RANDOMIZED APPROACH TO NONLINEAR INVERSION COMBINING SIMULTANEOUS RANDOM AND OPTIMIZED SOURCES AND DETECTORS

SELDIN S. ASLAN †, ERIC DE STURLER †, AND MISHA E. KILMER‡

Abstract. In partial differential equations-based (PDE-based) inverse problems with many measurements, we have to solve many large-scale discretized PDEs for each evaluation of the misfit or objective function. In the nonlinear case, each time the Jacobian is evaluated an additional set of systems must be solved. This leads to a tremendous computational cost, and this is by far the dominant cost for these problems.

Several authors have proposed to drastically reduce the number of systems to be solved by exploiting stochastic techniques [E. Haber, M. Chung, F. Herrmann, SIAM J. Optimiz., 22(2012), pp. 739-757] and posing the problem as a stochastic optimization problem [A. Shapiro, D. Dentcheva, and A. Ruszczyński, Lectures on Stochastic Programming: Modeling and Theory, SIAM, 2009]. In this approach, the misfit or objective function is estimated using only a few appropriately chosen random linear combinations of the sources, referred to as simultaneous random sources. For computing the Jacobian, we show that a similar approach can be used to reduce the number of additional adjoint solves for the detectors.

While others have reported good solution quality at a greatly reduced computational cost using these randomized approaches, for our problem of interest, diffuse optical tomography, the approach often does not lead to sufficiently accurate solutions. Therefore, we replace a few random simultaneous sources and detectors by simultaneous sources and detectors that are optimized to maximize the Frobenius norm of the sampled Jacobian after solving to a modest tolerance. This choice is inspired by (1) the regularized model problem solved in the TREGS nonlinear least squares solver [E. de Sturler and M. Kilmer, SIAM J Sci. Comput., 33(2011), pp. 3057-3086] used for minimization in our method and (2) the fact that these optimized directions correspond to the most informative data components.

Our approach leads to solutions of the same quality as obtained using all sources and detectors but at a greatly reduced computational cost, since a greatly reduced number of large-scale linear systems needs to be solved.

Key words. DOT, PaLS, stochastic programming, randomization, inverse problems, optimization

AMS subject classifications. 65F22, 65N21, 65N22, 65M32, 62L20, 90C15

1. Introduction. The solution of nonlinear inverse problems requires solving many large-scale discretized PDEs in the evaluation of the forward problem. In parameterized inverse problems, we can compute the response of the system for a particular input by numerically solving the PDE. The forward model used in this paper, see section 2, is already regularized using the parametric level set (PaLS) approach [1], and we focus on efficiently solving the nonlinear least squares problem

\[
\min_{\mathbf{p}} f(\mathbf{p}) := \min_{\mathbf{p}} \frac{1}{2}\|\mathbf{M}((\mathbf{p}) - \mathbf{d}\|_2^2,
\]

where \(\mathbf{M}(\mathbf{p})\) is the vector of computed measurements given by the forward model for the parameter vector \(\mathbf{p}\), and \(\mathbf{d}\) is the vector of measured data at the detectors.

Unfortunately, each evaluation of \(f(\mathbf{p})\) requires the solution of the PDE for all inputs. Moreover, to efficiently compute derivative information using the co-state approach [17], we also need to solve linear systems with the adjoint for each detector

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†Department of Mathematics, Virginia Tech, Blacksburg, VA 24061.

‡Department of Mathematics, Tufts University, Medford, MA 02115.
and each frequency. This leads to an enormous computational bottleneck, as rapid advances in technology allow for large numbers of sources and detectors. Multiply this by the number of frequencies, and the number of linear systems to solve in the solution of (1.1) is very large indeed. For the main application discussed in this paper, diffuse optical tomography (DOT), the number of sources and the number of detectors may each be a thousand or more; the number of frequencies used is typically modest (less than ten) [4].

Fortunately, solving the optimization problem does not require highly accurate steps. In particular, far from the minimizer, there is little use for computing accurate steps in a Newton-type method. For the solution to the minimization problem (1.1), we use the Trust region algorithm with REGularized model Solution (TREGS) [5] that has proven very effective for problems of this type. In a previous paper [4], we use reduced order models to approximate both the function evaluation as well as its derivatives to compute regularized Gauss-Newton steps in TREGS. In this paper, we explore an alternative approach, following the work by Haber, Chung, and Herrmann [7]. The main idea is to drastically reduce the number of systems to be solved by exploiting randomization [7] and posing the problem as a stochastic optimization problem [15]. In this approach, the misfit or objective function is estimated using only a few appropriately chosen random linear combinations of the sources, referred to as simultaneous random sources that are kept fixed over many optimization steps. This is referred to as the Sample Average Approximation (SAA) method in [15]. Simultaneous random sources have been well-studied in various papers (see [3, 13, 11, 14, 16] and the references within). While this approach seems to work well for direct current resistivity and seismic tomography [7], it often fails to reach the required accuracy for DOT. Therefore, we propose two innovations to this approach. In order to extend the approach to Newton-type methods, where we need to compute the Jacobian efficiently, we show that a similar approach can be used to reduce the number of additional adjoint solves for the detectors. This allows for a new stochastic optimization approach to minimize the residual norm for parameter inversion.

Simultaneous random sources and detectors provide moderately accurate solutions at a drastically reduced number of linear system solves. To overcome the convergence problems with simultaneous random sources and detectors, we solve for a fixed set of simultaneous random sources and detectors up to an intermediate tolerance. After reaching this intermediate tolerance, we replace a few random simultaneous sources and detectors by simultaneous sources and detectors that are optimized to maximize the Frobenius norm of the sampled Jacobian (see section 3); we refer to these as simultaneous optimized sources and detectors. This choice is inspired by (1) the regularized model problem solves in the TREGS nonlinear least squares solver [5] used for minimization in our method and (2) the fact that these optimized directions correspond to the most informative data components. After this update in simultaneous sources and detectors, convergence to a solution of the same quality as obtained using all sources and detectors is rapid.

This paper is organized as follows. In section 2, we briefly review DOT, PaLS, and TREGS. In section 3, we introduce a new randomized approach using simultaneous random sources and detectors in an SAA fashion. Further, we improve this approach by allowing the matrices of simultaneous random sources and detectors to be first downdated, then updated in an optimal way to obtain simultaneous optimized sources and detectors. Moreover, we also give an outline of our implementation strategies. In section 4, we demonstrate the effectiveness of combining simultaneous random sources and detectors.
sources and detectors with simultaneous optimized sources and detectors using three experiments. Finally, we draw some conclusions and discuss future work in Section 5.

2. Background on DOT, PaLS, and TREGS. We assume that the region to be imaged is a rectangular prism with sources and detectors on the top and or the bottom. We consider the diffusion model for the photon flux $\phi(x)$ obtained by an input source $g(x)$ as in [2]. Let the diffusion (or the scattering) and the absorption coefficients be given by $D(x)$ and $\mu(x)$, respectively. Then, the mathematical model of the problem in the frequency domain is given by

$$-\nabla \cdot (D(x)\nabla \phi(x)) + \mu(x)\phi(x) + \frac{i\omega}{\nu} \phi(x) = g(x),$$

for $x = (x_1, x_2, x_3)^T$ and $-a < x_1 < a$, $-b < x_2 < b$, $0 < x_3 < c$, $\phi(x) = 0$ if $0 \leq x_3 \leq c$ and either $x_1 = \pm a$, or $x_2 = \pm b$, $0.25\phi(x) + \frac{D(x)}{2} \frac{\partial \phi(x)}{\partial \xi} = 0$ for $x_3 = 0$, or $x_3 = c$,

where $\xi$ is the outward unit normal, $\omega$ is the frequency modulation of light and $\nu$ is the speed of light in the medium.

For simplicity, we assume in this paper that $D(x)$ is well-specified, and we only need to solve for the absorption, $\mu(x)$. In DOT, near infrared light is transmitted through the medium and measured at the detectors. Strong differences in absorption and scattering indicate the existence of anomalies, which might be cancerous regions in tissue. In [1, 4], PaLS are used to reduce the dimension of the search space for DOT. We parameterize the medium as in [1, 4], and solve for a modest number of parameters that describe the shape of potential anomalies (tumors), rather than solving for $\mu$ at every grid point. Hence, the parameterized absorption is defined as

$$\mu(x) = \mu(x; p),$$

where $p$ denotes the vector of parameters. Using PaLS, we parameterize the absorption $\mu(x; p)$ as follows.

