Error Bounds for Extended Source Inversion applied to an Acoustic Transmission Inverse Problem

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ABSTRACT

A simple inverse problem for the wave equation requires determination of both the wave velocity in a homogenous acoustic material and the transient waveform of an isotropic point radiator, given the time history of the wavefield at a remote point in space. The duration (support) of the source waveform and the source-to-receiver distance are assumed known. A least squares formulation of this problem exhibits the “cycle-skipping” behaviour observed in field scale problems of this type, with many local minima differing greatly from the global minimizer. An extended formulation, dropping the support constraint on the source waveform in favor of a weighted quadratic penalty, eliminates this misbehaviour. With proper choice of the weight operator, the velocity component at any local minimizer of this extended objective function differs from the global minimizer of the least-squares formulation by less than a linear combination of the source waveform support radius and data noise-to-signal ratio.

INTRODUCTION

Inverse problems based on wave equations (acoustic, elastic, Maxwell’s...) are commonplace in geophysics, nondestructive materials testing, medical imaging, and other areas of science and engineering in which wave motion plays an important role. These problems may be formulated as nonlinear least squares problems, requiring optimization of mean square misfit between observed and predicted data. Iterative local numerical optimization methods (relatives of Newton’s method) are feasible solution approaches for the computationally large variants of these nonlinear least squares problems that occur in seismology and medical imaging. However, local optimization produces only approximate stationary points, and these exhibit a tendency to stagnate at physically irrelevant solutions, under typical conditions of data acquisition. This “cycle-skipping” pathology can sometimes be overcome through use of information other than measured wave data, however it remains a serious obstacle to effective solution of field-scale inverse problems in wave propagation (Gauthier et al., 1986; Virieux and Operto, 2009; Fichtner, 2010; Plessix et al., 2010; Schuster, 2017).

Since numerical feasibility limits practical optimization approaches to search for stationary points, it is natural to explore alternatives to nonlinear least squares formulations for which approximate stationary points might perforce be acceptable solutions. Many such alternatives have been suggested and applied in both synthetic and field data tests, in some cases with excellent results (see Huang et al. (2019), Pladys et al. (2021) for recent reviews). However numerical tests are inevitably “a look in the rear view mirror”, with no guarantee...
that the next example will not behave quite differently. See Symes (2020) for an example of such an unpleasant surprise. Theoretical guarantees that stationary points are satisfactory solutions of specific inverse problems, in some specific sense and under specified conditions, are almost entirely absent from the literature.

This paper provides such a theoretical guarantee for a modification of least-squares data fitting via *modeling operator extension*, applied to a very simple example: recovery of the (spatially homogeneous) wave speed of an acoustic material model, together with the waveform of an isotropic point radiator (“wavelet”) with specified support, from the time history (“trace”) of the resulting pressure field at a single remote location. This is perhaps the simplest inverse wave propagation problem that exhibits cycle-skipping. While far too simple to have immediate practical application, it is a special case, or subproblem, of many field-scale inverse problems in industrial and academic seismology. It is also routinely used to illustrate cycle-skipping (see for example Virieux and Operto (2009), Figure 7). Modeling operator extension ideas underlie widely used techniques in seismic data processing, and have been applied to inversion for several decades (Symes, 2008). The particular approach used in this work is an example of *source extension*. Huang et al. (2019) review recent source extension contributions, some of which are closely related to the approach to single-trace transmission inversion studied here.

Model extension is only one of several ideas proposed to remedy cycle-skipping. For instance, measuring data misfit with versions of the Wasserstein metric from optimal transport theory, rather than the $L^2$ norm, also shows promise in mitigating cycle-skipping (Métivier et al., 2018; Yang et al., 2018; Ramos-Martinez et al., 2018; Wang and Wang, 2019; Engquist and Yang, 2021). Mahankali and Yang (2021) have established conditions under which the Wasserstein misfit is convex in a few parameters of simple models. Aside from the present paper, their work is one of the very few to give a complete mathematical justification (albeit also in very restricted circumstances) for application of local optimization to a nonlinear least squares alternative.

The next section precisely defines the single-trace transmission inverse problem, and the following section confirms the cycle-skipping behaviour of the obvious nonlinear least squares formulation, that is, that stationary points exist at arbitrarily large distance from any global minimizer (Theorem 1). The modeling operator extension used here simply consists in dropping the support constraint, thus allowing fit to any data with any wavespeed, by suitable choice of wavelet. The link between wave speed and data is re-established by supplementing the mean-square data misfit function with a suitable quadratic penalty on nonzero values of the wavelet far from the specified support. I show that any stationary point of the resulting penalty function deviates from the global solution of the original, constrained nonlinear least squares problem by an amount proportional to a combination of the support diameter and the relative data error, and this bound is sharp (Theorems 4 and 5). A solution of the original inverse problem (with wavelet support constraint) is recovered by truncating the wavelet obtained in the course of minimizing the penalty function (Theorem 6).

The elementary analysis developed here leans on the special features of the problem under study to achieve sharper results than will likely be possible in more general contexts. The Appendix recasts some of these constructions in a form that applies, at least formally, to more prototypical, larger-scale problems (Symes, 2014; ten Kroode, 2014), and suggests a route to achieving a similar, mathematically complete understanding of extension-based
approaches to applied wave propagation inverse problems.

AN ACOUSTIC TRANSMISSION INVERSE PROBLEM

According to linear acoustics, the causal pressure field \( p(x, t) \) due to an isotropic point radiator at \( x_s \in \mathbb{R}^3 \) with time-varying intensity (“wavelet”) \( w(t) \), propagating in an elastic fluid with slowness (reciprocal velocity) \( m \) and density 1 (in appropriate units), is the solution of the the initial value problem for the wave equation (Friedlander, 1958):

\[
\left( m^2 \frac{\partial^2 p}{\partial t^2} - \nabla^2 \right) p(x, t) = w(t)\delta(x - x_s),
\]

\[
p(x, t) = 0, \ t \ll 0.
\]

The solution is well-known, see for instance Courant and Hilbert (1962), Chapter VI, section 12, equation 47:

\[
p(x, t) = \frac{1}{4\pi |x - x_s|} w(t - m|x - x_s|),
\]

This trace of \( p \) at \( x_r \in \mathbb{R}^3 \) can be viewed as the result of applying an \( m \)-dependent linear operator \( F[m] \) to the wavelet \( w \):

\[
F[m]w(t) = p(x_r, t) = \frac{1}{4\pi r} w(t - mr)
\]

The slowness \( m \) must be positive, as follows from basic acoustics, and in fact reside in a range characteristic of the material model: for crustal rock, a reasonable choice would be \( m_{\text{min}} = 0.125 \), \( m_{\text{max}} = 0.6 \) s/km. The pressure trace \( p(x_r, \cdot) \) is square-integrable if and only if the same is true of the wavelet \( w \). Since the square-integral of the pressure trace is proportional to the accumulated energy transferred from the fluid to the sensor (Santosa and Symes, 2000), assume that \( w \in L^2(\mathbb{R}) \).

Natural choices for domain and range of \( F \) are thus

- \( M = (m_{\text{min}}, m_{\text{max}}) \), \( 0 < m_{\text{min}} \leq m_{\text{max}} \);
- \( W = L^2(\mathbb{R}) \);
- \( D = L^2([t_{\text{min}}, t_{\text{max}}]) \), \( t_{\text{min}} < t_{\text{max}} \);
- \( F : M \times W \to D \) as specified in 3.

