Estimating nuisance parameters in inverse problems

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Abstract

Many inverse problems include nuisance parameters which, while not of direct interest, are required to recover primary parameters. The structure of these problems allows efficient optimization strategies—a well-known example is variable projection, where nonlinear least-squares problems which are linear in some parameters can be very efficiently optimized. In this paper, we extend the idea of projecting out a subset over the variables to a broad class of maximum likelihood and maximum a posteriori likelihood problems with nuisance parameters, such as variance or degrees of freedom (d.o.f.). As a result, we are able to incorporate nuisance parameter estimation into large-scale constrained and unconstrained inverse problem formulations. We apply the approach to a variety of problems, including estimation of unknown variance parameters in the Gaussian model, d.o.f. parameter estimation in the context of robust inverse problems, and automatic calibration. Using numerical examples, we demonstrate improvement in recovery of primary parameters for several large-scale inverse problems. The proposed approach is compatible with a wide variety of algorithms and formulations, and its implementation requires only minor modifications to existing algorithms.

(Some figures may appear in colour only in the online journal)

1. Introduction

Many inverse problems can be formulated as optimization problems of the form

\[ \mathcal{P} = \min_{x \in \mathcal{X}, \theta} g(x, \theta), \]

where \( g : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R} \) is a twice differentiable function, \( \mathcal{X} \subseteq \mathbb{R}^n \), \( x \) is a primary set of parameters of interest, while \( \theta \in \mathbb{R}^k \) is a secondary set of nuisance parameters, such as variance parameters, application-specific tuning parameters, regularization parameters, or degrees of freedom parameters. In many settings, \( k \ll n \).
A rich source of examples in (1) is the class of separable least-squares problems [11], which has been an active research area over the last 40 years (see the review paper [12] and the many references therein; see also [6, 18]). A problem in this class is given by

\[
\min_{x, \theta} \| y - \Phi(x)\theta \|^2_2,
\]  

(2)

where the matrix \( \Phi(x) \) is parametrized by \( x \). Note that \( g \) has a very special form in this case, and \( X = \mathbb{R}^n \). For problems in this class, the major insight is to exploit the structure of the problem to obtain a reduced problem

\[
\min_x \| y - \Phi(x)\bar{\theta}(x) \|^2_2,
\]  

(3)

where

\[
\bar{\theta}(x) = \arg\min_{\theta} \| y - \Phi(x)\theta \|^2_2.
\]  

(4)

At first glance, this does not make the problem easier to solve. However, it turns out that (3) can be solved using black-box approaches designed to solve the problem for a fixed \( \theta \) as long as we re-evaluate \( \bar{\theta}(x) \) for any given \( x \). Problem (4) has a closed form solution, and as noted in [12], this approach converges much faster than optimization approaches to minimize the full functional (2) using descent methods for \( (x, \theta) \). Note that this approach does not alternate between \( x \) and \( \theta \). Instead, \( \theta \) is projected out, obtaining a reduced objective in \( x \) alone. In practice, this projection requires recomputing \( \bar{\theta}(x) \) every time \( x \) is updated.

In this paper, we consider the general class (1), where we can easily compute \( \bar{\theta}(x) = \arg\min_{\theta} g(x, \theta) \), either in a closed form or by solving a small auxiliary optimization problem. We show that many algorithms for solving instances of (1) with \( \theta \) fixed can be easily modified to solve the joint inverse problem in \( x \) and \( \theta \). We provide explicit details for several important classes of problems in (1), including variance and degrees of freedom (d.o.f.) estimation, and automatic calibration of nonlinear least-squares and robust inverse problem formulations.

The paper proceeds as follows. In section 2, we review the necessary theory underlying our approach to the entire class (1). In section 3, we discuss the role of nuisance parameters, such as variance and d.o.f., in maximum a posteriori likelihood (MAP) estimation formulations. We present two important applications in detail.