Let $\varphi : \mathbb{R}^+ \rightarrow \mathbb{R}$ be a smooth, compactly supported radial basis function (CSRBF), $\gamma$ be a positive, small, real number, and $\|x\|^4 := \sqrt{\|x\|^2 + \gamma^2}$ denote the (regularized) Euclidean norm. Then the PaLS function $\phi$ with a vector of unknown parameters $p_\varphi$ consisting of expansion coefficients $\alpha_j$, dilation coefficients $\beta_j$, and center locations $\chi_j$ is defined as

$$\phi(x; p_\varphi) := \sum_{j=1}^{m_0} \alpha_j \varphi(||\beta_j(x - \chi_j)||^4).$$

The PaLS approach uses an approximate Heaviside function $H_r(r)$, where $r$ is a scalar, to create a differentiable, but sharp transition from anomaly to background. The absorption $\mu(x; p)$ takes the value $\mu_{in}(x)$ if $x$ is inside the region and $\mu_{out}(x)$ if $x$ is outside the region,

$$\mu(x, p) = \mu_{in}(x)H_r(\phi(x, p_\varphi) - c) + \mu_{out}(x)(1 - H_r(\phi(x, p_\varphi) - c)),$$

where $c \in \mathbb{R}$ is a chosen cut-off parameter for the level set.

Figure 2.1 illustrates how PaLS represents the absorption field. Using PaLS, edges and complex boundaries can be captured with relatively few basis functions.
Fig. 2.1: (a) Surface and contour plot of a test anomaly on $100 \times 100$ mesh with 25 basis functions where the cut off is at $c = 0.15$. For simplicity, $p = p_c$. (b) The PaLS function of the test anomaly on the left. If $\phi(x, p) \geq 0.15$, then $x$ is inside the anomaly (light) and if $\phi(x, p) < 0.15$, then $x$ is outside the anomaly (dark).

The PaLS representation also regularizes the problem as a function of the number of basis elements used, hence no further regularization is needed. For further discussion of the PaLS parameters for DOT, we refer the reader to [1, 4].

Let $n_d$, $n_s$, and $n_\omega$ denote the number of detectors, sources, and frequencies, respectively. The discretization of (2.1) leads to computed measurements, $m_i(\omega_j, p) \in \mathbb{C}^{n_d}$ for each source term, $b_i$.

$$m_i(\omega_j, p) = C^T(i\omega_j E + A(p))^{-1} b_i,$$

where the rows of $C^T$ correspond to the detectors\(^1\). $A(p)$ derives from a finite difference discretization of the diffusion and absorption terms in (2.1), and $E$ derives from the frequency term in (2.1). $E$ is almost the identity except that it has zero rows for points on the boundary, $x_3 = 0, x_3 = c$, in (2.1); so, $E$ is singular.

For simplicity, we consider the nonlinear residual for a single frequency, $\omega_j = 0$. In vector form, the residual is defined as follows

$$r(p) = \begin{bmatrix} r_1(p) \\ \vdots \\ r_{n_s}(p) \end{bmatrix} = \begin{bmatrix} m_1(p) - d_1 \\ \vdots \\ m_{n_s}(p) - d_{n_s} \end{bmatrix} = \begin{bmatrix} C^T A^{-1}(p)b_1 - d_1 \\ \vdots \\ C^T A^{-1}(p)b_{n_s} - d_{n_s} \end{bmatrix},$$

where $r_i \in \mathbb{R}^{n_d}$, $d_i$ is the data vector with the measurements from the detectors corresponding to source $b_i$, and the nonlinear least squares problem (1.1) becomes

$$\min_p \frac{1}{2} \|r(p)\|_2^2.$$  

\(^1\)In general, we also split $m_i$ in its real and imaginary parts.
Let \( J \) be the Jacobian of \( r(p) \),
\[
J = \frac{\partial r(p)}{\partial p} = \left[ \frac{\partial r(p)}{\partial p_1} \ldots \frac{\partial r(p)}{\partial p_n} \right],
\]
where the components of \( J \) are given by small vectors
\[
J_{jk}(p) = \frac{\partial}{\partial p_k}(C^T A^{-1}(p)b_j) = -C^T A^{-1}(p) \frac{\partial A(p)}{\partial p_k} A^{-1}(p)b_j \in \mathbb{R}^{n_d}.
\]
Once \( r(p) \) and \( A^{-1}(p)b_j \) are available, evaluating \( J \) using the co-state approach \[17\] requires solving an additional \( n_d \cdot n_\omega \) adjoint systems for detectors.

We use TREGS \[5\] to solve the nonlinear least squares problem (2.6). The TREGS algorithm combines a trust region method with a regularized minimization of the Gauss-Newton (GN) model \[6\]. The local (GN) model at the current parameter vector, \( p_c \), is given by
\[
m_{GN}(p_c + \delta) \approx \frac{1}{2} r_c^T r_c + r^T J_c \delta + \frac{1}{2} \delta^T J_c^T J_c \delta,
\]
and its minimization is equivalent to the least squares problem \( J_c \delta \approx -r_c(p) \). The TREGS algorithm favors updates corresponding to (1) the large singular values and (2) the left singular vectors with large components in \( r \) as determined by a generalized cross validation-like (GCV) criterion. Since the Jacobian tends to be ill-conditioned, the emphasis on large singular values leads to relatively small steps that provide relatively large reductions in the GN model (2.9). We refer the reader to \[5\] for more details of TREGS.

3. A Randomized Approach. We recast the nonlinear least squares problem as a stochastic optimization problem using randomization to drastically reduce the number of large linear systems to solve in (2.5) and (2.8). The columns of \( B = [b_1, \cdots, b_n] \) are source terms, and we refer to any linear combination of these sources as a simultaneous source. Simultaneous random sources, \( Bw \), with \( w \in \mathbb{R}^{n_\omega} \) a random vector, have been used in several areas \[3, 12, 13, 7\]. In this section, we introduce the concept of simultaneous optimized sources and detectors to improve the rate of convergence of the optimization and the quality of the inverse solution.

3.1. A Stochastic Optimization Approach. To recast (2.5)–(2.6) as a stochastic optimization problem, we first write the residual in matrix form. For a single frequency, we get
\[
R(p) = [r_1(p) \ r_2(p) \cdots \ r_{n_\omega}(p)] = C^T A^{-1}(p)B - D,
\]
where the vectors \( r_i \in \mathbb{R}^{n_d} \) are defined in (2.5)\(^2\), and the columns of \( D = [d_1, \cdots, d_{n_\omega}] \) are the measurements corresponding to source \( b_i \). We have
\[
\min_p \| r(p) \|^2 = \min_p \sum_{j=1}^{n_\omega} \| C^T A^{-1}(p)b_j - d_j \|^2 = \min_p \| C^T A^{-1}(p)B - D \|^2. \quad (3.2)
\]
Each evaluation of the objective function requires solving \( n_\omega \cdot n_\omega \) linear systems. Haber et al. \[7\] reduce this cost using simultaneous random sources combined with (stochastic) trace estimators, following Hutchinson \[9\].

\(^2\)For multiple frequencies, we need to compute the residual for each frequency,
\[
[R(\omega_1, p) \ R(\omega_2, p) \cdots] = [C^T A^{-1}(\omega_1, p)B - D_1 \ C^T A^{-1}(\omega_2, p)B - D_2 \cdots].
\]
Let \( \mathbf{w} \) be a random vector with mean \( \mathbf{0} \) and identity covariance matrix, and let \( \mathbb{E} \) denote the expected value with respect to the random vector \( \mathbf{w} \). Then
\[
\mathbb{E}(\mathbf{w}^T \mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p})\mathbf{w}) = \text{trace}(\mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p})) = ||\mathbf{R}(\mathbf{p})||^2_F.
\]
As a particular choice, let each component of \( \mathbf{w} \) be independently and identically distributed (i.i.d) taking values from \( \{-1, +1\} \) with probability \( \frac{1}{2} \). Then, as shown in \cite{9}, \( \mathbf{w}^T \mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p})\mathbf{w} \) is a minimum variance and unbiased estimator of the trace of \( \mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p}) \). Thus, the nonlinear least squares problem can be written as a stochastic minimization problem
\[
\min_{\mathbf{p}} ||\mathbf{R}(\mathbf{p})||^2_F = \min \text{trace} \mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p}) = \min_{\mathbf{p}} \mathbb{E}(\mathbf{w}^T \mathbf{R}(\mathbf{p})^T \mathbf{R}(\mathbf{p})\mathbf{w}). \tag{3.3}
\]
For a random vector \( \mathbf{w} \) and simultaneous random source \( \mathbf{Bw} \), we have
\[
\mathbf{R}(\mathbf{p})\mathbf{w} = (\mathbf{C}^T \mathbf{A}^{-1}(\mathbf{p}) \mathbf{B} - \mathbf{D})\mathbf{w} = \mathbf{C}^T \mathbf{A}^{-1}(\mathbf{p}) \mathbf{Bw} - \mathbf{Dw}. \tag{3.4}
\]
So, computing \( ||\mathbf{R}(\mathbf{p})\mathbf{w}||^2_F \) requires a single PDE solve rather than \( n_s \) solves, which drastically reduces the cost of a function evaluation.