It is immediately evident from these choices and from the definition 3 that

\[
\text{for } m \in M, F[m] \text{ is bounded, and } \|F[m]\| = \frac{1}{4\pi r}.
\]

Since all possible data lie in the range of \( F[m] \) for any \( m \in M \), some restriction of the domain of \( F \) is necessary in order that fitting the data constrain \( m \). The constraint employed in this work is the specification of a maximum support radius \( \lambda_{\text{max}} > 0 \) (see the companion paper Symes et al. (2022) for a justification of this choice).

For \( \lambda \in (0, \lambda_{\text{max}}] \), define
• \( W_\lambda = \{ w \in W : \text{supp } w \subset [-\lambda, \lambda] \} \);

• \( F_\lambda = F|_{M \times W_\lambda} \).

In terms of this infrastructure, the inverse problem studied in this paper may be stated as

**Inverse Problem:** given data \( d \in D \), relative error level \( \epsilon \in [0, 1) \), and support radius \( \lambda \in (0, \lambda_{\text{max}}) \), find \((m, w) \in M \times W_\lambda \) for which

\[
\| F_\lambda[m]w - d \| \leq \epsilon \| d \|, \tag{5}
\]

Define the relative mean-square error \( e_\lambda : M \times W_\lambda \times D \rightarrow \mathbb{R}^+ \) by

\[
e_\lambda[m, w; d] = \frac{1}{2} \| F_\lambda[m]w - d \|^2/\| d \|^2, \tag{6}
\]

so that inequality \(5\) is equivalent to

\[
e_\lambda[m, w; d] \leq \frac{1}{2} \epsilon^2, \tag{7}
\]

Minimization of \( e_\lambda \) is the standard least-squares formulation of the Inverse Problem defined above: if the global minimum value of \( e_\lambda \) is less than \( \frac{1}{2} \epsilon^2 \), then the global minimizer is a solution of the Inverse Problem.

**Remark:** The constraint \( \epsilon < 1 \) imposed on the target noise level eliminates the obvious choice \((m, 0)\), which satisfies the data misfit constraint for any \( m \in M \) if \( \epsilon \geq 1 \).

**Remark:** I shall refer to the minimization of \( e_\lambda \) as “Full Waveform Inversion” or “FWI”, as this is the terminology used in the seismology literature to identify this and similar optimization problems.

The best case for data fitting is clearly the one in which the data can be fit precisely: that is, there exists \((m_*, w_*) \in M \times W_\lambda \) so that

\[
d = F_\lambda[m_*]w_. \tag{8}
\]

Such data \( d \) is **noise-free**, in the range of the map \( F_\lambda \). For such data a solution of the Problem Statement \(5\) exists with arbitrarily small \( \epsilon > 0 \).

**FULL WAVEFORM INVERSION**

While \( F \) is surjective, as noted above, it is very far from injective. On the other hand, under a constraint that will be assumed throughout, \( F_\lambda[m] \) is injective for each \( m \in M \) (in fact, \( 4\pi r F_\lambda[m] \) is an isometry):

**Proposition 1.** Suppose that

\[
[m_{\text{min}}r - \lambda_{\text{max}}, m_{\text{max}}r + \lambda_{\text{max}}] \subset [t_{\text{min}}, t_{\text{max}}]. \tag{9}
\]

Then \( F_\lambda[m] \) is coercive for every \( m \in M, \lambda \in (0, \lambda_{\text{max}}] \).
Remark: A useful consequence of the condition 9 for every \( m \in M \),
\[
\left[ -\lambda_{\text{max}}, -\lambda_{\text{max}} \right] \subset [t_{\text{min}} - m r, t_{\text{max}} - m r].
\] (10)

The first main result establishes the existence of large (100 \%) residual local minimizers for the basic FWI objective \( e_\lambda \), even for noise-free data.

**Theorem 1.** Suppose that \( 0 < \lambda \leq \lambda_{\text{max}} \), \( m_* \in M, w_* \in W_\lambda, d = F_\lambda [m_*] w_* \) is noise-free data per definition 8. Under assumption 9 for any \( m \in M \) with \( |m - m_*| r > 2\lambda \),
\[
\min_w e_\lambda [m, w; d] = e_\lambda [m, 0; d] = \frac{1}{2},
\] (11)
and any such \((m, 0)\) is a local minimizer of \( e_\lambda \) with relative RMS error = 1.0.

**Proof.** From the definition 3
\[
e_\lambda [m, w; d] = \frac{1}{32\pi^2 r^2 \|d\|^2} \int dt \ |w(t - m r) - w_*(t - m_* r)|^2.
\]
Since \( w_*, w \) vanish for \(|t| > \lambda\), \( F_\lambda [m_*] w_*(t) \) vanishes if \(|t - m_* r| > \lambda\) and \( F_\lambda [m] w \) vanishes if \(|t - m r| > \lambda\). So if \(|m r - m_* r| = |m - m_*| r > 2\lambda\), then \(|t - m r| + |t - m_* r| > |m r - m_* r| > 2\lambda\) so either \(|t - m r| > \lambda\) or \(|t - m_* r| > \lambda\), that is, either \( F_\lambda [m] w(t) = 0\) or \( F_\lambda [m_*] w_* = 0\). Therefore \( F_\lambda [m] w \) and \( F_\lambda [m_*] w_* \) are orthogonal in the sense of the \( L^2 \) inner product \( \langle \cdot, \cdot \rangle_D \) on \( D \):
\[
|m - m_*| r > 2\lambda \Rightarrow \langle F[m] w, F[m_*] w_* \rangle_D = 0
\] (12)
But \( d = F_\lambda [m_*] w_* \), so this is the same as saying that \( d \) is orthogonal to \( F[m] w \). So conclude after a minor manipulation that
\[
|m - m_*| r > 2\lambda \Rightarrow e_\lambda [m, w; d] = \frac{1}{32\pi^2 r^2 \|d\|^2} (\|w\|^2 + \|w_*\|^2).
\]
\[
= \frac{1}{2} \left( \frac{\|w\|^2}{\|w_*\|^2} + 1 \right)
\] (13)
That is, for slowness \( m \) in error by more than \( 2\lambda/r \) from the target slowness \( m_* \), the means square error (FWI objective) \( e_\lambda \) is independent of \( m \), and its minimum over \( w \) is attained for \( w = 0 \).

Therefore local minimizers of \( e_\lambda \) abound, as far as you like from the global minimizer \((m_*, w_*)\). Local exploration of the FWI objective \( e \) gives no useful information whatever about constructive search directions, and descent-based optimization tends to fail if the initial estimate \( m_0 \) is in error by more than \( 2\lambda/r \). In fact the actual behaviour of FWI iterations is worse (failure if \( m_0 \) is in error by “half a wavelength”), as follows from a more refined analysis of the cycle-skipping local behaviour of \( e_\lambda \) near its global minimizer.
EXTENDED SOURCE INVERSION

The phenomenon explained in the last section can be avoided by reformulating the inverse problem via an extended modeling operator and a soft (penalty) constraint to replace the support requirement. The extension simply amounts to dropping the support constraint, and replacing $W_\lambda$ and $F_\lambda$ by $W$ and $F$.

