to achieve an acceptable match between the approximate and exact

solutions (Figure 2).

Irrespective of the form of $\mathcal{G}$, regularization has the effect of smoothing the back-projected data

$\tilde{m}$, which leads to a smoother solution m. Further smoothing occurs for some data kernels (those

with oscillatory $\mathcal{B} = \omega^{-1}[\mathcal{G}^{\dagger}\mathcal{G} - 1]$), since the regularization also leads to a smoother

generalized inverse. Smoothing of $\tilde{m}$, which can be viewed as an approximate form of the

solution, is arguably the intent of regularization. Smoothing of $\mathcal{B}$, which represents the theory, is

arguably an undesirable side effect. This second kind of smoothing is of particular concern when

the averaging kernel $a(x)$ has side lobes, since spurious structure can be introduced into the theory, or when $a(x)$ has less than unit area, since structure can be suppressed. In the Case Studies, below, we derive analytic formulas for $a(x)$ for four common choices of prior information and analyze their properties to address these concerns. As we will put forward in more detail in the Discussion and Conclusions section, our overall opinion is that prior information that leads to an averaging kernel with unit area and without side lobes is the preferred choice, unless some compelling reason, specific to the particular inverse problem under consideration, indicates otherwise.

Four Case Studies

We discuss four possible ways of the quantifying the intuitive notion of a function being smooth. In all cases, we assume that the smoothing is uniform over x, which corresponds to the case where $\mathcal{L}$ has translational invariance, so smoothing is by convolution with a kernel $a(x)$ and the prior information is uncorrelated and with uniform variance σ_h^2. In Case 1, a smooth function is taken to be one with a small first-derivative, a choice motivated by the notion that a function that changes only slowly with position is likely to be smooth. In Case 2, a smooth function is taken as one with large positive correlations that decay with distance for points separated by less than some specified scale length. This choice is motivated by the notion that the function must be approximately constant, which is to say smooth, over that scale length. In Case 3, a smooth function is taken to be one with small second-derivative, a choice motivated by the notion that this derivative is large at peaks and troughs, so that a function with only small peaks and troughs is likely to be smooth. Finally, in Case 4, a smooth function is taken to be one that is similar to its localized average. This choice is motivated by the notion that averaging smoothes a function, so that any function that is approximately equal to its own localized average is likely to be

smooth. All four of these cases are plausible ways of quantifying smoothness. As we will show below, they all *do* lead to smooth solutions, but solutions that are significantly different from one another. Furthermore, several of these cases have unanticipated side effects. We summarize the smoothing kernels for each of these choices in Table 1.

Case 1. We take flatness (small first-derivative) as a measure of smoothness. The prior information equation is $\varepsilon \, dm/dx = 0$, where $\varepsilon = \sigma_d/\sigma_h$, so that $\mathcal{L} = \varepsilon \, d/dx$. The parameter ε quantifies the strength by which the flatness constraint is imposed. The smoothing kernel for this operator is (see Appendix):

$$a(x) = \frac{\varepsilon^{-1}}{2} \exp(-\varepsilon^{-1}|x|) \qquad (25)$$

The solution (Figure 3) is well-behaved, in the sense that the data are smoothed over a scale length ε without any change in their mean value (since $a(x)$ has unit area). Furthermore, the smoothing kernel monotonically decreases towards zero, without any side-lobes, so that the smoothing creates no extraneous features. The covariance and resolution of the estimated solution are

$$C_m(x) = \sigma_d^2 \, a(x) \quad \text{and} \quad R(x) = a(x) \qquad (26)$$

Note that the variance and resolution trade off, in the sense that the size of the variance is proportional to ε^{-1}, whereas the width of the resolution is proportional to ε; as the strength of the flatness constraint is increased, the size of the variance decreases and the width of the resolution increases.

The autocorrelation of the data, $X_d(x) = d(x) \star d(x)$, where $\star$ signifies cross-correlation, quantifies the scale lengths present in the observations. In general, the autocorrelation of the model parameters, $X_m(x) = m(x) \star m(x)$, will be different, because of the smoothing. The two are related by convolution with the autocorrelation of the smoothing kernel):

$$X_m(x) = [a(x) * d(x)] \star [a(x) * d(x)] = X_a(x) * X_a(x) \tag{27}$$

where $X_a(x) = a(x) \star a(x)$ (see Menke and Menke 2011, their Equation 9.24). The reader may easily verify (by direct integration) that the autocorrelation of equation (25) is:

$$X_a(x) = \frac{\varepsilon^{-2}}{4}(|x| + \varepsilon)\exp(-\varepsilon^{-1}|x|) \tag{28}$$

This is a monotonically declining function of $|x|$ with a maximum (without a cusp) at the origin. The smoothing broadens the autocorrelation (or auto-covariance) of the data in a well-behaved way.

The covariance function C_h associated with this choice of smoothing is (see equation A6):

$$C_h(x) = \sigma_d^2 \frac{\varepsilon^{-2}}{2}(C_0 - |x|) \quad \text{with } C_0 \text{ arbitrary} \tag{29}$$

Note that the product $\sigma_d^2\,\varepsilon^{-2}$ equals the prior variance σ_h^2.