In contrast to the approach in \cite{7}, we use a Newton-type method, so we also need to reduce the cost of Jacobian evaluations. Therefore, we propose a variation that also drastically reduces the cost of computing \( \mathbf{A}^{-T}(\mathbf{p}) \mathbf{C} \) for the Jacobian.

Let \( \mathbf{v} \in \mathbb{R}^{n_d} \) and \( \mathbf{w} \in \mathbb{R}^{n_s} \) with all components i.i.d uniformly from \( \{-1, +1\} \). Then,
\[
\mathbb{E}[(\mathbf{v}^T \mathbf{Rw})^2] = \mathbb{E} \left[ \left( \sum_{i=1}^{n_s} \sum_{j=1}^{n_d} v_i R_{ij} w_j \right)^2 \right] = \mathbb{E} \left[ \left( \sum_{j=1}^{n_s} \sum_{i=1}^{n_d} v_i R_{ij} w_j \right) \left( \sum_{k=1}^{n_s} \sum_{\ell=1}^{n_d} v_k R_{k\ell} w_{\ell} \right) \right] \nonumber \nonumber \nonumber
\]
\[
= \sum_{j,\ell=1}^{n_s} \sum_{i,k=1}^{n_d} R_{ij} R_{k\ell} \mathbb{E}[v_i v_j v_k w_{\ell}]. \tag{3.5}
\]
Since all components of \( \mathbf{v} \) and \( \mathbf{w} \) are independent and
\[
\mathbb{E}[v_i v_k] = \begin{cases} 0, & i \neq k \quad \text{and} \quad \mathbb{E}[w_j w_{\ell}] = \begin{cases} 0, & j \neq \ell \\ 1, & j = \ell, \end{cases} \end{cases}, \tag{3.6}
\]
we have
\[
\mathbb{E}[(\mathbf{v}^T \mathbf{Rw})^2] = \sum_{j,\ell=1}^{n_s} \sum_{i,k=1}^{n_d} R_{ij} R_{k\ell} \mathbb{E}[v_i v_k] \mathbb{E}[w_j w_{\ell}] = \sum_{j=1}^{n_s} \sum_{i=1}^{n_d} R_{ij}^2 = ||\mathbf{R}||_F^2. \tag{3.7}
\]

**Theorem 3.1.** Let \( \mathbf{W} \in \mathbb{R}^{n_s \times \ell_s}, \mathbf{V} \in \mathbb{R}^{n_d \times \ell_d}, \) and let all components of \( \mathbf{V} \) and \( \mathbf{W} \) be i.i.d uniformly from \( \{-1, +1\} \). Let \( \mathbf{R} \in \mathbb{R}^{n_d \times n_s} \). Then
\[
\frac{1}{\ell_s \ell_d} \mathbb{E}\left[||\mathbf{V}^T \mathbf{R} \mathbf{W}||^2_F\right] = ||\mathbf{R}||_F^2. \tag{3.8}
\]

**Proof.** The proof follows directly from the derivations above. \( \square \)
We typically need multiple \( \mathbf{w}_j \) and \( \mathbf{v}_j \) vectors to make the variance in our stochastic estimates sufficiently small. Hence, let

\[
\mathbf{W} = (\mathbf{w}_1 \mathbf{w}_2 \cdots \mathbf{w}_\ell),
\]

with \( \ell_s \ll n_s \), and replace the sources \( \mathbf{B} \) by simultaneous random sources \( \mathbf{BW} \). Similarly, let

\[
\mathbf{V} = (\mathbf{v}_1 \mathbf{v}_2 \cdots \mathbf{v}_\ell),
\]

with \( \ell_d \ll n_d \), and replace the detectors \( \mathbf{C} \) by simultaneous random detectors \( \mathbf{CV} \). So, given these simultaneous random sources and detectors, we have

\[
\frac{1}{\ell_s \ell_d} \min_{\mathbf{p}} \mathbb{E} \left[ \| \mathbf{V}^T \mathbf{R}(\mathbf{p}) \mathbf{W} \|^2_F \right] = \min_{\mathbf{p}} \| \mathbf{R}(\mathbf{p}) \|^2_F.
\]

Since TREGS has proven very effective for the nonlinear least squares problem in DOT with PaLS, we continue to use the TREGS algorithm in the stochastic minimization problem (3.11). We derive the least squares problem used in TREGS to compute a regularized Gauss-Newton update for the stochastic problem as follows. For any \( \mathbf{p} \),

\[
\| \mathbf{V}^T \mathbf{R}(\mathbf{p}) \mathbf{W} \|^2_F = \| (\mathbf{W}^T \otimes \mathbf{V}^T) \mathbf{r}(\mathbf{p}) \|^2_F.
\]

Using a first order approximation to \( \mathbf{r}(\mathbf{p} + \delta) \) gives

\[
(\mathbf{W}^T \otimes \mathbf{V}^T) \mathbf{r}(\mathbf{p} + \delta) \approx (\mathbf{W}^T \otimes \mathbf{V}^T) (\mathbf{r}(\mathbf{p}) + \mathbf{J} \delta),
\]

which leads to the least squares problem

\[
(\mathbf{W}^T \otimes \mathbf{V}^T) \mathbf{J} \delta \approx - (\mathbf{W}^T \otimes \mathbf{V}^T) \mathbf{r}(\mathbf{p}),
\]

instead of \( \mathbf{J} \delta \approx - \mathbf{r}(\mathbf{p}) \) as in (2.9). Note that setting up the least squares problem (3.13) does not require any computations beyond \( \mathbf{A}(\mathbf{p})^{-1} (\mathbf{BW}) \) and \( \mathbf{A}(\mathbf{p})^{-T} (\mathbf{CV}) \).

Two approaches to stochastic optimization are commonly used [15]. One approach, stochastic approximation (SA), uses a new random vector (or small set of random vectors) in each optimization step. The other approach, sample average approximation (SAA), uses a fixed set of random vectors over multiple (or many) optimization steps. We have experimented with both approaches, and the SAA approach seems to work better for our application. Hence, we use the SAA approach [15] to solve the stochastic problem (3.11). The SAA approach approximates (3.11) by the sample average problem. At each iteration, this approach requires solving only \( \ell_s + \ell_d \) linear systems for each frequency to estimate the objective function and the Jacobian rather than \( n_s + n_d \).

We give two representative solutions for our problem using the SAA approach in Figure 3.1. For DOT, the use of simultaneous random sources and detectors initially leads to good progress. However, later in the iteration the convergence slows down, and in many cases, for our problem, it does not lead to sufficiently accurate solutions. With the SAA approach, optimization (typically) does not reach the noise level. The standard optimization using all sources and all detectors does converge to the noise level. We will demonstrate this in section 4. In the next section, we provide a solution to this problem.
Fig. 3.1: Reconstruction of a test anomaly on $201 \times 201$ mesh with 32 sources, 32 detectors, using only the zero frequency.

(a) Initial configuration with 25 basis functions arranged in a $5 \times 5$ grid where 12 basis functions have positive expansion factors (visible as high absorption regions) and 13 basis functions have negative expansion factors (invisible). (b) True shape of the anomaly. (c) Reconstruction using the full order model. (d) and (e) are two reconstruction results using simultaneous random sources and detectors with $\ell_s = \ell_d = 10$.

3.2. Improving the Randomized Approach. In the standard SAA approach, when convergence slows down or a minimum is found for the chosen sample (but not for the true problem), we choose a new set of random simultaneous sources and detectors (a new sample) to improve the solution. However, for our problem this approach leads to slow convergence. We note that the (worst case) convergence rate for these stochastic methods is typically $O(N^{-1/2})$. Hence, after exploiting the relatively fast initial convergence for our problem, we want to avoid stagnation of convergence in the next phase. One approach is to add additional random simultaneous sources and detectors, that is, increasing the sample size, as proposed in [14] with good results. However, this requires progressively more, expensive solves. Therefore, for efficiency, we choose to keep the number of simultaneous sources and detectors fixed. To improve convergence, we exploit the (often fairly good) approximate solution after reaching a modest intermediate tolerance to obtain simultaneous sources and detectors that are optimized for convergence of the nonlinear least squares problem. We make this precise below.