The hard support constraint implicit in the choice of $W_\lambda$ as domain for the modeling operator is replaced by a soft constraint in the form of a quadratic penalty, with weight operator $A$:

$$Aw(t) = a(t)w(t), \ t \in \mathbb{R}. \quad (14)$$

Explicit choices for $a$ are discussed below.

With these choices, define

$$e[m, w; d] = \frac{1}{2} \| F[m]w - d \|^2 / \| d \|^2; \quad (15)$$
$$g[w; d] = \frac{1}{2} \| Aw \|^2 / \| d \|^2; \quad (16)$$
$$J_\alpha[m, w; d] = e[m, w; d] + \alpha^2 g[w; d]. \quad (17)$$

The main theoretical device used in the proofs of our main results on extended inversion is Variable Projection reduction of the penalty objective $J_\alpha$ (equation 17) to a function $\tilde{J}_\alpha$ of $m$ alone, by minimization over $w$:

$$\tilde{J}_\alpha[m; d] = \inf_w J_\alpha[m, w; d] \quad (18)$$

A minimizer $w$ on the right-hand side of definition 18 must solve the normal equation

$$(F[m]^T F[m] + \alpha^2 A^T A)w = F[m]^T d, \quad (19)$$

(here and in the following, the superscript $T$ signifies adjoint in the sense of domain and range Hilbert structures).

With $A$ of the form 14, $\tilde{J}_\alpha$ is explicitly computable. First observe that apart from amplitude, $F[m]$ is unitary: for $g \in D$,

$$F[m]^T g(t) = \left\{ \begin{array}{ll} \frac{1}{4\pi r} g(t + mr), & t \in [t_{\min} - mr, t_{\max} - mr], \\ 0, & \text{else}. \end{array} \right. \quad (20)$$

so

$$F[m]^T F[m] = \frac{1}{(4\pi r)^2} 1_{[t_{\min} - mr, t_{\max} - mr]} \quad (21)$$

in which $1_S$ denotes multiplication by the characteristic function of a measurable $S \subset \mathbb{R}$.

Therefore the normal equation for the minimizer on the RHS of equation 18 is

$$\left( \frac{1}{(4\pi r)^2} 1_{[t_{\min} - mr, t_{\max} - mr]} + \alpha^2 A^T A \right)w = F[m]^T d. \quad (22)$$
With these choices, the normal equation (22) becomes

\[
\left( \frac{1}{(4\pi r)^2} \mathbf{1}_{[\min - mr, \max - mr]} + \alpha^2 a^2 \right) w = F[m]^T d. \tag{23}
\]

Evidently, \( F^T F \) (the first summand in equation 23) is not coercive. If \( A \) is to yield small output for input localized near \( t = 0 \), as it must to play its desired role in replacing the hard support constraint, then \( A^T A \) must not be coercive either, that is, its spectrum must have zero as its infimum. Therefore an additional condition on \( A \) is required to enable application of the Lax-Milgram construction to the normal equation 19. This condition is an hypothesis of Proposition 2.

**Proposition 2.** Assume the conditions 3, 9, 14. Also assume that \( \lambda \in (0, \lambda_{\max}] \), \( \alpha > 0 \), and that \( C > 0 \) exists so that \( a \in L^\infty(\mathbb{R}) \) mentioned in equation 14 satisfies the condition

\[
a(t) \geq C \quad \text{for} \quad |t| \geq \lambda_{\max}.
\]

Then

1. the normal operator \( F[m]^T F[m] + \alpha^2 A^T A \) is invertible for any \( m \in M, \alpha > 0 \);
2. the solution \( w_\alpha[m; d] \in W \) of the normal equation 14 is given by

\[
w_\alpha[m; d](t) = \begin{cases} \left( \frac{1}{(4\pi r)^2} + \alpha^2 a^2(t) \right)^{-1} \frac{1}{4\pi} d(t + mr), t \in [\min - mr, \max - mr]; \\ 0, \text{ else}; \end{cases}
\]

3. if in addition \( d = F[m_*]w_*, w_* \in W_\lambda \) is noise-free, as in equation 8,

\[
w_\alpha[m, d](t) = \left( 1 + (4\pi r)^2 \alpha^2 a(t)^2 \right)^{-1} w_*(t + (m - m_*)r).
\]

**Proof.** The idea here is that \( F \) fails to be coercive just where \( A \) is coercive, and vis-versa.

1. Note that thanks to 10 if \( |t| \leq \lambda \leq \lambda_{\max} \), then \( \mathbf{1}_{[\min - mr, \max - mr]}(t) = 1 \), whereas if \( |t| > \lambda \), then \( a(t) \geq C \), whence

\[
\frac{1}{(4\pi r)^2} \mathbf{1}_{[\min - mr, \max - mr]} + \alpha^2 a^2 \geq \min\{ (4\pi r)^2, \alpha^2 \min\{ 1/(4\pi r)^2, C^2 \} \} > 0.
\]

Therefore the normal operator is invertible under the stated conditions.

2. From the identity 20

\[
\text{supp } F[m]^T d \subset [\min - mr, \max - mr].
\]

Define \( w_\text{tmp} \) to be the right-hand side of equation 25. Then from the previous observation and identity 20

\[
\text{supp } w_\text{tmp} \subset [\min - mr, \max - mr].
\]

From the identity 21 for any \( w \in W \),

\[
t \in [\min - mr, \max - mr] \Rightarrow F[m]^T F[m]w(t) = \frac{1}{(4\pi r)^2} w(t).
\]

It follows from this and the previous two observations that \( w_\text{tmp} \) solves the normal equation 19 and therefore that \( w_\alpha[m; d] = w_\text{tmp} \).
3. Follows by inserting the definition of $d$ in \eqref{eq:definition_d} and rearranging.

\begin{proof}

\end{proof}

**Theorem 2.** Assume the condition \( C > 0 \), and suppose that \( A \) is given by equation \eqref{eq:A} for \( a \in L^\infty(\mathbb{R}) \) satisfying condition \eqref{eq:condition_A}. Then

\begin{enumerate}
\item The reduced objective \( \tilde{J}_\alpha \) is given by
\begin{equation}
\frac{1}{2} \int_{t_{\text{min}}}^{t_{\text{max}}} dt \left( 4\pi r a(t - mr)^2 (1 + (4\pi r a(t - mr))^2)^{-2} d(t) \right)^2 \end{equation}
\end{enumerate}

\begin{proof}

These conclusions follow immediately from Proposition \ref{prop:conditions}. \end{proof}

If \( J_\alpha[\cdot; d] \) and \( \tilde{J}_\alpha[\cdot; d] \) were differentiable, then “local minimizer” in the conclusion of the preceding theorem could be replaced by “stationary point”. However, for the problem addressed in this paper, \( J_\alpha[\cdot; d] \) is not differentiable without added smoothness constraints on \( w \), whereas \( \tilde{J}_\alpha[\cdot; d] \) is differentiable for proper choice of penalty operator \( A \). This conclusion follows from properties of the modeling operator \( F \) shared with many other inverse problems in wave propagation, as explained in the Appendix.