Case 2: In Case 1, we worked out the consequences of imposing a specific prior information equation $\mathcal{L}m = 0$, among which was the equivalent covariance C_h. Now we take the opposite approach, imposing C_h and solving for, among other quantities, the equivalent prior information equation $\mathcal{L}m = 0$. We use a two-sided declining exponential function:

$$C_h(x - x') \;=\; \sigma_d^2\, \varepsilon^{-2} \exp(-\eta |x - x'|) \;=\; \sigma_d^2\, \frac{2\varepsilon^{-2}}{\eta}\, \frac{\eta}{2} \exp(-\eta |x - x'|) \tag{30}$$

This form of prior covariance was introduced by Abers et al. (1994). Here η^{-1} is a scale factor that controls decreases of covariance with separation distance $(x - x')$. The smoothing kernel is given by:

$$a(x) = \gamma^{-2} \frac{\beta\gamma}{2} \exp(-\beta\gamma |x|) \tag{31}$$

Where γ and β are functions of the smoothing weight ε and scale length η^{-1} (see equation A11) and $\gamma^{-2} = \int_{-\infty}^{\infty} g(x)\, dx$. This smoothing kernel (Figure 3) has the form of a two-sided, decaying exponential and so is identical in form to the one encountered in Case 1. As the variance of prior information is made very large, $\varepsilon^{-2} \to \infty$ and $\gamma^{-2} \to 1$, implying that the area under the smoothing kernel approaches unity – a desirable behavior for a smoothing function. However, as variance is decreased, $\varepsilon^{-2} \to 0$ and $\gamma^{-2} \to 0$, implying that the smoothing kernel is tending toward zero area – an undesirable behavior, because it reduces the amplitude of the smoothed function, as shown in Figure 3.

The behavior of the smoothing kernel at small variance can be understood by viewing the prior information as consisting of *two* equations, a flatness constraint of the form $\mathcal{L}_A m = \beta^{-1}\, dm/dx = 0$ (the same condition as in Case 1) and an additional *smallness* constraint of the form $\mathcal{L}_B m = \mu m = 0$, with $\mu^2 = \gamma^2 - 1$ by construction. When combined via equation (10b), the two equations lead to the same differential operator as in Case 1 (see equation A10) :

$$\left(\mathcal{L}_A^\dagger \mathcal{L}_A + \mathcal{L}_B^\dagger \mathcal{L}_B + 1\right) a(x) \;=\; \gamma^2 \left(-\beta^{-2}\gamma^{-2}\frac{d^2}{dx^2} + 1\right) a(x) \;=\; \delta(x) \tag{32}$$

Note that the strength of the smallness constraint is proportional to $\mu = \varepsilon \left(\frac{\eta}{2}\right)^{\frac{1}{2}}$, which depends

on both η and ε. The smallness constraint leads to a smoothing kernel with less than unit area,

since it causes the solution $m(x)$ to approach zero as $\varepsilon \to \infty$ and $\mu =\to \infty$. No combination of ε

and η can eliminate the smallness constraint while still preserving the two-sided declining

exponential form of the smoothing kernel.

Case 3: We quantify the smoothness of $m(x)$ by the smallness of its second-derivative. The

prior information equation is $\varepsilon \, d^2m/dx^2 = 0$, implying $\mathcal{L} = \varepsilon \, d^2/dx^2$. Since the second

derivative is self-adjoint, we have:

$$\mathcal{L}^{\dagger}\mathcal{L} = \varepsilon^2 \frac{d^4}{dx^4} \tag{33}$$

This differential equation yields the smoothing kernel:

$$a(x) = V \exp(-|x|/\lambda) \{\cos(|x|/\lambda) + \sin(|x|/\lambda)\} \tag{34}$$

See equation A15 for the definition of the constants V and λ. The covariance function C_h is given

by (see equation A17):

$$C_h(x) = -\sigma_d^{-2} \frac{\varepsilon^{-2}}{12} (C_0 - |x^3|) \quad \text{with } C_0 \text{ arbitrary} \tag{35}$$

This smoothing kernel arises in civil engineering, where it is represents the deflection $a(x)$ of a

elastic beam of flexural rigidity ε^2 floating on a fluid foundation, due to a point load at the origin

(Hetenyi 1979). In our example, the model $m(x)$ is analogous to the deflection of the beam and

the data to the load; that is, the model is a smoothed version of the data just as a beam's

deflection is a smoothed version of its applied load. Furthermore, variance is analogous to the

reciprocal of flexural rigidity. The beam will take on a shape that exactly mimics the load only in the case when it has no rigidity; that is, infinite variance. For any finite rigidity, the beam will take on a shape that is a smoothed version of the load, where the amount of smoothing increases with ε^2.

The area under this smoothing kernel can be determined by computing its Fourier transform, since area is equal to the zero-wavenumber value. Transforming position x to wavenumber k in (32) gives $(\varepsilon^2 k^4 + 1)a(k) = 1$, which imples $a(k = 0) = 1$; that is, the smoothing kernel has unit area. This is a desirable property. However, the smoothing kernel (Figure 3) also has small undesirable side-lobes.