The nonlinear least squares algorithm TREGS focuses on the dominant singular values of the Jacobian to compute good updates to the parameter vector [5]. The corresponding right singular vectors capture the directions in parameter space of largest sensitivity in the objective function. Hence, we want to update $W$ and $V$ so as to capture the largest singular values in $J$ while respecting the Kronecker product structure in (3.13). This is important for two reasons. (1) For the same (fixed) small number
of simultaneous sources and detectors, this gives us locally (at the current \( \mathbf{p} \)) the best approximation to what TREGS would do using all sources and detectors. (2) The directions corresponding to the dominant right singular vectors are best informed by the data. So, when a chosen intermediate tolerance is reached, our method computes the full Jacobian \( \mathbf{J} \) once and replaces the least effective directions in the \( \text{Range}(\mathbf{W}) \) and \( \text{Range}(\mathbf{V}) \) by directions that maximize

\[
||((\hat{\mathbf{W}}^T \otimes \hat{\mathbf{V}}^T)\mathbf{J})||^2_F,
\]

for the updated \( \hat{\mathbf{W}} \) and \( \hat{\mathbf{V}} \) (but with the same number of columns). This procedure can be carried out periodically or for a sequence of prescribed tolerances, but in our experiments it never needs to be done more than once.

For simplicity, the following discussion assumes that \( \mathbf{W} \in \mathbb{R}^{n_s \times \ell_s} \) and \( \mathbf{V} \in \mathbb{R}^{n_d \times \ell_d} \) have orthonormal columns. In our implementation, the length of the columns is \( n_s^{1/2} \) for \( \mathbf{W} \) and \( n_d^{1/2} \) for \( \mathbf{V} \), but as the columns in each matrix have equal norm, this has no effect on the analysis (and the issue could be remedied trivially by scaling all columns first). In addition, the columns of \( \mathbf{W} \) and \( \mathbf{V} \) are only orthogonal in expectation; \( \mathbf{E}(\mathbf{w}_j^T \mathbf{w}_i) = 0 \). However, for \( \ell_s \ll n_s \) and \( \ell_d \ll n_d \) the columns are close to orthogonal, and it appears that in practice the assumption (simplification) does not impact the effectiveness of our approach.

We want to update \( \mathbf{W} \) and \( \mathbf{V} \) to obtain \( \hat{\mathbf{W}} \in \mathbb{R}^{n_s \times \ell_s} \) and \( \hat{\mathbf{V}} \in \mathbb{R}^{n_d \times \ell_d} \) such that (3.14) is (approximately) maximized. There are several ways to do this. Since \( \hat{\mathbf{W}} \) and \( \hat{\mathbf{V}} \) would only be optimal at the current \( \mathbf{p} \), we choose to replace only a few components in the spaces spanned by the columns of \( \mathbf{W} \) and \( \mathbf{V} \). In practice, this seems to be sufficient. We provide some experimental results regarding the number of updated directions in section 4. In the remainder of this section, we first discuss downdating \( \mathbf{W} \) and \( \mathbf{V} \) and then updating \( \mathbf{W} \) and \( \mathbf{V} \).

**Removing Simultaneous Random Sources and Detectors.** We first consider truncating \( \mathbf{V}^{n_d \times \ell_d} \) to \( \hat{\mathbf{V}}^{n_d \times (\ell_d-s)} \) such that \( \text{Range}(\mathbf{V}) \subset \text{Range}(\hat{\mathbf{V}}) \) and \( ||(\mathbf{W}^T \otimes \hat{\mathbf{V}}^T)\mathbf{J})||^2_F \) is maximum. This is equivalent to the following optimization problem. Let \( S = \{ \mathbf{\Theta} \in \mathbb{R}^{d \times (\ell_d-s)} | \mathbf{\Theta}^T \mathbf{\Theta} = \mathbf{I} \} \) and \( \hat{\mathbf{V}} = \mathbf{V}_0 \). We want to find \( \mathbf{\Gamma} \) such that

\[
\mathbf{\Gamma} = \arg \max_{\mathbf{\Theta} \in S} ||(\mathbf{W}^T \otimes (\mathbf{V}_0^T)\mathbf{J})||^2_F.
\]

To solve (3.15) we need a variation of the min-max characterization of singular values.

**Lemma 3.2.** Let \( \mathbf{X} \in \mathbb{C}^{m \times n} \), let \( k \leq \min(m,n) \), and let \( T = \{ \mathbf{\Theta} \in \mathbb{C}^{m \times k} | \mathbf{\Theta}^* \mathbf{\Theta} = \mathbf{I} \} \). Furthermore, let the SVD of \( \mathbf{X} \) be given by \( \mathbf{X} = \mathbf{U} \Sigma \mathbf{Y}^* \) with \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_k \), \( \mathbf{U}_k = [\mathbf{u}_1 \mathbf{u}_2 \ldots \mathbf{u}_k] \) (the first \( k \) columns of \( \mathbf{U} \)) and \( \mathbf{Y}_k = [\mathbf{y}_1 \mathbf{y}_2 \ldots \mathbf{y}_k] \). Then

\[
\sum_{j=1}^{k} \sigma_j^2 = \max_{\mathbf{Z} \in T} ||\mathbf{Z}^* \mathbf{X}||^2_F,
\]

\[
\mathbf{U}_k = \arg \max_{\mathbf{Z} \in T} ||\mathbf{Z}^* \mathbf{X}||^2_F.
\]

Furthermore, any \( \tilde{\mathbf{U}}_k \in T \) with orthonormal columns such that \( \text{Range}(\mathbf{U}_k) = \text{Range}(\tilde{\mathbf{U}}_k) \) also solves (3.17).
Proof. Let \( Z \in T \), define the SVD \( Z^*X = \Phi \Omega \Psi^* \), and let \( \Psi_k = [\psi_1 \psi_2 \ldots \psi_k] \). Then

\[
\|Z^*X\|_F^2 = \sum_{j=1}^k \omega_j^2 = \|Z^*X\psi_k\|_F^2 \leq \sum_{j=1}^k \sigma_i^2,
\]

where the last inequality follows from Lemma 3.3.1 in [8]. However, for \( Z = U_k \) equality is obtained since \( U_k^*X = \text{diag}(\sigma_1,\ldots,\sigma_k)Y_k^* \). (Note that this choice for \( Z \) would give \( \Psi_k = Y_k \) up to non-uniqueness of the SVD.) □

The only complication in (3.15) now is the Kronecker structure of \( (W^T \otimes (V\tilde{\Gamma}))^T \), which we can remove by combining \( W \) and \( J \). For ease of exposition, we first consider a single simultaneous source \( \mathbf{w} \) and \( \ell_d \) simultaneous detectors. With \( J_{jk} \in \mathbb{R}^{n_d \times d} \) given by (2.8), and \( \mathbf{w}_i \) the \( i \)th component of \( \mathbf{w} \), we have

\[
\left[ w^T \otimes \tilde{V}^T \right] J = \left[ \begin{array}{cccc} w_1 \bar{v}_1^T & w_2 \bar{v}_1^T & \cdots & w_n \bar{v}_1^T \\ \vdots & \vdots & \ddots & \vdots \\ w_1 \bar{v}_{\ell_d-s}^T & w_2 \bar{v}_{\ell_d-s}^T & \cdots & w_n \bar{v}_{\ell_d-s}^T \end{array} \right] \left[ \begin{array}{cccc} J_{1,1} & J_{1,2} & \cdots & J_{1,n_p} \\ J_{2,1} & J_{2,2} & \cdots & J_{2,n_p} \\ \vdots & \vdots & \ddots & \vdots \\ J_{n_s,1} & J_{n_s,2} & \cdots & J_{n_s,n_p} \end{array} \right] = \left[ \begin{array}{c} \bar{v}_1^T \\ \vdots \\ \bar{v}_{\ell_d-s}^T \end{array} \right] \left[ \begin{array}{c} \mathbf{w} * J_1 \\ \mathbf{w} * J_2 \\ \vdots \\ \mathbf{w} * J_{n_p} \end{array} \right],
\]

(3.18)

where, for the vector \( \mathbf{w} \) and column \( J_k \), we define

\[
\mathbf{w} * J_k = w_1 J_{1,k} + w_2 J_{2,k} + \cdots + w_n J_{n_s,k} \quad \text{for } k = 1,2,\ldots,n_p.
\]

(3.19)

Furthermore, we define

\[
\hat{J} = \mathbf{w} * J = [\mathbf{w} * J_1 \mathbf{w} * J_2 \ldots \mathbf{w} * J_{n_p}].
\]

(3.20)

Using (3.20) and \( \tilde{V} = V\tilde{\Gamma} \), we can simplify (3.18),

\[
\left[ w^T \otimes \tilde{V}^T \right] J = \tilde{V}^T \hat{J} = \Gamma^T V^T \tilde{\Gamma},
\]

and as a result (3.15) reduces to

\[
\Gamma = \arg \max_{\Gamma \in S} \|\tilde{\Gamma}^T \tilde{V}^T \hat{J}\|^2_F.
\]

(3.21)

The solution of (3.21) follows directly from Lemma 3.2. Hence we have the following theorem.