\begin{proposition}

Assume the hypotheses of Proposition \ref{prop:conditions}. Then
\begin{align}
\bar{e}[m, w_\alpha[m, d]] &= \frac{1}{2} \int_{t_{\text{min}}}^{t_{\text{max}}} dt \left( 4\pi r a(t - mr)^2 (1 + (4\pi r a(t - mr))^2)^{-2} d(t) \right)^2, \\
\bar{p}[m, w_\alpha[m, d]] &= \frac{1}{2} \int_{t_{\text{min}}}^{t_{\text{max}}} dt \left( 4\pi r a(t - mr)^2 (1 + (4\pi r a(t - mr))^2)^{-2} d(t) \right)^2 \\
\bar{J}_\alpha[m, d] &= \frac{1}{2} \int_{t_{\text{min}}}^{t_{\text{max}}} dt \left( 4\pi r a(t - mr)^2 (1 + (4\pi r a(t - mr))^2)^{-2} d(t) \right)^2.
\end{align}

\begin{proof}

From equation \eqref{eq:definition_d},
\begin{equation}
F[m]w_\alpha[m, d](t) = \frac{1}{4\pi r} \left( \frac{1}{(4\pi r)^2 + \alpha^2 a^2 (t - mr)^2} \right)^{-1} \frac{1}{4\pi r} d(t),
\end{equation}
so
\begin{align}
(F[m]w_\alpha[m, d] - d)(t) &= (1 + (4\pi r a(t - mr))^2)^{-1} - 1) d(t) \\
&= -(4\pi r a(t - mr))^2 (1 + (4\pi r a(t - mr))^2)^{-1} d(t).
\end{align}
\end{proof}

\end{proposition}
Half the integral of the square of this data residual is $e[m, w_\alpha[m; d]; d]$, which proves identity 28.

To compute $p[m, w_\alpha[m; d]; d]$, note that

$$Aw_\alpha[m; d](t) = a(t) \left( \frac{1}{(4\pi r)^2} + \alpha^2 a^2(t) \right)^{-1} \frac{1}{4\pi r} d(t + mr)$$

$$= 4\pi r a(t)(1 + (4\pi r a(t))^2)^{-1} d(t + mr)$$

for $t \in [t_{\min} - mr, t_{\max} - mr]$, so squaring, integrating, and changing integration variables $t \mapsto t - mr$ gives the result 29.

That the VPM objective $\tilde{J}_\alpha$ is given by 30 follows from equations 27, 28, and 29.

**Theorem 3.** Suppose that in addition to the hypotheses of Theorem 2 a $\in W^{1,\infty}(\mathbb{R})$, then $\tilde{J}_\alpha[.; d] \in C^1(M)$.

**Proof.** Suppose first that $a \in C^1(\mathbb{R})$. Differentiation under the integral sign yields the expression for its derivative:

$$\frac{d}{dm} \tilde{J}_\alpha[m; d] = - \frac{(4\pi r \alpha)^2}{\|d\|^2} \int_{t_{\min}}^{t_{\max}} dt \left( a \frac{da}{dt} \right)(t - mr)(1 + (4\pi r a(t - mr))^2)^{-2} d(t)^2.$$ (31)

For $a \in W^{1,\infty}_{\text{loc}}(\mathbb{R})$ a limiting argument shows that the same expression gives the derivative of $\tilde{J}_\alpha$.

It will be useful to record expressions for the various components of $\tilde{J}_\alpha$ when the data is noise-free, that is, the context of Proposition 2 item 3:

**Corollary 1.** Assume the hypotheses of Proposition 2 item 3. Then noting that $\|d\| = \|w_*\|/(4\pi r)$

$$e[m, w_\alpha[m, d]; d] = \frac{\alpha^4}{2\|w_*\|^2} \int dt a(t - (m - m_*)r)^4(1 + (4\pi r)^2 \alpha^2 a(t - (m - m_*)r)^2)^{-2} w_*(t)^2.$$ (32)

$$p[m, w_\alpha[m, d]; d] = \frac{(4\pi r \alpha)^2}{2\|w_*\|^2} \int dt \frac{a(t - (m - m_*)r)^2}{(1 + (4\pi r)^2 \alpha^2 a(t - (m - m_*)r))^2} w_*(t)^2.$$ (33)

so

$$\tilde{J}_\alpha[m; d] = \frac{(4\pi r \alpha)^2}{2\|w_*\|^2} \int dt a(t - (m - m_*)r)^2(1 + (4\pi r)^2 \alpha^2 a(t - (m - m_*)r)^2)^{-1} w_*(t)^2.$$ (34)

Finally, if $a \in W^{1,\infty}(\mathbb{R})$, then $\tilde{J}_\alpha[.; d]$ is differentiable, and

$$\frac{d}{dm} \tilde{J}_\alpha[m; d] = - \frac{r(4\pi r \alpha)^2}{\|w_*\|^2} \int dt \frac{(a \frac{da}{dt})(t - (m - m_*)r)}{(1 + (4\pi r)^2 \alpha^2 a(t - (m - m_*)r))^2} w_*(t)^2.$$ (35)
Recall that the purpose of the penalty operator is to penalize energy away from \( t = 0 \). A simple multiplier of class \( W^{1, \infty} \) that accomplishes this goal (and produces a differentiable reduced objective \( \tilde{J}_\alpha \), thanks to Theorem \ref{theorem:support-tildeJ}) is

\[
a(t) = \min\{|t|, \tau\}. \tag{36}
\]

for suitable \( \tau > 0 \). In fact, the cutoff \( \tau \) will be chosen large enough to be effectively inactive: hindsight suggests

\[
\tau = \max\{|t_{\min} - m_{\min}r|, |t_{\min} - m_{\max}r|, |t_{\max} - m_{\min}r|, |t_{\max} - m_{\max}r|\}. \tag{37}
\]

Essentially this particular annihilator has been employed in earlier work on extended source inversion \cite{Plessix:2000a, Luo:2011a, Warner:2014a, Huang:2017b, Symes:2015a, Warner:2016a, Huang:2017b}.

**STATIONARY POINTS**

**Proposition 4.** Suppose that

1. \( m_* \in M \);
2. \( 0 < \mu \leq \lambda \), and \( w_* \in W_\mu \);
3. \( d_* = F[m_*]w_* \);
4. \( a(t) = \min\{|t|, \tau\} \) in the definition \ref{definition:multiplier} with \( \tau \) given by equation \ref{equation:cutoff} and
5. \( \alpha > 0 \).

Then for any \( m \in M \),

\[
|(m - m_*)r| > \lambda \Rightarrow \left| \frac{d}{dm} \tilde{J}_\alpha[m; d_*] \right| > \frac{r(4\pi r \alpha)^2(\lambda - \mu)}{(1 + (4\pi r \alpha)^2(\lambda + \mu)^2)^2}. \tag{38}
\]

**Proof.** As observed before, \( \text{supp } w_\alpha[m; d_*] \subset [t_{\min} - m_* r, t_{\max} - m_* r] \subset [-\tau, \tau] \), with \( \tau \) defined in \ref{equation:cutoff}. Therefore, \( a(t) = |t|, \ a a'(t) = t \) in the support of the integrand on the RHS of equation \ref{equation:Jtilde} which therefore becomes (after change of integration variable)

\[
\frac{d}{dm} \tilde{J}_\alpha[m; d_*] = -\frac{r(4\pi r \alpha)^2}{\|w_*\|^2} \int dt (1 + (4\pi r \alpha)^2(\lambda + \mu)^2)^{-2} w_*(t + (m - m_*))^2. \tag{39}
\]