Case 4: The prior information equation is that $m(x)$ is close to its localized average $s(x) *$ $m(x)$, where $s(x)$ is a localized averaging kernel. We use the same two-sided declining exponential as in Case 1 (equation 25) to perform the averaging:

$$s(x) = \frac{\eta}{2} \exp\{-\eta|x|\} \tag{36}$$

The prior information equation is then:

$$\mathcal{L}m = \varepsilon[\delta(x) - s(x)] * m = 0 \tag{37}$$

Both $s(x)$ and the Dirac delta function are symmetric, so the operator $\mathcal{L}$ is self-adjoint. The smoothing kernel for this case is:

$$s(x) = (1 - AD)\,\delta(x) - A\,\{S\,\sin(\eta q|x|/r) - C\,\cos(\eta q|x|/r)\}\exp(-\eta p|x|/r) \tag{38}$$

See equation A22 for the definition of constants A, D, S, C, q, and r. The smoothing kernel (Figure 3) consists of the sum of a Dirac delta function and a spatially-distributed function reminiscent to the elastic plate solution in Case 3. Thus, the function $m(x)$ is a weighted sum of

the data $d(x)$ and a smoothed version of that same data. Whether this solution represents a useful type of smoothing is debatable; it serves to illustrate that peculiar behaviors can arise out of seemingly innocuous forms of prior information. The area under this smoothing kernel (see equation A23) is unity, a desirable property. However, like Case 3, the solution also has small undesirable side-lobes.

Discussion and Conclusions

The main result of this paper is to show that the consequences of particular choices of regularization in inverse problems can be understood in considerable detail by analyzing the data smoothing problem in its continuum limit. This limit converts the usual matrix equations of generalized least squares into differential equations. Even though matrix equations are easy to solve using a computer, they usually defy simple analysis. Differential equations, on the other hand, often can be solved exactly, allowing the behavior of their solutions to be probed analytically.

A key result is that the solution to the general inverse problem depends on a smoothed version of the back-projected data $\tilde{m}$ and a smoothed version of the theory, as quantified by $\omega \mathcal{B}$ (equation 22). The leading order term reproduces the behavior of the simple $\mathcal{G} = 1$ data smoothing problem (considered in the case studies); that is, m_0 is just a smoothed version of $\tilde{m}$. However, in the general $\mathcal{G} \neq 1$ case, regularization (damping) also adds smoothing inside the generalized inverse $\mathcal{G}^{-g}$, making it in some sense "simpler". Furthermore, the higher order terms, which are important when $\mathcal{G}^\dagger \mathcal{G}$ is dissimilar from 1, are preferentially smoothed. In all cases, the smoothing is through convolution with $a(x)$, the solution to the simple $(1 + \mathcal{L}^\dagger \mathcal{L}) m = \delta$

problem. Thus, the solution to the simple problem controls the way smoothing occurs in the more general one.

We have also developed the link between prior information expressed as a constraint equation of the form $\mathbf{Hm} = \mathbf{h}$ and of that same prior information expressed as a covariance matrix $\mathbf{C_h}$. Starting with a particular $\mathbf{H}$ or $\mathbf{C_h}$, we have worked out the corresponding $\mathbf{C_h}$ or $\mathbf{H}$, as well as the smoothing kernel. This smoothing kernel is precisely equivalent to the Green function, or generalized inverse familiar from the classic, linear algebraic approach.

An interesting result is that prior information implemented as a prior covariance with the form of a two-sided declining exponential function, is exactly equivalent to a pair of constraint equations, one of which suppresses the first derivative of the model parameters and the other that suppresses their size. In this case, the smoothing kernel is a two-sized declining exponential with an area less than or equal to unity; that is, it both smoothes and reduces the amplitude of the observations.

Our results allow us to address the question of which form of regularization best implements an intuitive notion of smoothing. There is, of course, no authoritative answer to this question. Any of the four cases we have considered, and many others besides, implements reasonable forms of smoothing; any one of them might arguably be *best* for a specific problem. Yet simpler is often better. We put forward first-derivative regularization as an extremely simple and effective choice, with few drawbacks. The corresponding smoothing kernel has the key attributes of unit area and no side-lobes. The scale length of the smoothing depends on a single parameter, ε. Its only drawback is that it possesses a cusp at the origin, which implies that it suppresses higher wavenumbers relatively slowly, as k^{-2}. Its autocorrelation, on the other hand, has a simple

maximum (without a cusp) at the origin, indicating that it widens the auto-covariance of the observations in a well-behaved fashion.

Furthermore, first-derivative regularization has a straightforward generalization to higher dimensions. One merely writes a separate first-derivative equation for each independent variable (say, x, y, z):

$$\mathcal{L}_A m = \varepsilon \frac{\partial}{\partial x} m = 0 \quad \text{and} \quad \mathcal{L}_B m = \varepsilon \frac{\partial}{\partial y} m = 0 \quad \text{and} \quad \mathcal{L}_C m = \varepsilon \frac{\partial}{\partial z} m = 0 \tag{39}$$

The least-squares minimization will suppress the sum of squared errors of these equations, which is to say, the Euclidian length of the gradient vector ∇m. According to (equation 12), the smoothing kernel satisfies the Screened Poisson equation:

$$\left(\nabla^2 - \varepsilon^{-2} \right) a(\mathbf{x}) = -\varepsilon^{-2} \delta(\mathbf{x}) \tag{40}$$

which has two- and three-dimensional solutions (Wikipedia, 2014) :

$$a_{2D}(\mathbf{x}) = \frac{\varepsilon^{-2}}{2\pi} K_0(\varepsilon^{-1} r) \quad \text{and} \quad a_{3D}(\mathbf{x}) = \frac{\varepsilon^{-2}}{4\pi r} \exp(-\varepsilon^{-1} r) \quad \text{with} \quad r = |\mathbf{x}| \tag{41}$$

Here, K_0 is the modified Bessel function. Both of these multidimensional smoothing kernels, like the 1D version examined in Case 1, have unit area and no side-lobes, indicating that first-derivative regularization will be effective when applied to these higher-dimensional problems.