1. Variance estimation for multiple data sets (see [5]).
2. Estimation of variance and d.o.f. for Student’s \( t \) formulations (see [14]).

Both are illustrated on a seismic imaging problem where the data are contaminated with various types of noises.

In section 4, we discuss the automatic calibration problem, where the forward model includes calibration parameters that need to be estimated. We illustrate the approach on a seismic imaging problem where the calibration parameters are frequency-dependent source-weights.

Finally, we discuss other possible applications and present conclusions.

2. General formulation

We consider problems of the form (1), and assume that for any given \( x \in X \), one can easily find

\[
\tilde{\theta}(x) = \arg\min_{\theta} g(x, \theta).
\]  

(5)
This condition can be relaxed, and \( \hat{\theta}(x) \) can be considered a local minimum. Rather than working to solve (1), we can instead focus on the reduced objective
\[
\tilde{g}(x) = g(x, \hat{\theta}(x)).
\]
(6)
This approach is justified by the following theorem, adapted from [4, theorem 2].

**Theorem 2.1.** Suppose that \( \mathcal{U} \subset \mathbb{R}^n \) and \( \mathcal{V} \subset \mathbb{R}^k \) are open, and \( g(x, \theta) \) is twice continuously differentiable on \( \mathcal{U} \times \mathcal{V} \). Define the optimal value function
\[
\tilde{g}(x) = \min_{\theta} g(x, \theta).
\]
(7)
Suppose that \( \bar{x} \in \mathcal{U} \) and \( \bar{\theta} \in \mathcal{V} \) are such that \( \nabla_{\theta} g(\bar{x}, \bar{\theta}) = 0 \) and \( \nabla_{\theta}^2 g(\bar{x}, \bar{\theta}) \) is positive definite. Then there exist neighborhoods of \( \bar{x} \) and \( \bar{\theta} \) and a twice continuously differentiable function \( \tilde{\theta} : \mathcal{U} \to \mathcal{V} \), where \( \tilde{\theta}(x) \) is the unique minimizer of \( g(x, \cdot) \) on \( \mathcal{V} \).

Then \( \tilde{g}(x) \) is twice continuously differentiable with
\[
\nabla_x \tilde{g}(\bar{x}) = \nabla_x g(\bar{x}, \bar{\theta}(\bar{x}))
\]
(8)
\[
\nabla_x^2 \tilde{g}(\bar{x}) = \nabla_x^2 g(\bar{x}, \bar{\theta}(\bar{x})) + \nabla^2_{x,\theta} g(\bar{x}, \bar{\theta}(\bar{x})) \nabla_{\theta} \bar{\theta}(\bar{x}).
\]
(9)

**Remark 2.2.** Theorem 2.1 provides sufficient conditions for existence of the first and second derivatives of \( \tilde{g} \). In practice, these derivatives may exist even if the smoothness hypotheses are not satisfied. Consider \( g(\theta, x) = \frac{\theta^2}{2} + \theta^2 - |\theta|^2 \). In this case, \( |\hat{\theta}(x)| = \frac{\theta^2}{2} \), so \( \tilde{g}(x) = \frac{\theta^2}{2} \) is smooth even though \( g(x, \theta) \) is not.

Theorem 2.1 suggests a natural approach to designing algorithms for minimizing \( \tilde{g}(x) \). In the unconstrained case (i.e. \( \mathcal{X} \) is the whole space), consider iterative methods of the form
\[
x^{k+1} = x^k - \gamma_k H_k^{-1} \nabla \tilde{g}(x^k) = x^k - \gamma_k H_k^{-1} \nabla g(x^k, \bar{\theta}(x^k)).
\]
(10)
Here, \( \gamma_k \) is a step length which can be chosen using one of several line search routines. Specifically, \( H_k = I \) yields Cauchy’s steepest descent, \( H_k = \nabla^2 \tilde{g}(x^k) \) yields a modified Newton method and approximations to \( H_k \) that use only first-order derivative information yield Gauss–Newton (GN) or Levenberg–Marquardt-type methods (see e.g. [17]). A quasi-Newton method such as BFGS or L-BFGS (see [17]) may be similarly implemented using only information from (8).