Recall that \( w_*(t + (m - m_*)r) \) vanishes if \( |t + (m - m_*)r| > \lambda \). Therefore the integral on the RHS of equation \ref{equation:Jtilde} can be re-written

\[
= -\frac{r(4\pi r \alpha)^2}{\|w_*\|^2} \int_{-(m - m_*)r - \lambda}^{-(m - m_*)r + \lambda} dt (1 + (4\pi r \alpha)^2(\lambda + \mu)^2)^{-2} w_*(t + (m - m_*))^2
\]

Suppose that \( \mu \leq \lambda \) and \( w_* \in W_\mu \). If \( m > m_* + \lambda/r \), then \( t + (m - m_*)r \in \text{supp } w_* \) implies \( -\mu - \lambda < t < \mu - \lambda < 0 \), so

\[
t(1 + (4\pi r \alpha)^2(\lambda + \mu)^2)^{-2} \Rightarrow (\mu - \lambda)(1 + (4\pi r \alpha)^2(\mu + \lambda)^2)^{-2} < 0
\]

in the support of the integrand in equation \ref{equation:Jtilde}. Arguing similarly for \( m < m_* - \lambda/r \), obtain a similar inequality, implying the conclusion \ref{equation:stationarity}. \qed
Theorem 4. Suppose that

1. \( m_* \in M \);
2. \( 0 < \lambda \), and \( w_* \in W_\lambda \);
3. \( d_* = F[m_*]w_* \);
4. \( a(t) = \min\{|t|, \tau\} \) in the definition \( [14] \) with \( \tau \) given by equation \( [37] \);
5. \( \alpha > 0 \); and
6. \( m \in M \) is a stationary point of \( \tilde{J}_\alpha[\cdot; d_*] \).

Then \( |m - m_*| < \lambda/r \).

Proof. Follows directly from Proposition 4 by taking \( \mu = \lambda \).

The preceding theorem established that a proper choice of annihilator leads to a reduced penalty objective all of whose stationary points are within \( O(\lambda) \) of the target slowness \( m_* \), provided that the data are noise-free in the sense of equation \( [8] \). This result leaves open two questions:

- how does one use this reduced penalty minimization to produce a solution of the inverse problem as in problem statement \( [5] \)?
- how does one answer the same question for noisy data?

The next result answers the first question, in the case of noise-free data:

Proposition 5. Suppose that \( a \) is given by definition \( [26] \), \( \alpha, \mu \in (0, \lambda_{\text{max}}] \), \( d \) is given by \( [8] \) with \( w_* \in W_\mu \), and \( m \) is a stationary point of \( \tilde{J}_\alpha[\cdot; d] \). Then \( (m, w_\alpha[m; d]) \) is a solution of the inverse problem \( [7] \) for any \( \lambda \geq 2\mu \) and

\[
\epsilon \geq \frac{(8\pi\mu\alpha)^2}{1 + (8\pi\mu\alpha)^2}.
\] (40)

Proof. From the assumption \( w_* \in W_\mu \) and Theorem \( [4] \) \(|(m - m_*)r| \leq \mu\). From the identity \( \supp w_\alpha[m; d] \subset [(m - m_*)r - \mu, (m - m_*)r + \mu] \subset [-2\mu, 2\mu] \). Because of the support limitation, \( a(t) = |t| \) in the interval of integration appearing in \( [22] \) so

\[
\epsilon[m, w_\alpha[m; d]; d] = 8\pi^2 r^2 \alpha^4 \int_{-\mu}^{\mu} dt \frac{|t - (m - m_*)r|^4}{(1 + (4\pi r)^2 \alpha^2 |t - (m - m_*)r|^2)^2} w_\alpha(t)^2
\]

\[
\leq \frac{1}{2} \|d\|^2 \left( \frac{(8\pi\rho \alpha)^4}{1 + (8\pi\rho \alpha)^2} \right).
\]
The inequality 40 can be interpreted as a bound on $\alpha$, given $\epsilon$ and $\lambda$, for a stationary point of $\tilde{J}_\alpha$ to yield a solution of the inverse problem: one obtains a solution, provided that $\alpha$ is sufficiently small. On the other hand, it is clear that $\alpha$ cannot be too large if stationary points of $\tilde{J}_\alpha$ are to yield solutions: the integrand in 32 is increasing in $\alpha$ for every $t$ and $m$, and the multiplier 
\[
t(t) \mapsto (4\pi r \alpha (t - (m - m_*) r))^4 (1 + (4\pi r)^2 \alpha^2 |t - (m - m_*) r|^2)^{-2}
\] tends monotonically to 1 as $\alpha \to \infty$, uniformly on the complement of any open interval containing $t = (m - m_*) r$. Therefore

\[
\lim_{\alpha \to \infty} e[m, w_\alpha[m; d]; d] = \frac{1}{2} \frac{1}{(4\pi r)^2} \|w_*\|^2 = \frac{1}{2} \|d\|^2. \tag{41}
\]

Consequently, there exists $\alpha_{\text{max}}(\epsilon, \lambda, d)$ so that

\[
e[m, w_\alpha[m; d]; d] \leq \frac{1}{2} \epsilon^2 \|d\|^2 \Rightarrow \alpha \leq \alpha_{\text{max}}(\epsilon, \lambda, d).
\]

The existence of this limiting penalty weight has been inferred indirectly. Fu and Symes (2017) describe a constructive algorithm for its approximation, which is used in the companion paper Symes et al. (2022) to dynamically adjust $\alpha$ in the course of optimization of $\tilde{J}_\alpha$.

I turn now to the second issue identified above, the effect of noise. Suppose that the data trace $d$ takes the form

\[
d = F[m_*] w_* + n = d_* + n, \tag{42}
\]

with $m_* \in M, w_* \in W''_\mu, 0 < \mu < \lambda$, and noise trace $n \in D$. Since no support assumptions can be made about $n$, equation 25 implies that $w_\alpha[m; d] \notin W_\lambda$ for any values of $\alpha$ and $\lambda$. Therefore minimization of $\tilde{J}_\alpha$ cannot by itself yield a solution of the inverse problem as defined in the problem statement 5. In this section, I explain how a solution may nonetheless be constructed from a stationary point of $\tilde{J}_\alpha$.

First, examine the effect of additive noise on the estimation of the slowness $m$. In expressing the result, use the dimensionless relative data error

\[
\eta = \frac{\|n\|}{\|d_*\|}. \tag{43}
\]

Proposition 6. Assume the hypotheses of Proposition 4, and that $d$ is given by definition 42. Suppose that $m \in M$ is a stationary point of $\tilde{J}_\alpha[; d]$, and that

\[
\eta(1 + \eta) \leq \frac{16}{3\sqrt{3}} \frac{4\pi r \alpha (\lambda - \mu)}{(1 + (4\pi r \alpha (\lambda + \mu))^2)^2}. \tag{44}
\]

Then

\[
|m - m_*| \leq \frac{\lambda}{r} \tag{45}
\].
Proof. From equation 31, \( d\tilde{J}_\alpha / dm \) is the value of a quadratic form in \( d \) with (indefinite) symmetric operator \( B = \text{multiplication by} \ b(t; m, \alpha) = -\frac{(4\pi r\alpha)^2(t - mr)}{1 + (4\pi r\alpha(t - mr))^2} \)