**Theorem 3.3.** Let \( J \) and \( J_{j,k} \) be defined by (2.7) and (2.8) respectively, let \( \hat{J} \) be defined as in (3.20) for a single simultaneous source \( \mathbf{w} \), and let \( \mathbf{V} \in \mathbb{R}^{n_d \times \ell_d} \) have orthonormal columns. Furthermore, let

\[
\mathbf{V}^T \hat{J} = \Phi \Omega \Psi^T.
\]

(3.22)

Then the solution to (3.15) for a single simultaneous source is given by

\[
\Gamma = [\phi_1 \phi_2 \ldots \phi_{\ell_d-s}].
\]

(3.23)
Proof. The proof follows from (3.18), (3.20), and Lemma 3.2. □

Next we consider the general case of (3.15), that is, for multiple simultaneous sources. Using (3.18), we have
\[
\begin{bmatrix}
W^T \otimes \tilde{V}^T
\end{bmatrix} J = \begin{bmatrix}
w_1^T \otimes \tilde{V}_1^T \\
w_2^T \otimes \tilde{V}_2^T \\
\vdots \\
w_{\ell_s}^T \otimes \tilde{V}_{\ell_s}^T
\end{bmatrix} = \begin{bmatrix}
\tilde{V}_1^T \tilde{J}_1 \\
\tilde{V}_2^T \tilde{J}_2 \\
\vdots \\
\tilde{V}_{\ell_s}^T \tilde{J}_{\ell_s}
\end{bmatrix},
\]
where the matrices \(\tilde{J}_i\) are defined as
\[
\tilde{J}_i = w_i \ast J \quad \text{for} \quad i = 1, \ldots, \ell_s. \quad \text{(cf. (3.20))}
\]

**Theorem 3.4.** Let \(J\) be defined by (2.7), let \(\tilde{J}_k\) be defined as in (3.25), and let \(W \in \mathbb{R}^{n_s \times \ell_s}\) and \(V \in \mathbb{R}^{n_d \times \ell_d}\) have orthonormal columns. Furthermore, define the SVD
\[
V^T \begin{bmatrix}
\tilde{J}_1 \\
\tilde{J}_2 \\
\vdots \\
\tilde{J}_{\ell_s}
\end{bmatrix} = \Phi \Omega \Psi^T.
\]
Then the solution to (3.15) is given by
\[
\Gamma = [\varphi_1 \varphi_2 \ldots \varphi_{\ell_d-s}].
\]

Proof. The proof mostly follows the proof of Theorem 3.3.

\[
\| (W^T \otimes \tilde{V}^T) J \|_F^2 = \left\| \begin{bmatrix}
\tilde{V}_1^T \tilde{J}_1 \\
\tilde{V}_2^T \tilde{J}_2 \\
\vdots \\
\tilde{V}_{\ell_s}^T \tilde{J}_{\ell_s}
\end{bmatrix} \right\|_F^2 = \left\| \tilde{V}^T \begin{bmatrix}
\tilde{J}_1 \\
\tilde{J}_2 \\
\vdots \\
\tilde{J}_{\ell_s}
\end{bmatrix} \right\|_F^2 = \left\| \Gamma^T V^T \begin{bmatrix}
\tilde{J}_1 \\
\tilde{J}_2 \\
\vdots \\
\tilde{J}_{\ell_s}
\end{bmatrix} \right\|_F^2,
\]
which puts the problem in the form of Lemma 3.2. Hence the solution is given by (3.27). □

Next, consider truncating \(W_n \times \ell_s\) to \(\tilde{W}_n \times (\ell_s-s)\) such that \(\text{Range}(\tilde{W}) \subset \text{Range}(W)\) and \(\| (\tilde{W}^T \otimes \tilde{V}^T) J \|_F^2\) is maximized. This is equivalent to the following optimization problem. Let \(S = \{ \Theta \in \mathbb{R}^{\ell_s \times (\ell_s-s)} | \Theta^T \Theta = I \}\) and \(\tilde{W} = W \Gamma\). We want to find \(\Gamma\) such that
\[
\Gamma = \arg \max_{\Gamma \in S} \| (\tilde{W} \Gamma)^T \otimes \tilde{V}) J \|_F^2.
\]

We combine \(V\) and \(J\) to remove the Kronecker structure. For ease of exposition, we first consider \(\ell_s\) simultaneous sources and a single simultaneous detector \(v\).

\[
\begin{bmatrix}
\tilde{W}^T \otimes v^T
\end{bmatrix} J = \begin{bmatrix}
\tilde{W}_1^T \otimes v^T \\
\tilde{W}_2^T \otimes v^T \\
\vdots \\
\tilde{W}_{\ell_s-s}^T \otimes v^T
\end{bmatrix} = \tilde{W}^T \begin{bmatrix}
v^T J_{1,1} & v^T J_{1,2} & \ldots & v^T J_{1,n_p} \\
v^T J_{2,1} & v^T J_{2,2} & \ldots & v^T J_{2,n_p} \\
\vdots & \vdots & \ddots & \vdots \\
v^T J_{n_s,1} & v^T J_{n_s,2} & \ldots & v^T J_{n_s,n_p}
\end{bmatrix} = \tilde{W}^T J,
\]

(3.30)
where we define, for convenience and later use, the notation
\[ \tilde{J} = v \odot J = \begin{bmatrix} v^T J_{1,1} & v^T J_{1,2} & \cdots & v^T J_{1,n_p} \\ v^T J_{2,1} & v^T J_{2,2} & \cdots & v^T J_{2,n_p} \\ \vdots & \vdots & \ddots & \vdots \\ v^T J_{n_s,1} & v^T J_{n_s,2} & \cdots & v^T J_{n_s,n_p} \end{bmatrix}. \] (3.31)

We now define for multiple detectors
\[ \tilde{J}_k = v_k \odot J \quad \text{for} \quad k = 1, \ldots, \ell_d. \] (3.32)

Hence, we obtain
\[ \begin{bmatrix} \tilde{W}^T \otimes V^T \end{bmatrix} = \begin{bmatrix} \tilde{W}^T J_1 \\ \tilde{W}^T J_2 \\ \vdots \\ \tilde{W}^T J_{\ell_d} \end{bmatrix}. \]

**Theorem 3.5.** Let \( J \) be defined by (2.7), let \( \tilde{J}_k \) be defined as in (3.31) and (3.32), and let \( W \in \mathbb{R}^{n_s \times \ell_s} \) and \( V \in \mathbb{R}^{n_d \times \ell_d} \) have orthonormal columns. Furthermore, define the SVD
\[ W^T \left[ \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_d} \right] = \Phi \Omega \Psi^T. \] (3.33)

Then the solution to (3.29) is given by
\[ \Gamma = [\varphi_1 \varphi_2 \ldots \varphi_{\ell_s-s}]. \] (3.34)

**Proof.** We use the definition of the Frobenius norm to put the problem in the form of Lemma 3.2.

\[ \| (W^T \otimes V^T) J \|_F^2 = \left\| \begin{bmatrix} \tilde{W}^T J_1 \\ \tilde{W}^T J_2 \\ \vdots \\ \tilde{W}^T J_{\ell_d} \end{bmatrix} \right\|_F^2 = \left\| W^T \left[ \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_d} \right] \right\|_F^2 = \left\| \Gamma_2^T W^T \left[ \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_d} \right] \right\|_F^2. \]

Therefore, the solution is given by (3.34). \( \Box \)