If \( \mathcal{X} \) is a closed and bounded set that allows a simple projection, such as a set of box constraints \( \{x : l \leq x \leq u\} \), an ellipsoidal set \( \{x : ||x||_M \leq \tau\} \), or the 1-norm ball \( \{x : ||x||_1 \leq \tau\} \), this can be exploited to solve (1). For example, we can use a modified projected gradient method
\[
x^{k+1} = P_{\mathcal{X}}[x^k - \gamma_k \nabla \tilde{g}(x^k)],
\]
(11)
or an appropriately modified projected quasi-Newton method, such as the one described in [22]. The point is that the structure of \( \mathcal{X} \) does not enter into the computation of (8) or (9), so a natural strategy is to compute these quantities first and then apply methods that exploit the structure of \( \mathcal{X} \). Moreover, we show in the next corollary that the point \( (\bar{x}, \theta(\bar{x})) \) satisfies the first-order necessary conditions for the original (constrained) problem.

**Corollary 2.3.** Suppose the hypotheses of theorem 2.1 hold, and the additional constraint \( x \in \mathcal{X} \) is imposed, where \( \mathcal{X} \) is a closed convex set. If \( \bar{x} \) satisfies the first-order necessary conditions for \( \tilde{g}(x) \), then \( (\bar{x}, \theta) \) with \( \theta = \theta(\bar{x}) \) satisfies the first-order necessary conditions for \( g(x, \theta) \).
Proof. The first-order necessary conditions for (1) are

\[
\begin{align*}
\nabla \theta g(\bar{x}, \bar{\theta}) &= 0 \\
- \nabla_x g(\bar{x}, \bar{\theta}) &\in N_X(\bar{x}),
\end{align*}
\]

where \( N_X(\bar{x}) \) is the normal cone to \( X \) at the point \( \bar{x} \) (see [21] for details). The first-order necessary condition for \( \bar{x} \) to be a minimizer of the reduced objective (6) is

\[
- \nabla_x \tilde{g}(\bar{x}) \in N_X(\bar{x}).
\]

(13)

Since we have \( \nabla_x \tilde{g}(\bar{x}) = \nabla_x g(\bar{x}, \bar{\theta}) \) by theorem 2.1, \((\bar{x}, \bar{\theta}(\bar{x}))\) satisfies (12) if and only if \( \bar{x} \) satisfies (13). On the other hand, \( \bar{\theta}(\bar{x}) \) satisfies the first equation of (12) by construction. \( \square \)

Thus, for many applications (both constrained and unconstrained), we can systematically extend standard algorithms for minimizing \( g(x, \theta) \) with \( \theta \) fixed to extended problems (1).

Note that this is not equivalent to an alternating approach, where \( x \) and \( \theta \) are updated in an alternating fashion. Rather, \( \theta \) is updated continuously as a function of \( x \). The beauty of this approach is that the optimization algorithm used to minimize the modified objective \( \tilde{g}(x) \) can be agnostic to the existence of the auxiliary parameter \( \theta \).

In the following sections, we present some applications and provide full algorithmic details and numerical work.

3. Complicating parameters in maximum likelihood estimation

Many inverse problems can be formulated as maximum likelihood (ML) problems within a statistical modeling framework (see e.g. [23, 25]). Given data \( y \), we want to solve for parameters of interest \( x \), using the fact that the parameters are related to the data via a (possibly nonlinear) forward model:

\[
d = F(x) + \epsilon.
\]

(14)

The \( \epsilon \) term in (14) reflects a statistical model of the discrepancy between the model \( F(x) \) and the true data \( d \). Independent, identically distributed (i.i.d.) Gaussian errors \( \epsilon \sim N(0, \sigma^2 I) \) are a common choice, and even though the variance parameter \( \sigma^2 \) is unknown, it does not affect the ML formulation in \( x \). This is not true if the data come from different sources, with each group having its own parameter \( \sigma_i^2 \).