Therefore

\[
\left| \frac{d}{dm} \tilde{J}_\alpha[m; d] - \frac{d}{dm} \tilde{J}_\alpha[m; d_*] \right| = |\langle (d + d_*), B(d - d_*) \rangle| \leq \max_{t \in \mathbb{R}} |b(t; m, \alpha)| \eta(1 + \eta) \|d_*\|^2 \tag{46}
\]

A straightforward calculation shows that

\[
\max_{t \in \mathbb{R}} b(t; m, \alpha) = \frac{3\sqrt{3}}{16} 4\pi r\alpha.
\]

For a stationary point \( m \) of \( \tilde{J}_\alpha \cdot d \), the inequality 46 implies

\[
\left| \frac{d}{dm} \tilde{J}_\alpha[m; d_*] \right| \leq \frac{3\sqrt{3}}{16} 4\pi r\alpha(1 + \eta) \|d_*\|^2
\]

On the other hand, the conclusion 38 of Proposition 4 implies that if also

\[
\frac{3\sqrt{3}}{16} 4\pi r\alpha(1 + \eta) \|d_*\|^2 \leq \frac{\lambda - \mu}{(1 + (4\pi r\alpha\lambda_{\max})^2\alpha^2(\lambda + \mu)^2)^2} \|d_*\|^2
\]

then \( |m - m_*| \leq \lambda / r \). Rearranging, obtain the conclusion.

Corollary 2. Assume the hypotheses of Proposition 4 in particular that \( m \) is a stationary point of \( \tilde{J}_\alpha \cdot d \), \( d = d_* + n \). Then

\[
|m - m_*| \leq \frac{\mu}{r} + \frac{\eta}{\alpha} \left( \frac{3\sqrt{3}(1 + \eta)}{64\pi r^2} (1 + (8\pi r\alpha\lambda_{\max})^2)^2 \right)
\]

Proof. Assume that \( \lambda \) is chosen to obtain equality in the condition 44, substitute the bound \( 2\lambda_{\max} \) for \( \lambda + \mu \) in the denominator, solve for \( \lambda \) and substitute in inequality 45.

Remark: This bound suggests that error in the estimate of \( m \) due to data noise is a decreasing function of \( \alpha \), at least for small \( \alpha \). This result is intuitively appealing, and is supported by numerical evidence. It may be taken as a justification for the discrepancy-based algorithm for adjusting \( \alpha \) during inversion (Fu and Symes, 2017), used in the companion paper (Symes et al., 2022).

Theorem 5. Assume that

1. \( \alpha, \mu > 0 \),
2. \( m_* \in M, w_* \in W_\mu \),
3. \( d_* = F[m_*]w_* \),
4. \( n \in D \) and \( d = d_* + n \).
Set \( \eta = \| n \| / \| d_s \| \). Assume that \( \eta \) satisfies inequality
\[
\eta < \frac{\sqrt{5} - 1}{2},
\]
and that \( m \) is a stationary point of \( \tilde{J}_\alpha[\cdot; d] \). Then
\[
|m - m_*| \leq \left( 1 + \frac{2\eta(1 + \eta)}{1 - \eta(1 + \eta)} \right) \frac{\mu}{r}.
\]

Proof. of Theorem 5. Write \( \lambda = (1 + \delta)\mu \), and \( x = 4\pi r \alpha \mu \). Then the right-hand side of equation 44 may be written as
\[
\frac{16}{3\sqrt{3}} \frac{4\pi r \alpha (\lambda - \mu)}{(1 + (4\pi r \alpha (\lambda + \mu))^2)^2} = D \frac{x}{(1 + C^2 x^2)^2},
\]
where
\[
D = \frac{16}{3\sqrt{3}} \delta, \quad C = 2 + \delta.
\]
The positive stationary point of the quantity on the right-hand side of 50 is a maximum, and occurs at \( x = 1/(\sqrt{3}C) \), that is
\[
4\pi r \alpha \mu = \frac{1}{\sqrt{3}(2 + \delta)}.
\]
Thus
\[
1 + C^2 x^2 = \frac{4}{3}
\]
hence the maximum value is
\[
\frac{D 3\sqrt{3}}{16C} = \frac{\delta}{2 + \delta}.
\]
This maximum value must be larger than the left hand side of inequality 44, that is,
\[
\eta(1 + \eta) \leq \frac{\delta}{2 + \delta},
\]
in order that there be any solutions at all, but the right hand side is less than 1. This observation establishes the necessity of hypothesis 48 of the theorem. Solving this above inequality for \( \delta \) and unwinding the definitions, one finds that the right-hand side of inequality 44 is bounded by 49, so appeal to Proposition 6 finishes the proof.

Remark. That is, with the choice of penalty multiplier a given in equation 36 and support radius \( \mu \) of the “noise-free” wavelet \( w_* \), \( J_\alpha \) has no local minima with slownesses further than \( (1 + O(\eta))\mu/r \) from the slowness used to generate the data.

Remark. The estimate \( |m - m_*| r < \mu(1 + O(\eta)) \) for local minima of \( J_\alpha \) is sharp: it is possible to choose \( w_* \in W_\mu \) so that \( \mu - |m - m_*| r \) is as small as you like. In particular, the “exact” or “true” slowness \( m_* \) is not necessarily the only slowness component of a local minimizer, or even the slowness component of any local minimizer, and in particular is not (necessarily) the slowness component of a global minimizer of \( J_\alpha \).
Remark. No similar bound could hold for much larger noise levels than specified in condition 48, the right-hand side of which is a bit larger than 0.6. For example, if the noise is the predicted data for the same wavelet \( w^\ast \) with a substantially different slowness \( m^\flat \), that is, \( n = F[m^\flat]w^\ast \), then a simple symmetry argument shows that if there is a local minimizer of \( J_\alpha[\cdot , \cdot ; d^\ast + n] \) with slowness near \( m^\ast \), there must also be a minimizer with slowness near \( m^\flat \), so that the difference with \( m^\ast \) is not constrained at all by the assumed support radius of \( w^\ast \). So for this example with 100% noise, no bound of the type given by conclusion 2 could possibly hold. The companion paper (Symes et al., 2022) illustrates this phenomenon numerically.

Remark. Note that \( \alpha \) plays no role in the conclusions of this theorem. It is only required that \( \alpha > 0 \).

Remark: I emphasize that Theorem 5 states sufficient conditions for a bound on the slowness error \( |m - m^\ast| \) in terms of the relative data noise level \( \eta \), giving an additional “fudge factor” beyond the support size \( \mu \) of the noise-free wavelet \( w^\ast \) for an interval within which the slowness error is guaranteed to lie.

Conclusion 1 in Theorem 5 constrains the range of noise level to which these results apply to a bit more than 60%. That is, the bound given by conclusion 2 is useful only for small noise. In the limit as \( \eta \to 0 \), conclusion 2 becomes \( \lambda/\mu \gtrsim 1 + 2\eta \), that is, the “fudge factor” beyond the noise-free bound is approximately twice the noise level.

On the other hand, stronger bounds than given by Theorem 5 are possible, given additional constraints on the noise \( n \). A natural example is uniformly distributed random noise, filtered to have the same spectrum as the source. The expression 31 implies that the interaction of noise \( n \) and signal \( d^\ast \) in the derivative of \( \bar{J}_\alpha \) is local, so that the coefficient of \( \eta \) on the left-hand side of inequality 44 is effectively much less that 1, resulting in a larger range of allowable \( \eta \). While I will not formulate such a result, one of the numerical examples in the companion paper (Symes et al., 2022) suggests its feasibility.