**Adding Simultaneous Optimized Sources and Detectors.** Next, we consider extending \( V_{n_d \times \ell_d} \) to \( V_{n_d \times (\ell_d+s)} \) in directions that orthogonal to the current space \( V \) such that \( \| (W^T \otimes V^T) J \|_F^2 \) is maximized. This is equivalent to the following optimization problem. Let \( S = \{ \Theta \in \mathbb{R}^{n_d \times s} \mid \Theta^T \Theta = I \} \), \( Q_s = [q_1 q_2 \ldots q_s] \) such that \( Q_s = V_c \Gamma \), and \( [V V_c] \) is orthogonal. We want to find \( \Gamma \in S \) such that
\[ \Gamma = \arg \max_{\Gamma \in S} \| (W^T \otimes \left[ V V_c \tilde{\Gamma}^T \right]) J \|_F^2. \] (3.35)
Combining \( \mathbf{W} \) and \( \mathbf{J} \) using \( \hat{\mathbf{J}}_i = \mathbf{w}_i \ast \mathbf{J} \), see (3.25), we get

\[
\begin{bmatrix}
\mathbf{w}_1^T \otimes \mathbf{V}_1^T \\
\mathbf{w}_1^T \otimes \hat{\mathbf{q}}_1^T \\
\vdots \\
\mathbf{w}_\ell^T \otimes \mathbf{V}_1^T \\
\mathbf{w}_\ell^T \otimes \hat{\mathbf{q}}_1^T \\
\vdots \\
\mathbf{w}_\ell^T \otimes \hat{\mathbf{q}}_s^T
\end{bmatrix}\mathbf{J} = 
\begin{bmatrix}
\mathbf{V}_1^T \\
\hat{\mathbf{q}}_1^T \\
\vdots \\
\mathbf{q}_1^T \\
\vdots \\
\hat{\mathbf{q}}_s^T
\end{bmatrix}[\mathbf{w}_1 \ast \mathbf{J} \; \mathbf{w}_2 \ast \mathbf{J} \; \cdots \; \mathbf{w}_\ell \ast \mathbf{J}]^T
\] = \[\mathbf{V}_1^T [\hat{\mathbf{J}}_1 \; \hat{\mathbf{J}}_2 \; \cdots \; \hat{\mathbf{J}}_s] \]_F^2 + \parallel \mathbf{Q}_s^T [\hat{\mathbf{J}}_1 \; \hat{\mathbf{J}}_2 \; \cdots \; \hat{\mathbf{J}}_s] \parallel^2_F.
\]

(3.36)

Since the first term is fixed, we maximize the second term in (3.36). Taking \( \mathbf{Q}_s = \mathbf{V}_c\Gamma \), we get

\[
\Gamma = \arg \max_{\Gamma \in \mathcal{S}} \parallel \mathbf{V}_c^T [\hat{\mathbf{J}}_1 \; \hat{\mathbf{J}}_2 \; \cdots \; \hat{\mathbf{J}}_s] \parallel^2_F.
\]

(3.37)

The solution of (3.37) now follows from Lemma 3.2.

**Theorem 3.6.** Let \( \mathbf{J} \) be defined by (2.7) and (2.8), let \( \hat{\mathbf{J}}_k \) be defined as in (3.25) and let \( \mathbf{W} \in \mathbb{R}^{n_s \times \ell} \) and \( \mathbf{V} \in \mathbb{R}^{n_d \times \ell_d} \) have orthonormal columns and \( [\mathbf{V} \; \mathbf{V}_c] \) be orthogonal. Furthermore, let

\[
\mathbf{V}_c^T [\hat{\mathbf{J}}_1 \; \hat{\mathbf{J}}_2 \; \cdots \; \hat{\mathbf{J}}_s] = \Phi \Omega \Psi^T.
\]

(3.38)

Then the solution to (3.35) is given by

\[
\Gamma = [\varphi_1 \; \varphi_2 \; \cdots \; \varphi_s].
\]

(3.39)

**Proof.** The proof follows directly from (3.36) and (3.37), and Lemma 3.2. \( \square \)

The final derivation we discuss is to add simultaneous optimized sources. Consider extending \( \mathbf{W}^{n_s \times \ell} \) to \( \mathbf{W}^{n_s \times (\ell+s)} \) so that \( (\mathbf{W}^T \otimes \mathbf{V})^T \mathbf{J} \parallel^2_F \) is maximized. This is equivalent to the following optimization problem. Let \( \mathcal{S} = \{ \Theta \in \mathbb{R}^{n_s \times s} \mid \Theta^T \Theta = \mathbf{I} \} \) and \( \mathbf{Q}_s = [\bar{\mathbf{q}}_1 \; \bar{\mathbf{q}}_2 \cdots \bar{\mathbf{q}}_s] \) such that \( \mathbf{Q}_s = \mathbf{V}_c \Gamma \) where \( [\mathbf{W} \; \mathbf{W}_c] \) is orthogonal. We want to find \( \Gamma \in \mathcal{S} \) such that

\[
\Gamma = \arg \max_{\Gamma \in \mathcal{S}} \parallel (\mathbf{W} \; \mathbf{W}_c \Gamma^T \otimes \mathbf{V})^T \mathbf{J} \parallel^2_F.
\]

(3.40)
Combining \( V \) and \( J \) using \( \tilde{J}_k = v_k \otimes J \), see (3.32), we get

\[
\begin{bmatrix}
\| W^T \otimes V^T \|_F^2 \\
\| \tilde{q}_1^T \otimes V^T \|_F^2 \\
\vdots \\
\| \tilde{q}_s^T \otimes V^T \|_F^2
\end{bmatrix} J = \begin{bmatrix}
W^T \\
\tilde{q}_1^T \\
\vdots \\
\tilde{q}_s^T
\end{bmatrix} \begin{bmatrix}
\tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_s}
\end{bmatrix}.
\]

\[
= \| W^T \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_s} \|_F^2 + \| \tilde{Q}_s^T \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_d} \|_F^2.
\]

(3.41)

Since the first term is fixed, we maximize the second term in (3.41). Taking \( \tilde{Q}_s = W_c \Gamma \), we get

\[
\Gamma = \arg \max_{\Gamma \in \mathcal{S}} \| \tilde{W}_c^T \tilde{J}_1 \tilde{J}_2 \ldots \tilde{J}_{\ell_d} \|_F^2.
\]

(3.42)

The solution of (3.42) follows from Lemma 3.2.

**Theorem 3.7.** Let \( J \) be defined by (2.7) and (2.8), let \( \tilde{J}_k \) be defined as in (3.31) and (3.32), and let \( W \in \mathbb{R}^{n_s \times \ell_s} \) and \( V \in \mathbb{R}^{n_d \times \ell_d} \) have orthonormal columns and \([W \ W_c]\) be orthogonal. Furthermore, let

\[
W_c^T \begin{bmatrix}
\tilde{J}_1 \\
\tilde{J}_2 \\
\vdots \\
\tilde{J}_{\ell_d}
\end{bmatrix} = \Phi \Omega \Psi^T.
\]

(3.43)

Then the solution to (3.40) is given by

\[
\Gamma = [\varphi_1 \varphi_2 \ldots \varphi_s].
\]

(3.44)

**Proof.** The proof follows directly from (3.41), (3.42) and Lemma 3.2. \( \square \)

**3.3. Implementation.** We outline the efficient computation of several critical parts of the algorithm.

**3.3.1. Computation of the residual and Jacobian.** We estimate the norm of the residual using

\[
(W^T \otimes V^T) r(p) = \begin{bmatrix}
V^T C^T A^{-1}(p) B w_1 - D w_1 \\
\vdots \\
V^T C^T A^{-1}(p) B w_{\ell_s} - D w_{\ell_s}
\end{bmatrix} = \begin{bmatrix}
V^T C^T z_1 - D w_1 \\
\vdots \\
V^T C^T z_{\ell_d} - D w_{\ell_d}
\end{bmatrix},
\]

(3.45)

where we solve \( A(p) z_i = B w_i \) for \( z_i, i = 1 \ldots \ell_s \). This reduces the number of large solves from \( n_s \) to \( \ell_s \) per frequency. To compute the Jacobian, we solve the systems, \( A^T(p) y_j = C v_j \) for \( y_j, j = 1 \ldots \ell_d \). This reduces the additional number of large solves from \( n_d \) to \( \ell_d \) per frequency. We can use iterative solvers or direct sparse solvers depending on the size of the system [10]. To obtain the \( k \)-th column of \( (W^T \otimes V^T) J \), we compute

\[
\begin{bmatrix}
y_1^T \frac{\partial A(p)}{\partial p_k} z_1 \\
y_2^T \frac{\partial A(p)}{\partial p_k} z_1 \\
\vdots \\
y_{\ell_d}^T \frac{\partial A(p)}{\partial p_k} z_1
\end{bmatrix},
\]

(3.46)
where $\frac{\partial A(p)}{\partial p_k}$ is a diagonal matrix if we only invert for absorption. If we also invert for diffusion, this matrix has 5 (in 2D) or 7 (in 3D) diagonals. Moreover, after a few iterations, the changes in $A(p)$ are highly localized, and $\frac{\partial A(p)}{\partial p_k}$ contains mostly zero coefficients; see [4]. In that case, we first find the few nonzero components of $\frac{\partial A(p)}{\partial p_k}$ for each $k$, and the corresponding nonzeros in $z_i$ and $y_j$. Then, compute $y_i^T \frac{\partial A(p)}{\partial p_k} z_j$ exploiting the fact that there are few nonzero components in $\frac{\partial A(p)}{\partial p_k} z_j$.