More generally, \( \epsilon_i \) may come from a range of parametric distributions. The Student’s \( t \) distribution has been applied in many instances where large measurement errors are common or unexplained artifacts in the data are an issue [1, 2, 14]. These applications require estimates for d.o.f. and variance parameters even with the i.i.d. assumption on the errors.

If we take \( \theta \) to be unknown nuisance parameters, the general ML formulation for estimating \( x \) in model (14) takes the form (1). The method proposed in this paper is well suited for online estimation of \( \theta \), and in the remainder of the section we provide full exposition for the multiple sources of error example and for Student’s \( t \) hyperparameter estimation.

3.1. Variances in multiple data sets

Estimating variance parameters in multiple datasets is an important problem in many areas, including drug and tracer kinetics [5], and geophysics. In this section, we review the formulation presented in [5] and show that the algorithm derived in [5] follows immediately from the general approach we propose here, i.e. it is a GN method of form (10). We present a numerical example, illustrating the importance of variance parameter estimation for a large-scale geophysical inverse problem. We also extend the approach to the (fully observed) multivariate Gaussian case with correlations between measurement errors.
We are given $M$ experiments indexed by $i$, each of which yields $N_i$ measurements and has its own variance parameter $\sigma_i$. All experiments share a common set of primary parameters $x$:

$$d_i = F_i(x) + \epsilon_i,$$

where $d_i \in \mathbb{R}^{N_i}$, $F_i(x)$ is the modeling operator for the $i$th experiment and $\epsilon_i \sim \mathcal{N}(0, \sigma_i^2 I)$. If the variance parameters are fixed, the ML estimation problem for $x$ is given by

$$\min_x \frac{1}{\sigma_i^2} \|d_i - F_i(x)\|^2_2. \quad (16)$$

The joint ML estimation problem for $x$ and $\sigma^2 = \{\sigma_i^2\}$ is given by

$$\min_{\sigma^2, x} g(x, \sigma^2) := \sum_{i=1}^{M} \left( N_i \log (2\pi \sigma_i^2) + \frac{1}{\sigma_i^2} \|d_i - F_i(x)\|^2_2 \right). \quad (17)$$

This is a special example of (1).

With $x$ fixed, (17) separates and (5) has a closed form solution, which we find by taking the gradient with respect to each $\sigma_i^2$ and setting it to 0:

$$\tilde{\sigma}_i^2(x) = \frac{1}{N_i} \|d_i - F_i(x)\|^2_2. \quad (18)$$

This quantity is precisely the population variance estimate. The modified problem (6) is now given by

$$\min_x \tilde{g}(x) := \sum_{i=1}^{M} \left( N_i \log (2\pi \tilde{\sigma}_i^2(x)) + N_i \right). \quad (19)$$

The gradient of this objective is given by

$$\nabla_x \tilde{g}(x) = -\sum_{i=1}^{M} \frac{1}{\tilde{\sigma}_i^2(x)} \nabla F_i(x)(d_i - F_i(x)), \quad (20)$$

while the GN Hessian approximation is given by

$$H(x) = \sum_{i=1}^{M} \frac{1}{\tilde{\sigma}_i^2(x)} \nabla F_i(x)\nabla F_i(x)^T.$$

Note that this approximation to $\nabla_x^2 \tilde{g}$ ignores the term $\nabla_x^2 \tilde{g}(\tilde{x}, \tilde{\theta} (\tilde{x}))\nabla_x \tilde{g} (\tilde{x})$ in (9) and is equivalent to the one used in [5], which we show by forming the GN subproblem:

$$\min_x \sum_{i=1}^{M} \frac{1}{\tilde{\sigma}_i^2(x_k)} \|d_i - F_i(x_k) - \nabla F_i(x_k)^T x\|^2_2. \quad (21)$$

This expression matches [5, (12)] up to a constant. However, while in [5] the subproblem (21) came about via a cleverly constructed proxy objective for (17), we can now view it as a natural GN approximation to the modified objective (19).