Unless the data is noise-free, there is no reason to suppose that the estimated wavelet \( w_\alpha[m;d] \) (Theorem 2) will lie in \( W_\lambda \), unless the support of the noise \( n \) is restricted. In order to construct a solution of the inverse problem 5 project \( w_\alpha[m;d] \) onto \( W_\lambda \). For sufficiently large \( \lambda, \epsilon \), the result is a solution of the inverse problem:

**Theorem 6.** Assume the hypotheses of Theorem 5 and that inequality 48 holds, and \( \mu \in (0, \lambda_{\text{max}}] \). Then the pair

\[
(m, 1_{[-\lambda, \lambda]}w_\alpha[m,d])
\]

solves the inverse problem as stated in 5 if

\[
\left( 2 + \frac{2\eta(1 + \eta)}{1 - \eta(1 + \eta)} \right) \mu \leq \lambda \leq \lambda_{\text{max}},
\]

and

\[
\epsilon \geq \frac{(8\pi r\alpha \lambda)^2}{1 + (8\pi r\alpha \lambda)^2} + \eta.
\]

**Proof.** of Theorem 6 From Theorem 2

\[
w_\alpha[m;d](t) = (1 + (4\pi r\alpha t)^2)^{-1}(w^\ast(t + (m - m^\ast)) + 4\pi r\eta(t + mr))
\]
\[ w_\alpha[m; d_*] + (1 + (4\pi r \alpha t)^2)^{-1}4\pi r n(t + mr) \]

From Theorem 5,

\[ |m - m_*| \leq \left( 1 + \frac{2\eta(1 + \eta)}{1 - \eta(1 + \eta)} \right) \frac{\mu}{r} \]

which from assumption 51 is

\[ = \left( 2 + \frac{2\eta(1 + \eta)}{1 - \eta(1 + \eta)} \right) \frac{\mu}{r} - \frac{\mu}{r} \leq \left( \frac{\lambda}{\mu} - 1 \right) \frac{\mu}{r} \]

That is,

\[ |m - m_*| r \leq \lambda - \mu. \]

From Theorem 2,

\[ \text{supp } w_\alpha[m; d_*] \subset [-\mu - (m - m_*)r, \mu - (m - m_*)r] \subset [-\lambda, \lambda] \]

so

\[ E_{\lambda}w_\alpha[m; d](t) = w_\alpha[m; d_\alpha](t) + E_{\lambda}(1 + (4\pi r \alpha t)^2)^{-1}4\pi r n(t + mr) \]

From the definition of \( F[m] \), for any \( t_1 < t_2, w \in W \),

\[ F[m]1_{[t_1, t_2]}w = 1_{[t_1 + mr, t_2 + mr]}F[m]w \]

Thus the data residual after projection is

\[ F[m]E_{\lambda}w_\alpha[m; d] - d(t) = F[m]w_\alpha[m; d_\alpha](t) - d_\alpha(t) \]

\[ + 1_{[-\lambda + mr, \lambda + mr]}(4\pi r \alpha(t - mr))^2(1 + (4\pi r \alpha(t - mr))^2)^{-1}n(t) \]

\[ - (1 - 1_{[-\lambda + mr, \lambda + mr]}n(t) \]

From 32 and the bound on \( m - m_* \),

\[ \| F[m]E_{\lambda}w_\alpha[m; d_*] \| = (4\pi r \alpha)^4 \int_{-\lambda + (m - m_*)r}^{\lambda + (m - m_*)r} dt \]

\[ \times (1 + (4\pi r \alpha)^2(t - (m - m_*)r)^2)^{-1}d_\alpha(t)^2 \]

\[ \leq (4\pi r \alpha)^4 \| d_* \|^2 \]

Similarly, the norm squared of the sum of the last two terms is

\[ \leq (4\pi r \alpha)^2 \| 1_{[-\lambda + mr, \lambda + mr]}n \|^2 + \| (1 - 1_{[-\lambda + mr, \lambda + mr]}n \| \]

Without additional hypotheses to outlaw the accumulation of \( n \) near \( t = mr \), all that can be said is that this is

\[ \leq \max\{ (4\pi r \alpha)^2, 1 \} \| n \|^2 \]

Putting this all together,

\[ \| F[m]E_{\lambda}w_\alpha[m; d] - d \| \leq (4\pi r \alpha)^2 \| d_* \| + \max\{ 4\pi r \alpha, 1 \} \| n \| \]

\[ \leq ((4\pi r \alpha)^2 + \max\{ 4\pi r \alpha, 1 \} \eta) \| d_* \|. \]

If the right-hand side is to be less than \( \| d_* \| \) as required by the definition 5 of the inverse problem, then necessarily \( 4\pi r \alpha \lambda < 1 \), so the right hand side in the preceding inequality is bounded by the right hand side of assumption 52 of the theorem. Therefore this assumption implies that the relative residual is \( \leq \epsilon \). \qed
Remark: Note that the sufficient condition \( \lambda \) for \( \lambda \) is independent of \( \alpha \). It follows that for any choice of \( \lambda \) consistent with this bound, \( (m, 1_{[\lambda, \lambda]}w_\alpha[m, d]) \) is a solution of the inverse problem for any \( \epsilon > 0 \) provided that \( \alpha \) is chosen sufficiently small \( O(\sqrt{\epsilon}) \).

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APPENDIX: ABSTRACT STRUCTURE OF THE GRADIENT

The inverse problem studied here is far too simple to have any direct use in applications. Its simplicity allows a rather complete account of its properties, as the reader has seen in the preceding pages. However this discussion has touched on features found in more complex and prototypical problems:

- Nested optimization (variable projection method, Golub and Pereyra (2003)) based on a model decomposition into inner and outer variables seems to be very important: in some cases, such as the simple problem presented here, the decomposition is obvious (inner variable = wavelet, outer variable = slowness), in others less so (Symes, 2008; Terentyev, 2017).

- The extended modeling operator must be surjective, or at least have a dense range, for each value of the outer variable, so that data may be fit well even for a poor initial guess of the outer variable, for the extended inversion approach to be successful.

- Because of this data-fitting assumption, a straightforward algorithm for scaling the quadratic penalty, based on the Discrepancy Principle, is available - see Fu and Symes (2017); Symes (2021); Symes et al. (2022). This scaling varies dynamically during iterative optimization, in effect changing the objective function sporadically as the iteration converges.

- The derivative of the extended modeling operator with respect to the outer variable is well-approximated by the composition of the extended modeling operator itself and a pseudodifferential operator of order 1 (Symes, 2014; ten Kroode, 2014).

- The choice of the penalty operator, controlling the extended degrees of freedom, is critical: in order to produce an objective immune from cycle-skipping, this penalty operator must be (pseudo-) differential of order zero (Stolk and Symes, 2003). A smooth multiplier $a$, as in equation 14, is a special case.

The expression 31 for the derivative of the reduced objective $\tilde{J}_\alpha$ is the result of elementary manipulations, based on the explicit expression 3 for the modeling operator $F$. In this appendix I give an alternative derivation that generalizes to extended inversion formulations for much less constrained physics. I will point out the additional reasoning necessary to reach similar conclusions in these more complex instances of extended inversion, as presented for example in Stolk and Symes (2003); Stolk et al. (2009); Symes (2014); ten Kroode (2014); Huang et al. (2017, 2018a,b, 2019).