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Appendix: Derivations of Smoothing Kernels and Covariances for Case Studies

Case 1: First derivative minimization

The operator $\mathcal{L} = \varepsilon\, \mathrm{d}/\mathrm{d}x$ has translational invariance, so we expect that the smoothing kernel $a(x, x') = a(x - x')$ depends only upon the separation distance $(x - x')$ (as also will C_h, P_h, Q_h and R). Without loss of generality, we can set $x' = 0$, so that equation (13) becomes:

$$\left(-\varepsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + 1 \right) a(x) = \delta(x) \tag{A1}$$

Here, we utilize the relationship that $(d/dx)^\dagger = -d/dx$. The solution to this well-known 1D Screened Poisson equation is:

$$a(x) = \frac{\varepsilon^{-1}}{2} \exp(-\varepsilon^{-1}|x|)$$

(A2)

This solution can be verified by substituting it into the differential equation:

$$\frac{da}{dx} = -\frac{\varepsilon^{-2}}{2} \operatorname{sgn}(x) \exp(-\varepsilon^{-1}|x|) \quad \text{and} \quad \frac{d^2a}{dx^2} = \frac{\varepsilon^{-3}}{2} \exp(-\varepsilon^{-1}|x|) - \varepsilon^{-2}\delta(x)$$

(A3)

$$\text{so} \quad -\varepsilon^2 \frac{\varepsilon^{-3}}{2} \exp(-\varepsilon^{-1}|x|) - \varepsilon^2(-\varepsilon^{-2})\,\delta(x) + \frac{\varepsilon^{-1}}{2} \exp(-\varepsilon^{-1}|x|) = \delta(x)$$

Here, we have relied on the fact that $(d/dx)|x| = \operatorname{sgn}(x)$ and $(d/dx)\operatorname{sgn}(x) = 2\delta(x)$. Note that $a(x)$ is a two-sided declining exponential with unit area and decay rate ε^{-1}. Because of the translational invariance, the integral in equation (11) has the interpretation of a convolution. The solution is the observed data $d(x)$ convolved with this smoothing kernel:

$$m(x) = a(x) * d(x)$$

(A4)

The variance C_h of the prior information satisfies (equation 15a):

$$-\sigma_d^{-2}\,\varepsilon^2 \frac{d^2}{dx^2}\,C_h(x) = \delta(x)$$

(A5)

This is a 1D Poisson equation, with solution:

$$C_h(x) = \sigma_d^2 \frac{\varepsilon^{-2}}{2}(C_0 - |x|) \quad \text{with } C_0 \text{ arbitrary}$$

(A6)

This solution can be verified by substituting it into the differential equation:

$$\frac{dC_h}{dx} = -\sigma_d^2 \frac{\varepsilon^{-2}}{2} \operatorname{sgn}(x) \quad \text{and} \quad \frac{d^2C_h}{dx^2} = -\sigma_d^2\,\varepsilon^{-2}\,\delta(x)$$

(A7)

25

$$\text{thus} \quad -\sigma_d^{-2}\, \varepsilon^2 \frac{d^2}{dx^2} C_h(x) \;=\; -\sigma_d^{-2}\, \varepsilon^2(-\sigma_d^2\, \varepsilon^{-2})\, \delta(x) \;=\; \delta(x)$$

The covariance $C_h(x - x')$ implies that the errors associated with neighboring points of the prior

information equation $m(x) = 0$ are highly and positively correlated, and that the degree of

correlation declines with separation distance, becoming negative at large separation.

Finally, we note that the operator $\mathcal{L} = \varepsilon\, d/dx$ is not self-adjoint, so that it is not the continuous

analog of the symmetric matrix $\mathbf{C}_h^{-1/2}$. As described earlier, we can construct a symmetric

operator by introducing a unary transformation. $\mathcal{L}$ is antisymmetric in x, but we seek a

symmetric operator, so the correct transformation it is the Hilbert transform, $\mathcal{H}$; that is, the linear

operator that phase-shifts a function by $\pi/2$. It obeys the rules $\mathcal{H}^\dagger = -\mathcal{H}$, $\mathcal{H}^\dagger \mathcal{H} = 1$ and

$\mathcal{H}(d/dx) = (d/dx)\mathcal{H}$. The modified operator $\mathcal{L}_{sa} = \varepsilon\, \mathcal{H} d/dx$ *is* self-adjoint and satisfies

$\mathcal{L}_{sa}^\dagger \mathcal{L}_{sa} = \mathcal{L}^\dagger \mathcal{L}$.

Case 2: Exponentially decaying covariance

For a covariance described by a two-sided declining exponential function:

$$C_h(x - x') = \varepsilon^{-2} \exp(-\eta|x - x'|) = \frac{2\varepsilon^{-2}}{\eta}\, \frac{\eta}{2} \exp(-\eta|x - x'|) \qquad \text{(A8)}$$

By comparing equtions (A1) and (A2), we find that this prior covariance is the inverse of the

operator:

$$\mathcal{L}^\dagger \mathcal{L} = \frac{\eta \varepsilon^2}{2}\left(-\eta^{-2} \frac{d^2}{dx^2} + 1\right) \qquad \text{(A9)}$$

The smoothing kernel solves the equation:

$$\gamma^2 \left(-\beta^{-2}\gamma^{-2}\frac{d^2}{dx^2} + 1 \right) a(x) = \delta(x)$$