3.3.2. Replacing Simultaneous Random Sources and Detectors by Simultaneous Optimized Sources and Detectors. Given the general discussion in section 3.2, replacing simultaneous random sources and detectors by optimized sources and detectors can be done in several ways. Experiments suggest that using a two-phase alternating approach gives good reconstruction results. In phase one, we alternately remove one source, then one detector, and so on. In phase two, we alternately add one source, then one detector, and so on. This choice requires the SVD of four small matrices. The sizes of these matrices are given in Table 3.1. The cost of these computations is negligible compared with the solution of many large PDEs. Therefore, the main cost of our algorithm is the number of PDE solves for the function and Jacobian evaluations. Section 4 includes a detailed discussion of the computational cost.

| Method            | Sizes for SVD |
|-------------------|---------------|
| Removing detectors| $\ell_d \times (\ell_s n_p)$ |
| Removing sources  | $\ell_s \times (\ell_d n_p)$ |
| Adding detectors  | $(n_d - (\ell_s - s)) \times (\ell_s - s) n_p$ |
| Adding sources    | $(n_s - (\ell_d - s)) \times (\ell_d - s) n_p$ |

Table 3.1: Sizes of matrices for SVD computations to replace simultaneous random sources and detectors by simultaneous optimized sources and detectors.

4. Numerical Experiments. We discuss three examples to demonstrate the effectiveness of combining simultaneous random sources and detectors with simultaneous optimized sources and detectors. We show that using simultaneous optimized sources and detectors not only produces reconstruction results that are close to those obtained using all sources and all detectors, but it also reduces the computational cost. The experimental set up we use is that described in [4], in which model reduction was proposed as an alternative approach to reduce the cost of the inversion process in DOT.

All experiments are carried out on a 201×201 grid, which yields 40,401 degrees of freedom in the forward model (2.1). The model has 32 sources, 32 detectors, and we use only the zero frequency. For each test case, we construct anomalies in the pixel basis, and we add a small normally distributed random heterogeneity to both the background and to the anomaly to make the medium inhomogeneous. This ensures a modest mismatch between the exact image and the representation we use to reconstruct the image, so that we avoid the so-called ‘inverse crime’. We use this absorption image to compute the true measured data. We also add $\delta = 0.1\%$ white
noise to the measured data which is the same noise level as in [4]. PaLS [1] and TREGS [5] are used to reconstruct the absorption images. Our model has 25 CSRBFs, which leads to 100 parameters (four per 2D basis function) for the nonlinear optimization. We use the same starting guess for each example (see Figure 4.1), with 25 basis functions arranged in a $5 \times 5$ grid, where 12 basis functions have a positive expansion coefficient (visible as high absorption regions) and 13 basis functions have a negative expansion coefficient (invisible).

**Fig. 4.1:** Initial configuration with 25 basis functions arranged in a $5 \times 5$ grid where 12 basis functions have a positive expansion factors (visible) and 13 basis functions have negative expansion factors (invisible).

We use 10 simultaneous random sources and detectors in each example. As discussed in section 3.2, we replace simultaneous random sources and detectors by simultaneous optimized sources and detectors after a chosen intermediate tolerance has been reached. We find that, in general, the noise level $\delta$ is a good choice as the intermediate tolerance ($\|r(p)\|_2^2 = \delta$). Since the PaLS representation regularizes the problem, we consider the problem converged when the squared residual norm falls below $\delta^2$ (the factor $\frac{1}{2}$ in (1.1) is dropped for convenience). We run each experiment for 50 trials. In each trial, the simultaneous random sources and detectors are chosen independently to get representative reconstruction results.

**Example 1.** The true absorption image for Example 1 is given in Figure 4.2a. We report the reconstruction results using simultaneous random sources and detectors and combined with simultaneous optimized sources and detectors in Tables 4.1-4.3. We also include the reconstruction results using all sources and all detectors for comparison (see Figure 4.2b). As can be seen in Figure 4.2c at the intermediate tolerance, SAA gives a good localization of the anomaly; however, there is no further improvement using SAA (see Figure 4.2d).

While initially the SAA estimate is unbiased, bias arises as we optimize for a specific small set of simultaneous random sources and detectors [15]. The algorithm stops prematurely as the bias, a systematic underestimation of the error/misfit [15, Section 5.1.2], makes it appear as if convergence has been reached. This can make a big difference since it is usually the case that substantial improvement in the shape of the anomaly occurs towards the end of the iterative process. Figure 4.5 demonstrates how poor the reconstructions using only the SAA approach can be at the convergence tolerance when underestimation is severe. To make a fair comparison in terms of the number of large systems solved, we solve the full system on the side to check convergence of the SAA approach. Table 4.1 shows that in terms of the true function evaluation, the SAA approach does not reach to the convergence tolerance. Once we replace a few sources and detectors, this is no longer an issue (see Table 4.1). In Table 4.2, we give the average ratio of the number of times when the estimated residual
|            | SAA Approach | Simult Rand & Optimized Src/Det |
|------------|--------------|----------------------------------|
| Iter       | True $\|\mathbf{r}\|_2^2 (\delta^2)$ | Estimated $\|\mathbf{r}\|_2^2 (\delta^2)$ | Iter | True $\|\mathbf{r}\|_2^2 (\delta^2)$ | Estimated $\|\mathbf{r}\|_2^2 (\delta^2)$ |
| Example 1  |       |                                  |       |                                  |                                  |
| 1          | 118980     | 60504                            | 10    | 298.46                           | 313.03                           |
| 7          | 4508.8     | 2943                             | 14    | 166.06                           | 156.42                           |
| 13         | 78.698     | 42.345                           | 16    | 5.951                            | 6.251                            |
| 19         | 1.607      | 1.069                            | 19    | 2.392                            | 2.576                            |
| 20         | 1.735      | 0.845                            | 20    | 0.738                            | 0.806                            |
| Example 2  |       |                                  |       |                                  |                                  |
| 1          | 89777      | 119030                           | 9     | 278.26                           | 554.33                           |
| 6          | 26144      | 31707                            | 13    | 46.7                             | 105.78                           |
| 11         | 278.69     | 432.4                            | 18    | 3.58                             | 7.642                            |
| 17         | 1.9412     | 1.869                            | 21    | 2.838                            | 2.999                            |
| 18         | 1.838      | 0.977                            | 22    | 0.428                            | 0.960                            |
| Example 3  |       |                                  |       |                                  |                                  |
| 1          | 90913      | 30028                            | 9     | 1188.7                           | 1084.7                           |
| 7          | 9017.3     | 2708.3                           | 16    | 292.4                            | 264.67                           |
| 14         | 116.22     | 33.279                           | 21    | 17.268                           | 35.567                           |
| 20         | 2.4558     | 1.1767                           | 26    | 12.522                           | 13.947                           |
| 21         | 1.2917     | 0.9255                           | 27    | 0.128                            | 0.242                            |

Table 4.1: Subset of results for Example 1, 2 and 3. The comparison of the true objective function $\|\mathbf{r}\|_2^2$ and its SAA estimate relative to the stopping criterion $(\delta^2)$ for selected iterations. For the SAA approach, the estimated residual is obtained with 10 simultaneous random sources and detectors. The estimated residual for combining simultaneous random and optimized sources and detectors that we report here are those obtained when replacing 2 random sources and 2 detectors by optimized sources and detectors for Example 1; replacing 1 random source and 1 detector by an optimized source and detector for Example 2; and replacing 3 random sources and 3 detectors by optimized sources and detectors for Example 3.

underestimates the true residual to the total number of iterations using 50 trials for each example. Clearly, there is a large improvement to be gained by replacing a very small number of simultaneous random sources and detectors.

The main purpose of the SAA approach and our modification is to reduce the large number of discretized PDE solves that is necessary for the inversion. In Table 4.3, we give a comparison of the total number of PDE solves for Example 1. Our approach reduces both the computational cost and the number of large-scale linear systems that needs to be solved.