Recall that $w_\alpha[m;d]$ is the solution of the normal equation 19. The reduced objective $\tilde{J}_\alpha$ is given by

$$\tilde{J}_\alpha[m;d] = J_\alpha[m,w_\alpha[m;d];d]$$

$$= \frac{1}{2}(\|F[m]w_\alpha[m;d] - d\|^2 + \alpha^2\|Aw[m;d]\|^2)$$

(equation 27)

$$= \frac{1}{2}(\|d\|^2 - \langle d, F[m]w_\alpha[m;d] \rangle),$$

after a little algebra.
As mentioned above, $F : M \times W \to D$ is not differentiable. Neither is $w_\alpha : M \times D \to W$, as follows immediately from the identity \[25\] However $F w_\alpha : M \times D \to D$ is differentiable, hence so is $\tilde{J}_\alpha : M \times D \to \mathbb{R}$ thanks to the identity \[53\] under the conditions on the multiplier $a$ identified in Theorem \[53\]

For the model problem studied in the body of this paper, a simple argument justifies this conclusion. To sideline some technical details, assume that $a \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R})$ and $a(t) = t$ for $|t| < \tau$ and $|a(t)| \geq \tau$ for $|t| \geq \tau$, with $\tau$ defined in equation \[37\] Then Proposition \[2\] item \[1\], implies that

$$F[m]w_\alpha[m; d] = F[m](F[m]^T F[m] + \alpha^2 A^T A)^{-1} F[m]^T d.$$ \[54\]

The normal operator and its inverse are multiplication operators, whereas $F$ and $F^T$ are scaled shift operators, inverse to each other except for scale. From this it is easy to see that the operator on the RHS of equation \[54\] is multiplication by a smooth function, with its arguments shifted by $m r$. Such an operator is smooth in $m$, hence so is $F w_\alpha$.

Since $\tilde{J}_\alpha$ and its gradient depend smoothly on their arguments, it is possible to derive an alternate expression assuming that $d \in H^1(\mathbb{R})$, then extend it by continuity to $d \in L^2(\mathbb{R})$. Note that if $w \in H^1(\mathbb{R})$, then differentiable, and

$$(D(F[m]w)\delta m)(t) = F[m](Q[m]\delta m)w(t),$$ \[55\]

where

$$(Q[m]\delta m)w = r\delta m \frac{d w}{d t}.$$ \[56\]

That is, $DF[m]\delta m$ factors into $F[m]$ following $Q[m]\delta m$, where the latter a skew-adjoint differential operator of order 1, depending linearly on $\delta m$.

Assume that $d \in H^1(\mathbb{R})$. From equation \[25\] it follows that $w[m; d] \in H^1(\mathbb{R})$ and moreover that $m \mapsto w_\alpha[m; d]$ is differentiable as a map from $\mathbb{R}^+$ to $L^2(\mathbb{R})$. From equation \[27\]

$$\tilde{J}_\alpha[m; d] = \frac{1}{2} \left( \|F[m]w[m; d] - d\|^2 + \alpha^2 \|Aw[m; d]\|^2 \right),$$

whence $m \mapsto \tilde{J}_\alpha[m; d]$ is differentiable. A standard calculation invoking the normal equation \[19\] shows that

$$D\tilde{J}_\alpha[m; d] \delta m = \langle D(F[m]w_\alpha[m; d]) \delta m, F[m]w_\alpha[m; d] - d \rangle$$

$$= \langle F[m](Q[m]\delta m)w_\alpha[m; d], F[m]w_\alpha[m; d] - d \rangle$$

$$= \langle (Q[m]\delta m)w_\alpha[m; d], F[m]^T (F[m]w_\alpha[m; d] - d) \rangle$$

$$= -\alpha^2 \langle (Q[m]\delta m)w_\alpha[m; d], A^T Aw_\alpha[m; d] \rangle$$

$$= \alpha^2 \langle w_\alpha[m; d], (Q[m]\delta m)A^T Aw_\alpha[m; d] \rangle$$

(\text{using antisymmetry of $Q$})

$$= \alpha^2 \langle w_\alpha[m; d], [(Q[m]\delta m), A^T A]w_\alpha[m; d] \rangle + \alpha^2 \langle (Q[m]\delta m)w_\alpha[m; d], A^T Aw_\alpha[m; d] \rangle$$

Rearranging,

$$d\tilde{J}_\alpha[m; d] \delta m = \frac{1}{2} \alpha^2 \langle w_\alpha[m; d], [(Q[m]\delta m), A^T A]w_\alpha[m; d] \rangle.$$ \[57\]
Since $Q$ is a differential operator of order 1, and $A^T A$ an operator of order 0, the commutator has order 0. That is, the RHS of equation \ref{eq:5.7} defines a continuous quadratic form in $d$ with respect to the $L^2$ norm. As shown above, the same is true of the left hand side. Therefore their extensions by continuity to $d \in L^2(\mathbb{R})$ are the same, and the identity \ref{eq:5.7} holds for $d \in L^2(\mathbb{R})$.

Making the identity \ref{eq:5.7} explicit by means of equation \ref{eq:5.6} and $A^T A = t^2$, substituting the expression \ref{eq:2.5} for $w_\alpha[m; d]$, and rearranging: one obtains precisely the expression \ref{eq:3.1}.

Similar reasoning can be applied to some of the other extended inversion settings mentioned at the beginning of this appendix. Provided that the outer parameter $m$ consists of (or parametrizes) smooth coefficients in the principal part of the governing system of wave equations, $F$ is a microlocally elliptic Fourier Integral Operator (FIO) (Duistermaat, 1996). The canonical relation of $F$ takes on the role of the shift operator $t \to t - mr$, and has the properties necessary to conclude that the composition of $F$ and $F^T$ in both orders is pseudodifferential, at least in an open conic subset of the cotangent bundle. If $A^T A$ is pseudodifferential, then so is the normal operator, and it is microlocally elliptic, so positive-definite when restricted to a suitable subspace of the inner parameter $w$, which appears in the hyperbolic system as components of a right-hand side or boundary condition. The inverse in the RHS of equation \ref{eq:5.4} must be replaced by a microlocal parametrix. Thanks to Egorov’s Theorem (Taylor, 1981), a special case of the rules for composing FIOs, the operator on the RHS of equation \ref{eq:5.4} is a pseudodifferential operator whose symbol is algebraic in geometric optics quantities, hence depends smoothly on the coefficients in the system of wave equations, and therefore on $m$, as does $F w_\alpha$.

Microlocal ellipticity of $F$ implies an analogue of relation \ref{eq:5.5} in which $Q$ is an essentially skew-symmetric pseudodifferential operator of order 1. Since the derivation the gradient identity \ref{eq:5.7} is algebraic, it holds approximately in these more general cases, with lower-order (smoother) error terms. See Symes (2015); ten Kroode (2014); Symes (2014) for details in several specific cases, and for a similar calculation of the Hessian. For these examples, the principal symbol of $Q$ can be computed explicitly, as a function of the geodesic distance (traveltime) function. Consequently, the analog of $\tilde{J}_\alpha$ is tangent to second order to the Hessian of an objective formulated in terms of traveltime. This relation explains the ability of the variant of extended inversion studied in the cited references to recover kinematically accurate velocity fields. Of course, that is what is shown in detail in this paper for the very simple model problem studied here.