**Example: full waveform inversion**

Full waveform inversion (FWI) is an approach to obtain gridded subsurface velocity parameters from seismic data. Experiments are conducted by placing explosive sources on the surface and recording the reflected waves with an array of receivers on the surface. FWI is naturally cast as a nonlinear least-squares optimization problem [24, 20], and fits in the framework described above. The data, $d_i$, in this case represents the Fourier transform of the recorded time series for frequency $i$. The corresponding modeling operator, $F_i(x) = P A_i(x)^{-1} Q_i$, inverts a discretized
Helmholz operator $A_i(x)$ for the $i$th frequency and the gridded velocity field $x$, and samples the wavefield at the receiver locations. Here, $P$ denotes the sampling operator and each column of the matrix $Q_i$ is a gridded source function.

To illustrate the approach, we use a subset of the well-known Marmousi benchmark model, depicted in figure 1(a). The model is discretized on a $201 \times 301$ grid with 10 m grid spacing. We generate data for 151 sources, 301 receivers (i.e. $N_i = 151 \times 301$)—all equi-spaced and located at the surface—and $M = 12$ frequencies between 3 and 25 Hz. Typically, the data have a lower signal-to-noise ratio for the low and high frequencies. To emulate this situation, we add Gaussian noise to the measurements with variance $\sigma_i \sim (i - 6)^2$. We use an L-BFGS method to solve both the modified optimization problem (19) and the original problem (16) for a fixed $\sigma_i = 1$ for all $i$. The results after 50 iterations are shown in figures 1(b) and (c). The corresponding error between the reconstructed and true model is shown in figure 1(d). Finally, we show the estimated variance in the final model for both reconstructions in figure 1(e). The reconstruction obtained by solving the modified problem is clearly better. Interestingly enough, the variance estimates for both models are almost identical. This means that at least for this application, solving (16) with an incorrect variance and then trying to improve on the solution using an updated variance estimate does not work as well as updating the variance estimates on the fly as one solves (19).

3.2. Correlated multivariate observations

The results from the previous case can be generalized to variance estimation in a multivariate inverse problem setting with correlated errors. Consider the model (15), where now we take
\( \epsilon_i \sim N(0, \Sigma) \). In this case, all of the \( \epsilon_i \) are of the same dimension. The ML objective corresponding to (17) is given by

\[
\min_{\Sigma, x} g(x, \Sigma) := \left( M \log(2\pi \det(\Sigma)) + \sum_{i=1}^{M} (d_i - F_i(x))^T \Sigma^{-1} (d_i - F_i(x)) \right).
\] (22)

The point here is that despite the generalization to full \( \Sigma \), we still have a closed form solution analogous to (18):

\[
\Sigma(x) = \arg\min_{\Sigma} g(x, \Sigma) = \frac{1}{M} \sum_{i=1}^{M} (d_i - F_i(x))(d_i - F_i(x))^T.
\] (23)

The fastest way to see this is to take the derivative of (22) with respect to \( \Sigma \) (rather than with respect to \( \Sigma^{-1} \)):

\[
\frac{d}{d\Sigma^{-1}} g(x, \Sigma) = -M\Sigma + \frac{d}{d\Sigma^{-1}} \text{tr} \left( \sum_{i=1}^{M} \Sigma^{-1} (d_i - F_i(x))(d_i - F_i(x))^T \right)
\]

\[
= -M\Sigma + \sum_{i=1}^{M} (d_i - F_i(x))(d_i - F_i(x))^T = 0.
\]

For details on matrix derivatives, see e.g. [19]. Therefore, the variable projection method can be applied to (22) with respect to \( \Sigma^{-1} \) (rather than with respect to \( \Sigma \)).