(A10)

$$\text{with } \beta^2 = 2\eta\varepsilon^{-2} \text{ and } \gamma^2 = \left(1 + \frac{\eta\varepsilon^2}{2} \right)$$

By analogy to equations (A1) and (A2), the smoothing kernel is:

$$a(x) = \gamma^{-2}\frac{\beta\gamma}{2}\exp(-\beta\gamma|x|)$$

(A11)

An operator $\mathcal{L}$ that reproduces the form of $\mathcal{L}^\dagger\mathcal{L}$ given in equation (A9) is:

$$\mathcal{L} = \lambda\left(\eta^{-1}\frac{d}{dx} + 1 \right) \quad \text{with} \quad \lambda^2 = \eta/2\varepsilon^{-2}$$

(A12)

The function P_h solves equation (15b), $\mathcal{L}^\dagger P_h = \delta(x)$, which for the operator in (30) has the

form of a one-sided exponential:

$$P_h(x) = \alpha\lambda^{-1}H(-x)\exp(\eta x)$$

(A13)

Here, $H(x)$ is the Heaviside step function. Because of the translational invariance, the inner

product in equation (14) relating P_h to C_h is a convolution. That, together with the rule that the

adjoint of a convolution is the convolution backwards in time, implies that $C_h(t) = P_h(-t) *$

$P_h(t) = P_h(t) \star P_h(t)$, where $\star$ signifies cross-correlation. The reader may easily verify that the

autocorrelation of equation (31) reproduces the formula for C_h given in (25). Unfortunately, its

Hilbert transform cannot be written as a closed-form expression, so no simple formula for the

symmetrized form of P_h, analogous to $\mathbf{C}_h^{1/2}$, can be given.

Case 3: Second derivative minimization

The smoothing kernel $a(x)$ satisfies the differential equation:

$$\left(\varepsilon^2 \frac{d^4}{dx^4} + 1\right) a(x) = \delta(x) \tag{A14}$$

This well-known differential equation has solution (Hetenyi 1979; see also Menke and Abbott 1989; Smith and Wessel 1990; Menke, 2014):

$$a(x) = V \exp(-|x|/\lambda) \{\cos(|x|/\lambda) + \sin(|x|/\lambda)\}$$

$$\lambda = (2\varepsilon)^{1/2} \quad \text{and} \quad V = \frac{\lambda^3}{8\varepsilon^2} \tag{A15}$$

The variance C_h of the prior information satisfies equation (15a):

$$\sigma_d^{-2} \, \varepsilon^2 \frac{d^4}{dx^4} C_h(x) = \delta(x) \tag{A16}$$

And by analogy to (A6) has solution:

$$C_h(x) = -\sigma_d^2 \frac{\varepsilon^{-2}}{12} (C_0 - |x^3|) \quad \text{with } C_0 \text{ arbitrary} \tag{A17}$$

This solution can be verified by substituting it into the differential equation:

$$\frac{d^3 C_h}{dx^3} = \sigma_d^2 \frac{\varepsilon^{-2}}{2} \operatorname{sgn}(x) \quad \text{and} \quad \frac{d^2 C_h}{dx^2} = \sigma_d^2 \, \varepsilon^{-2} \, \delta(x) \tag{A18}$$

$$\text{thus} \quad \sigma_d^{-2} \, \varepsilon^2 \frac{d^4}{dx^4} C_h(x) = \sigma_d^{-2} \varepsilon^2 (\sigma_d^2 \, \varepsilon^{-2}) \, \delta(x) = \delta(x)$$

This function implies a steep drop off in covariance between neighboring points and increasingly great anticorrelation with distance.

Case 4: Damping towards localized average

From equation (37), we find that the smoothing kernel $a(x)$ satisfies:

$$\mathcal{L}^{\dagger}\mathcal{L}\, a + a = \varepsilon^2 [\delta(x) - s(x)] * [\delta(x) - s(x)] * a + a = \delta(x) \qquad \text{(A19)}$$

We now make use of the fact that the operator $\mathcal{L}_s = 1 - \eta^{-2} d^2/dx^2$ is the inverse to convolution by $s(x)$. Applying $\mathcal{L}_s$ twice to (37) yields the differential equation:

$$(1 + \varepsilon^2)\eta^{-4}\frac{d^4 a}{dx^4} - 2\eta^{-2}\frac{d^2 a}{dx^2} + a = f(x) \quad \text{with} \quad f(x) = \mathcal{L}_s \mathcal{L}_s \delta(x) \qquad \text{(A20)}$$

We solve this equation by finding its Green function (that is, solving (39) with $f(x) = \delta(x)$) and then by convolving this Green function by the actual $f(x)$. This Green function can be found using Fourier transforms, with the relevant integral given by equation 3.728.1 of Gradshteyn and Ryzhik (1980) (which needs to be corrected by dividing their stated result by a factor of 2). The result is:

$$a(x) = (1 - AD)\, \delta(x) - A\, \{S\, \sin(\eta q |x|/r) - C\, \cos(\eta q |x|/r)\} \exp(-\eta p |x|/r) \qquad \text{(A21)}$$

where:

$$S = \left(\frac{\eta}{r}\right)^4 p\{(p^4 - q^4) - 2q^2(p^2 + q^2)\}$$

$$C = \left(\frac{\eta}{r}\right)^4 q\{(p^4 - q^4) + 2p^2(p^2 + q^2)\}$$

$$A = \varepsilon^2 \eta^{-4} \times \frac{2}{\pi}\left(\frac{\eta^4}{\varepsilon^2 + 1}\right) \times \left(\frac{\pi}{4uv}\right) \times 2\left(\frac{\eta}{r}\right)$$

or $\qquad A = \left(\frac{\varepsilon^2}{\varepsilon^2+1}\right)\left(\frac{\eta}{uvr}\right)$ (A22)

$$D = 4\left(\frac{\eta}{r}\right)^3 pq(p^2 + q^2)$$

$$u = \frac{2\varepsilon\eta^2}{\varepsilon^2 + 1} \quad \text{and} \quad v = \frac{\eta^2(\varepsilon^2 + 1)^{1/2}}{r^2}$$

$$r = (\varepsilon^2 + 1)^{1/2} \quad \text{and} \quad p = \left(\frac{r+1}{2}\right)^{1/2} \quad \text{and} \quad q = \left(\frac{r-1}{2}\right)^{1/2}$$

We determine the area under the smoothing kernel by taking the Fourier transform of (A20):

$$\left((1 + \varepsilon^2)\eta^{-4}k^4 - 2\eta^{-2}k^2 + 1\right)a(k) = 1 - 2\eta^{-2}k^2 + \eta^{-4}k^4 \qquad \text{(A23)}$$

and evaluating it at zero wavenumber. Thus, $a(k = 0) = 1$; that is, the area is unity.

Figure captions

Figure 1. Telegraph signal inverse problem. (A) The true model, $m^{true}(x)$ is a spike. (B) The observed data $d^{obs}(x)$ are the true data $g(x) * m^{true}(x)$ plus random noise. (C) An undamped inversion yields an estimated model $m^{est}(x)$. (D) A damped inversion with $L = \varepsilon \, d/dx$ and $\varepsilon = 0.1$ yields a smoother estimated model. (E) The first 2 terms of the series approximation for the generalized inverse yield a solution substantially similar to the one in (D).

Figure 2. Gravity inverse problem. (A) The true model, $m^{true}(x)$ represents density. (B) The observed data $d^{obs}(x)$ is the true data predicted by Newton's Law, plus random noise. (C) An undamped inversion yields an estimated model $m^{est}(x)$ that is very noisy. (D) A damped inversion with $L = \varepsilon \, d/dx$ and $\varepsilon = 0.1$ suppresses the noise, yielding an improved estimated model. (E) The first 20 terms of the series approximation for the generalized inverse yield a solution substantially similar to the one in (D).

Figure 3. The data smoothing problem implemented using each of the four cases. $\varepsilon = 3$ and $\alpha = 0.4$. A) The true model $m^{true}(x) = \sin(A\pi x^2)$ (black line) has noise added with standard deviation 0.2 to produce the hypothetical data $d^{obs}(x)$ (black circles), to which the different smoothing solutions are applied to produce estimated models (colored lines). For cases 1-4, the smoothed solutions have posterior r.m.s. errors of 0.10, 0.44, 0.07, and 0.19, respectively. B-E) Numerical (grey) and analytic (colored) versions of the smoothing kernels, $a(x)$ for each of the four smoothing schemes considered. The two versions agree closely.