Additionally, combining simultaneous random and simultaneous optimized sources and detectors drastically improves the reconstruction results of the SAA approach. Figure 4.2 also shows that replacing a few random sources and detectors by optimized sources and detectors leads to solutions of the same quality as obtained using all sources and detectors.

**Example 2 and Example 3.** In Example 2, we discuss reconstruction results for an image with multiple anomalies. In Figure 4.3, we show the reconstruction results for combining simultaneous random and simultaneous optimized sources and detectors. The true absorption image is given in Figure 4.3a. We also include the reconstruction result using all sources and all detectors for comparison. The results show similar behavior as was observed in Example 1 for a fixed set of simultaneous random sources and detectors. In Table 4.4, we give the total number of PDE solves.
Fig. 4.2: Results for Example 1. Reconstruction of a test anomaly on $201 \times 201$ mesh with 32 sources and detectors, 25 basis functions, and using only the zero frequency. The SAA approach uses 10 simultaneous random sources and detectors.

(a) True shape of the anomaly. (b) Reconstruction using all sources and all detectors. (c) Reconstruction using SAA approach at intermediate tolerance. (d) Reconstruction using the SAA approach after the maximum iterations. (e) Reconstruction with SAA and replacing 1 simultaneous random source and detector by a simultaneous optimized source and detector. (f) Reconstruction with SAA and replacing 2 simultaneous random sources and detectors by simultaneous optimized sources and detectors. (g) Reconstruction with SAA and replacing 3 simultaneous random sources and detectors by simultaneous optimized sources and detectors.

required for each approach for Example 2.

The true shape of the absorption and the reconstruction results for Example 3 are given in Figure 4.4. We give the total number of PDE solves for each approach in Table 4.5.
| Example 1 | Example 2 | Example 3 |
|-----------|-----------|-----------|
| (m/n)     | (m/n)     | (m/n)     |
| Replacing 1 src/1 det | 9/14 | 9/14 | 7/12 |
| Replacing 2 srcs/2 dets | 7/14 | 6/14 | 5/13 |
| Replacing 3 srcs/3 dets | 4/16 | 4/15 | 2/13 |
| SAA       | 24/28     | 24/28     | 23/28 |

Table 4.2: The average number of times (m) that the estimated residual underestimates the true residual out of the total number of iterations (n) on average for 50 trials to reach the stopping criterion, $\delta^2$.

|             | Iteration Number | Function Evaluations | Jacobian Evaluations | Total PDE Solves | Tol  |
|-------------|------------------|----------------------|----------------------|------------------|------|
| SAA* (intermediate tol) | 9 | 10 | 5 | 150 | $\delta^2$ |
| Replacing 1 src/1 det | 23 | 25 | 12 | 434 | $\delta^2$ |
| Replacing 2 srcs/2 dets | 23 | 25 | 12 | 434 | $\delta^2$ |
| Replacing 3 srcs/3 dets | 25 | 27 | 13 | 464 | $\delta^2$ |
| All srcs/All dets | 71 | 72 | 47 | 3808 | $\delta^2$ |
| SAA** | 28 | 29 | 18 | 470 | $\delta^2$ |
| SAA *** | (92) | (93) | (67) | 1700 | $\delta^2$ |

Table 4.3: Example 1 Results. The total number of iterations, function evaluations, Jacobian evaluations and PDE solves required on average for 50 trials to reach the stopping criterion, $\delta^2$.

* The first row gives the costs to reach the intermediate tolerance for the SAA approach, $\delta$.

** Since the SAA estimate becomes biased and underestimates the objective function, the algorithm stops prematurely.

*** The SAA approach measuring the convergence with the true objective function. Parentheses indicate that the SAA approach does not reach the tolerance.

Fig. 4.3: Results for Example 2. Reconstruction of a test anomaly on 201 × 201 mesh with 32 sources and detectors, 25 basis functions, and using only the zero frequency.

(a) True shape of the anomaly. (b) Reconstruction using all sources and all detectors. (c) Reconstruction with SAA and replacing 1 simultaneous random source and detector by optimized source and detector.
Fig. 4.4: Results for Example 3. Reconstruction of a test anomaly on $201 \times 201$ mesh with 32 sources and detectors, 25 basis functions, and using only the zero frequency. 
(a) True shape of the anomaly. (b) Reconstruction using all sources and all detectors. (c) Reconstruction with SAA and replacing 3 simultaneous random sources and detectors by optimized sources and detectors.

Table 4.4: Example 2 Results. The total number of iterations, function evaluations, Jacobian evaluations and PDE solves required on average for 50 trials to reach the stopping criterion, $\delta^2$.

| Method                     | Iteration Number | Function Evaluations | Jacobian Evaluations | Total PDE Solves | Tol |
|---------------------------|------------------|----------------------|----------------------|------------------|-----|
| SAA (intermediate)        | 9                | 10                   | 5                    | 150              | $\delta$ |
| Replacing 1 src/1 det     | 23               | 25                   | 12                   | 434              | $\delta^2$ |
| Replacing 2 srcs/2 dets   | 23               | 25                   | 12                   | 434              | $\delta^2$ |
| Replacing 3 srcs/3 dets   | 24               | 26                   | 13                   | 454              | $\delta^2$ |
| All srcs/All dets         | 97               | 98                   | 69                   | 5344             | $\delta^2$ |
| SAA*                      | 28               | 29                   | 16                   | 450              | $\delta^2$ |
| SAA**                     | (92)             | (93)                 | (65)                 | 1580             | $\delta^2$ |

* The first row gives the costs to reach the intermediate tolerance for the SAA approach $\delta$. ** Since the SAA estimate becomes biased and underestimates the objective function, the algorithm stops prematurely. *** The SAA approach measuring the convergence with the true objective function. Parentheses indicate that the SAA approach does not reach the tolerance.

Fig. 4.5: Example of poor SAA reconstructions for each test case. Reconstruction of a test anomaly on $201 \times 201$ mesh with 32 sources and detectors, 25 basis functions, and using only the zero frequency.
|                              | Iteration Number | Function Evaluations | Jacobian Evaluations | Total PDE Solves | Tol  |
|------------------------------|------------------|----------------------|----------------------|------------------|------|
| SAA (intermediate)           | 10               | 11                   | 5                    | 160              | $\delta$ |
| Replacing 1 src/1 det        | 22               | 24                   | 11                   | 414              | $\delta^2$ |
| Replacing 2 srcs/2 dets      | 23               | 25                   | 11                   | 424              | $\delta^2$ |
| Replacing 3 srcs/3 dets      | 23               | 25                   | 12                   | 434              | $\delta^2$ |
| All srcs/All dets            | 25               | 26                   | 14                   | 1280             | $\delta^2$ |
| SAA*                         | 28               | 29                   | 16                   | 450              | $\delta^2$ |
| SAA**                        | (96)             | (97)                 | (68)                 | 1650             | $\delta^2$ |

Table 4.5: Example 3 Results. The total number of iterations, function evaluations, Jacobian evaluations and PDE solves required on average for 50 trials to reach the stopping criterion, $\delta^2$.

* The first row gives the costs to reach the intermediate tolerance for the SAA approach, $\delta$.
** Since the SAA estimate becomes biased and underestimates the objective function, the algorithm stops prematurely.
*** The SAA approach measuring the convergence with the true objective function. Parentheses indicate that the SAA approach does not reach the tolerance.
5. Conclusions and Future Work. We use the SAA approach to estimate the objective function and the Jacobian using only a few simultaneous random sources and detectors in DOT problems. While this approach is reasonably effective for the application in [7], it does not work quite that well for DOT. Since convergence to the noise level slows down for later iterations, and the SAA approach regularly does not converge to the noise level, we propose using simultaneous optimized sources and detectors. With the addition of optimized directions, we observed faster convergence and good quality reconstructions and robustness. This technique could be quite useful in other applications as well. Although the approach has proved successful experimentally, we aim to understand the underlying theory better. In the future, we plan to analyze, more fundamentally, what are the most effective simultaneous sources and detectors for fast convergence of the inverse problem: randomized, optimized (and in what sense), and their combination.

We intend to update the TREGS algorithm and study how small we can make the number of simultaneous sources and detectors (random and optimized) and still obtain good solutions and fast convergence. We report results for two-dimensional DOT. We are currently adapting our approach for three-dimensional DOT that drastically increase the ratio of the number of all sources and detector to the number of simultaneous number of simultaneous random sources and detectors. Moreover, finding more appropriate stopping criteria for the randomized approach may also improve our results.

As shown in [4], parametrized interpolatory model reduction can also reduce the cost of inversion process in DOT. We are currently working on combining model reduction with the randomized approach.
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