3.3. Degrees of freedom and variance estimation for Student’s t formulations

Many applications require robust formulations to obtain reasonable results with noisy data or in cases where a portion of the data is unexplained by the forward model (e.g. in the presence of coherent artifacts). A useful way to derive these formulations is to begin with the statistical model (15) where the noise term \( \epsilon_i \) is modeled using a particular parametric density, and then formulate the MAP likelihood problem. The least-squares formulation corresponds to a Gaussian assumption on \( \epsilon_i \) (see section 3.1), while assuming that a Laplacian distribution leads to a 1-norm penalty on the data-misfit.

As shown in [2, theorem 2.1], in cases where unexplained artifacts may be large or constitute a significant portion of the data, it is better to use heavy-tailed densities. A prime example is the Student’s \( t \), whose density is given by

\[
p(y, \sigma^2, k) = \frac{\Gamma((k+1)/2)}{\Gamma(k/2)\sqrt{\pi k} \sigma^k} \left( 1 + \frac{y^2}{\sigma^2 k} \right)^{-(k+1)/2}.
\] (24)

This density was first successfully used in [14] in the data fitting context. The d.o.f. parameter \( k \) was seen as a tuning parameter, smoothly transitioning between heavy-tailed and near-Gaussian behavior; \( k \) and \( \sigma \) were fit using expectation maximization (EM) and scoring methods. This density was also successfully used in the Kalman smoothing context [8], where it was suggested that the EM algorithm can be used to fit meta-parameters. Recent work using the Student’s \( t \) distribution [2, 3, 1] has side-stepped the problem, using fixed values for \( \sigma \) and \( k \).
In this section, we show that the general projection approach can be used to solve the joint inverse problem, treating scale and d.o.f. as nuisance parameters. We propose a novel simple method, different from EM or scoring methods discussed in [14], for estimating scale and d.o.f. for any given set of residuals. Given the model (15), the full MAP Student’s t estimation problem is given by

$$
\min_{x, k, \sigma^2} g(x, \sigma^2, k) := -n \log \left( \frac{\Gamma \left( \frac{k+1}{2} \right)}{\Gamma \left( \frac{k}{2} \right) \sqrt{\pi k}} \right) + \frac{n}{2} \log(\sigma^2) + \frac{k+1}{2} \sum_{i=1}^{n} \log \left( 1 + \frac{r_i^2}{\sigma^2 k} \right),
$$

where $r_i = d_i - F_i(x)$. Following the philosophy presented in the paper, we solve the problem by defining the modified objective

$$
\tilde{g}(x) = g(x, \sigma^2(x), k(x))
$$

with

$$
(\sigma^2(x), k(x)) = \arg\min_{\sigma^2, k} g(x, \sigma^2, k).
$$

The two-dimensional optimization problem in $(\sigma^2, k)$ required to evaluate $\tilde{g}(x)$ can be solved using a customized routine or a black-box optimization code. An application is presented below.

**Example: traveltime tomography**

We consider a cross-well traveltime tomography problem. In this case, sources and receivers are placed in vertical wells and the data consist of picked traveltime of first arrivals. Since the data are typically very noisy, a portion of the traveltimes may be picked erroneously, motivating the use of robust penalties for the inversion. The traveltimes are computed by a geometric optics approach, where wave propagation is modeled via rays. The traveltime between a given source and receiver is simply the integral of the reciprocal velocity along the corresponding ray-path. By assuming small perturbations of a known background velocity, we arrive at a linear modeling operator with a fixed ray geometry. The data are the traveltime perturbations, while the primary parameter of interest is the velocity perturbation, both taken with respect to a known background model.