Table 1. Comparison of smoothing kernels for the different choices of smoothing scheme for the four cases considered. The plotted smoothing kernels were calculated with the choices $\varepsilon = 3$ and $\eta = 0.4$ and are plotted at the same scale, in the x-range of ± 40 units.
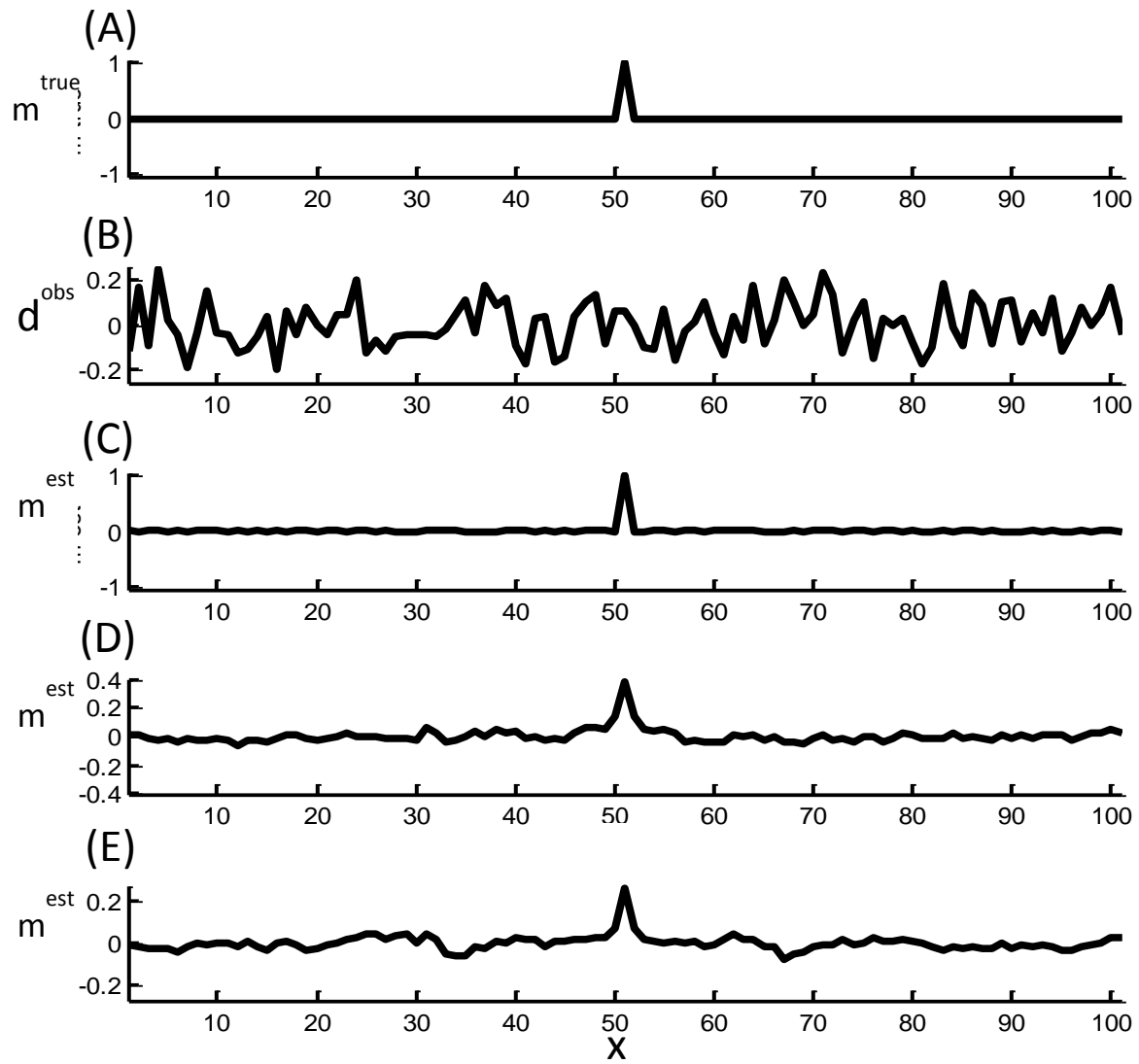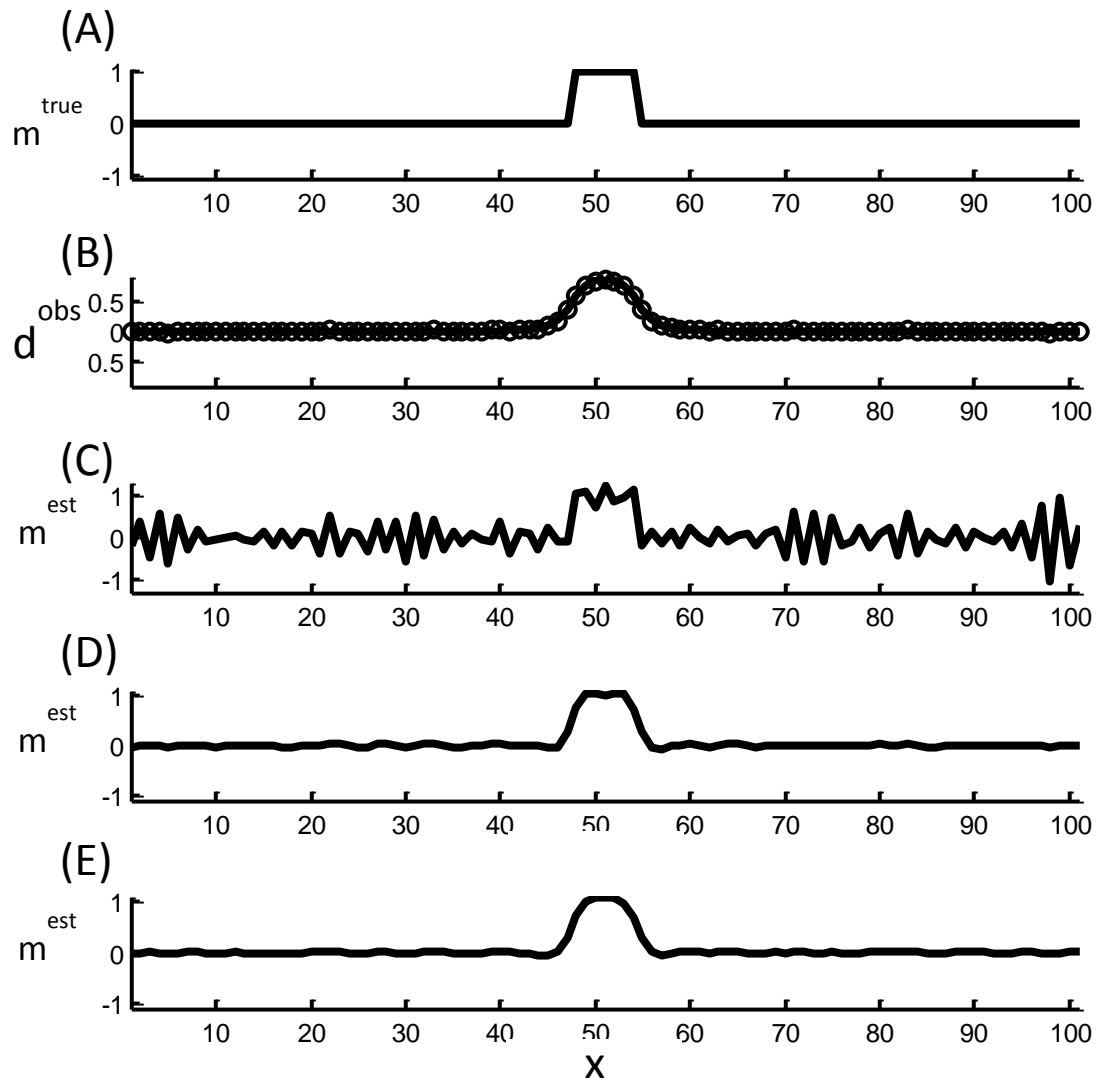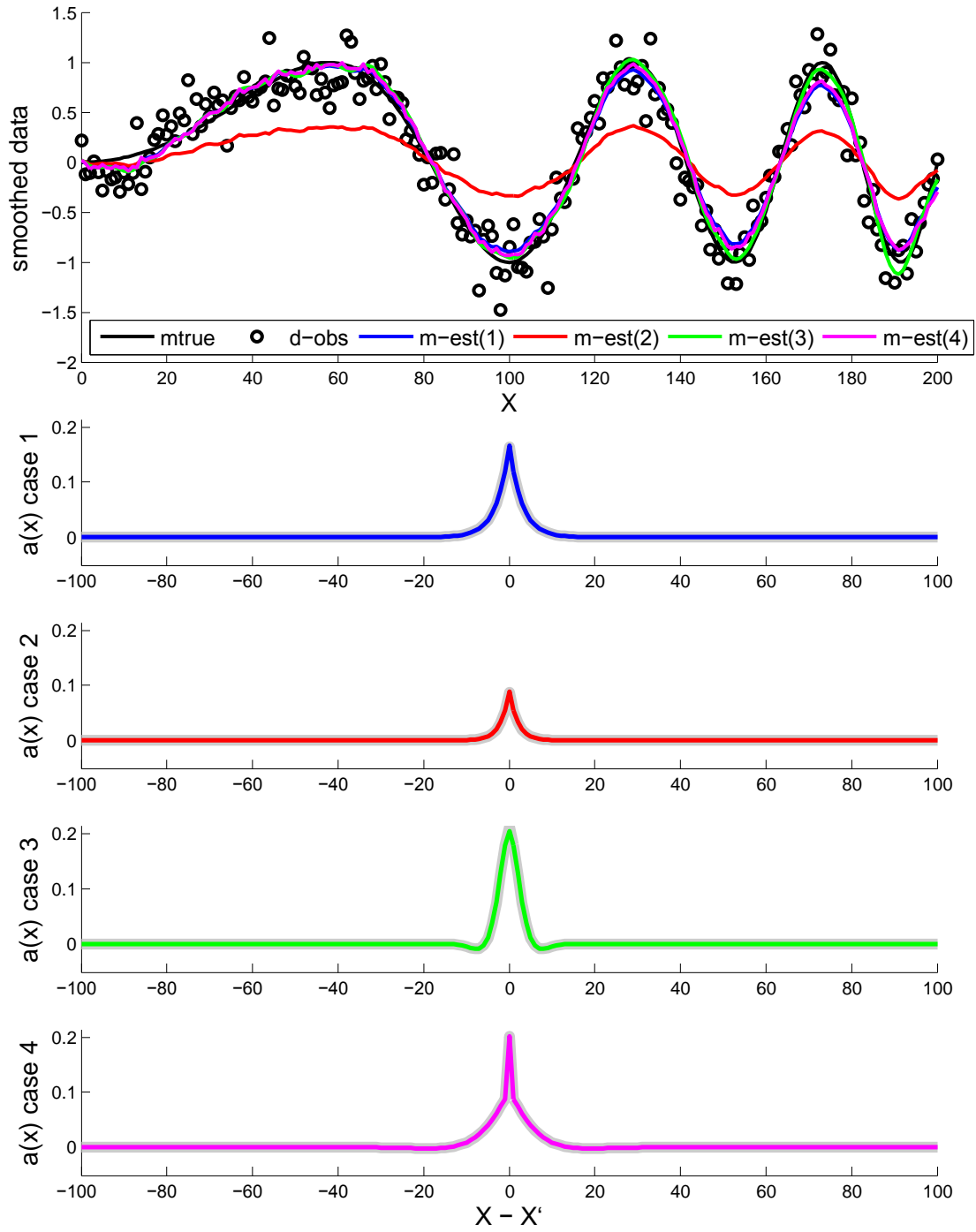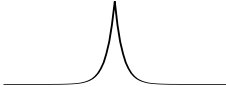
Figure 1.

Figure 2.

Figure 3.
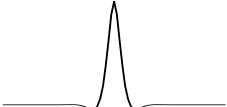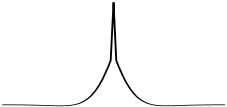
Table 1.

Case	1	2	3	4
Constraint	1st derivative damping	Exponentially declining spatial covariance	2nd derivative damping	Damping towards localized average $s(x)$
Constraint equation	$\varepsilon \dfrac{d}{dx} = 0$	$C_h(x) = \sigma_h^2 \exp(-\eta\lvert x - x'\rvert)$ with $\sigma_h^2 = \sigma_d^2\, \varepsilon^{-2}$	$\varepsilon \dfrac{d^2}{dx^2} = 0$	$\varepsilon[\delta(x) - s(x)] * m = 0$
$a(x) =$				
Comments	No side lobes Unit area	No side lobes Area $= \dfrac{2}{2+\eta\varepsilon^2} < 1$	Side lobes Unit area	Side lobes Unit area