In this example, we consider a constant background velocity, so that the ray paths are straight lines. The modeling operator is therefore essentially a Radon transform, which is often used in medical x-ray imaging applications. The true velocity perturbation is discretized on a $51 \times 51$ grid and is shown in figure 2(a). The corresponding data for 51 sources and receivers and the added outliers are shown in figure 2(b). We regularize the inversion by inverting the primary parameters on a coarser grid of size $26 \times 26$. We then interpolate back to the fine grid using 2D cubic interpolation. The modified optimization problem is now given by

$$
\min_{x} \rho_{\theta}(\Delta T - A x),
$$

where $\Delta T \in \mathbb{R}^{2601}$ are the measured traveltime perturbations, $x \in \mathbb{R}^{676}$ is the velocity perturbation, $A$ is the modeling operator which combines the Radon transform and interpolation and $\tilde{\theta} = (\tilde{\sigma}^2, \tilde{k})$ is obtained by solving (26) using a Nelder–Mead method [16].

Note that we may treat $\theta$ as fixed when designing an algorithm to solve (27), as long as the parameters are re-estimated at every evaluation of $\rho_{\theta}(r)$ and its derivatives. To solve (27), we use a modified GN algorithm which calculates the updates by solving

$$
(A^T H_\theta(r_k)A) \Delta x_k = A^T \nabla \rho_{\theta}(r_k),
$$

where $H_\theta(r_k) = (A^T A(r_k) + \lambda I)$. This expression can be used to update $x_k$.
Figure 2. (a) Velocity perturbation in m/s used to generate the observed data. (b) The corresponding traveltime perturbations in black (o) and the outliers in red (+).

Figure 3. Results for traveltime tomography. (a) Least-squares reconstruction, (b) Student’s $t$ reconstruction with fixed $\theta$ estimated at the initial residual and (c) Student’s $t$ reconstruction where $\theta$ is re-estimated at every iteration.

where $r_k = \Delta T - A x_k$ and $H_{\theta}$ is a positive approximation of the Hessian $\nabla^2 \rho_\theta$ (see also section 4). We solve the subproblems using CG.

We compare the following three approaches: (i) least-squares, shown in figure 3(a), (ii) Student’s $t$ with a fixed $\theta$ which is estimated once at the initial residual, shown in figure 3(b), and (iii) Student’s $t$ where we estimate $\theta$ at each iteration, shown in figure 3(c). All results are obtained after 20 GN iterations, each using 10 CG iterations to solve the subproblem.

In order to understand the difference between the latter two cases, we show histograms of the initial and final residuals as well as the influence function $(\nabla \rho)(\gamma f)$ for the corresponding $\theta$ in figures 4(a)–(c). Clearly, re-fitting the $\theta$ at each iteration allows the inversion to home in on the good data while ignoring the outliers.

4. Automatic calibration

In this section, we consider the case where the forward model includes a calibration factor $\alpha$:

$$d = F(x, \alpha) + \epsilon.$$  

(29)
In the case of the nonlinear data-fitting problem described earlier, the modified objective is given by

$$
\min_x \tilde{g}(x) = \rho(d - F(x, \tilde{a})) \quad \text{(30)}
$$

where

$$
\tilde{a}(x) = \arg\min_{a} \rho(d - F(x, a)) \quad \text{(31)}
$$

The motivating example that led us to consider this class of problems is presented below.

4. Example: FWI with source estimation

Seismic data can be interpreted as the Green function of the subsurface, parametrized by $x$, convolved with an unknown (bandlimited) source signature. In the frequency domain, we can model the unknown source signature by multiplication with a complex scalar for each frequency. The problem of interest is now formulated as

$$
\min_{x, \alpha} \left\{ g(x, \alpha) := \sum_{i=1}^{M} \rho(d_i - \alpha_i F_i(x)) \right\} \quad \text{(32)}
$$

where the index $i$ runs over frequency. Just as in the variance parameter case, the parameters $\alpha_i$ are linked only through the parameters $x$, and for a given $x$ the problem decouples completely, giving

$$
\tilde{a}_i(x) = \arg\min_{\alpha} \rho(d_i - \alpha_i F_i(x)) \quad \text{(33)}
$$

We consider the least-squares and Student’s $t$ penalty, and use a scalar Newton-type method to solve (33):

$$
\alpha_i^{v+1} = \alpha_i^{v} - \left( \nabla \rho(r_i^v(x)) \right) / \left( \langle F_i(x), H F_i(x) \rangle \right) \quad \text{(34)}
$$

where $r_i^v(x) = d_i - \alpha_i^v F_i(x)$, $\nabla \rho$ is the gradient of the penalty function and $H$ is (a positive definite approximation of) the Hessian $\nabla^2 \rho$. In particular, we have

- least-squares: $\rho(r) = \frac{1}{2} \sum r_i^2$, $\nabla \rho_i = r_i$, and $H_{ii} = 1$.
- Student’s $t$: $\rho(r) = \frac{1}{2} \sum \log(k + r_i^2)$, $\nabla \rho_i = r_i / (k + r_i^2)$ and $H_{ii} = 1 / (k + r_i^2)$.
For more details on the Student’s $t$ approach, we refer to [2]. We generate seismic data for the velocity model depicted in figure 5(a) with a time-domain finite difference code. The data consist of 141 sources and 281 receivers, and has a recording time of 4 s. Ten per cent of the data is corrupted with large outliers.

We invert the data in several stages, moving from low to high frequencies. Each stage uses only a few frequencies and the output is used as initial guess for the subsequent stage. This is a well-known strategy in FWI to avoid local minima [7]. We use an L-BFGS method to solve the resulting optimization problems, starting from the initial model shown in figure 5(b). The results are shown in figures 5(c) and (d). The Student’s $t$ approach recovers the most important features of the model, whereas the least-squares approach leads to a very noisy model.

5. Discussion and conclusions

Many inverse problems involve nuisance parameters that are not of primary interest but can have significant influence on the estimation of primary parameters. Common examples include variance, d.o.f. and calibration parameters. These issues arise in a great variety of applications, including pharmacokinetic modeling [5], seismic inverse problems [24], dynamic systems [9], uncertainty quantification [10] and optimal experimental design [13].

In this paper, we proposed a straightforward approach to fitting these nuisance parameters on the fly, while solving the overall inverse problem. Specifically, we formulated the problem as a joint optimization over primary parameters $x$ and nuisance parameters $\theta$, and showed that for a large class of problems, one can simply project out the $\theta$ parameters by solving (5). In the least-squares case, this idea has been carefully studied under the name variable projection [18, 12]. As we showed, these ideas extend nicely to the entire class (1). In particular, theorem 2.1 and corollary 2.3 characterize the general approach and are the basis for algorithm design of first- and second-order methods.

An immediate consequence of the work is the ability to modify first- and second-order algorithms that exploit particular application structure to also fit nuisance parameters. We demonstrated this in practice using several (large-scale) inverse problems.
In the case of variances in multiple datasets, the proposed approach matches the algorithm proposed in [5], and therefore the development we presented provides an alternative (and significantly simpler) derivation. We have also shown that the approach can be easily extended to estimate covariances between error sources in the case where we have multivariate observations in section 3.2.

In the case of Student’s $t$ parameters, it is interesting to note that when estimating d.o.f. for fixed residuals, our approach matches the one used in the MASS library of the R programming language [26]. To our knowledge, this approach has not been used for fitting d.o.f. in general inverse problems, and in fact Lange, Little and Taylor [14], who first proposed Student’s $t$ inversion, advocated a very different (EM-type) approach for d.o.f. fitting.

From a theoretical point of view, the method we propose can be used to solve a variety of inverse problems from the general class (1). From a practical point of view, the main selling point of the proposed approach is the ability to modify existing methods to solve for nuisance parameters on the fly.

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