DERIVATIVE-FREE OPTIMIZATION OF NOISY FUNCTIONS VIA QUASI-NEWTON METHODS

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Abstract. This paper presents a finite difference quasi-Newton method for the minimization of noisy functions. The method takes advantage of the scalability and power of BFGS updating, and employs an adaptive procedure for choosing the differencing interval $h$ based on the noise estimation techniques of Hamming [14] and Moré and Wild [30]. This noise estimation procedure and the selection of $h$ are inexpensive but not always accurate, and to prevent failures the algorithm incorporates a recovery mechanism that takes appropriate action in the case when the line search procedure is unable to produce an acceptable point. A novel convergence analysis is presented that considers the effect of a noisy line search procedure. Numerical experiments comparing the method to a model based trust region method are presented.

Key words. derivative-free optimization, nonlinear optimization, stochastic optimization

AMS subject classifications. 90C56, 90C53, 90C30

1. Introduction. The BFGS method has proved to be a very successful technique for nonlinear continuous optimization, and recent work has shown that it is also very effective for nonsmooth optimization [20, 24, 25]—a class of problems for which it was not designed for and for which few would have predicted its success. Moreover, as we argue in this paper, the BFGS method with finite difference approximations to the gradient can be the basis of a very effective algorithm for the derivative-free optimization of noisy objective functions.

It has long been recognized in some quarters [12] that one of the best methods for (non-noisy) derivative-free optimization is the standard BFGS method with finite difference gradients. However, its application in the noisy case has been considered problematic. The fact that finite differences can be unstable in the presence of noise has motivated the development of alternative methods, such as direct search methods [10, 17, 18, 22, 26, 41] and model based trust region methods [7–9, 27, 28, 36, 37, 40], which use function evaluations at well spread out points—an indispensable feature when minimizing noisy functions. These algorithms do not, however, scale well with the number of variables.

In contrast, the L-BFGS method for deterministic optimization is able to build useful quadratic models of the objective function at a cost that is linear in the dimension $n$ of the problem. Motivated by this observation, we propose a finite difference quasi-Newton approach for minimizing functions that contain noise. To ensure the reliability of finite difference gradients, we determine the differencing interval $h$ based on an estimate of the noise level (i.e., the standard deviation of the noise). For this purpose, we follow the difference-table technique pioneered by Hamming [14], as improved and extended by Moré and Wild [30]. This technique samples the objective

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function $f$ at a small number ($4 - 10$) of equally spaced points along a random direction, and estimates the noise level from the columns of the difference table. Our optimization algorithm is adaptive, as it re-estimates the noise level and differencing interval $h$ during the course of the optimization, as necessary.

An important ingredient in the method is the line search, which in our approach serves the dual purpose of computing the length of the step (when the interval $h$ is adequate) and determining when the differencing interval $h$ is not appropriate and should be re-estimated. When the line search is unable to find an acceptable point, the method triggers a recovery procedure that chooses between several courses of action. The method must, in general, be able to distinguish between the case when an unsuccessful step is due to a poor gradient approximation (in which case $h$ may need to be increased), due to nonlinearity (in which case $h$ should be maintained and the steplength $\alpha_k$ shortened), or due to the confusing effects of noise.

We establish two sets of convergence results for strongly convex objective functions; one for a fixed steplength strategy and one in which the steplength is computed by an Armijo backtracking line search procedure. The latter is novel in the way it is able to account for noisy function evaluations during the line search. In both cases, we prove linear convergence to a neighborhood of the solution, where the size of the neighborhood is determined by the level of noise.

The results of our numerical experiments suggest that the proposed algorithm is competitive, in terms of function evaluations, with a well-known model based trust region method, and that it scales better with the dimension of the problem and parallelizes easily. Although the reliability of the noise estimation techniques can be guaranteed only when the noise in the objective function is i.i.d., we have observed that the algorithm is often effective on problems in which this assumption is violated.

Returning to the first paragraph in this section, we note that it is the power of quasi-Newton methods, in general, rather than the specific properties of BFGS that have proven to be so effective in a surprising number of settings, including the subject of this paper. Other quasi-Newton methods could also prove to be useful. The BFGS method is appealing because it is simple, admits a straightforward extension to the large-scale setting, and is supported by a compact and elegant convergence theory.

The paper is organized into 6 sections. We conclude this section with some background and motivation for this work. In Section 2 we compare the performance of finite difference L-BFGS and a model based trust region method on smooth objective functions that do not contain noise. Section 3 presents the algorithm for the minimization of noisy functions, which is analyzed in Section 4. Section 5 reports the results of numerical experiments, and Section 6 summarizes the main findings of the paper.

1.1. Background. Although not a mainstream view, the finite difference BFGS method is regarded by some researchers as one of the most effective methods for derivative-free optimization of smooth functions that do not contain noise, and countless users have employed it knowingly or unknowingly in that setting. To cite just one example, if a user supplies only function values, the `fminunc` MATLAB function automatically invokes a standard finite difference BFGS method. (In fact, the motivation for the research reported in this paper stems from the competition established in 2015 to test algorithms for black-box (non-noisy) optimization http://bbcomp.ini.rub.de/.

The winner was the finite difference BFGS method for bound constrained optimization implemented in the KNITRO package [5].)

Nevertheless, much research has been performed in the last two decades to de-
sign other approaches for derivative-free optimization [9, 38], most prominently di-
rect search methods [10, 17, 18, 22, 26, 41] and model based trust region methods
[7–9, 27, 28, 36, 37, 40]. Earlier approaches include the Nelder-Mead method [33],
simulated annealing [21] and genetic algorithms [3, 16].

Model based trust region (MB) methods are more robust in the presence of noise
than other techniques for derivative-free optimization. This was demonstrated by
Moré and Wild [29] who report that the NEWOA [37] implementation of the MB
approach was more reliable and efficient in the minimization of both smooth and
noisy functions than the direct search method implemented in APPSPACK [13] and
the Nelder-Mead method NMSMAX [15]. Their experiments show that direct search
methods are slow and unable to scale well with the dimension of the problem; their
main appeal is that they are robust due to their expansive exploration of \( \mathbb{R}^n \), and are
easy to analyze and implement. In spite of its efficiency, the MB approach is limited by
the high linear algebra cost of the iteration; straightforward implementations require
\( O(n^9) \) operations, and although this can be reduced to \( O(n^4) \) operations by updating
factorizations, this cost is still high for large dimensional problems.

An established finite difference BFGS algorithm is the Implicit Filtering
method of Kelley [6, 19], which is designed for the case when noise decays as the iterates
approach the solution. That method enjoys deterministic convergence guarantees to
the solution, which are possible due to the assumption that noise can be diminished at
any iteration, as needed. In this paper we assume that noise in the objective function
does not decay to zero, and establish convergence to a neighborhood of the solution,
which is the best we can hope for in this setting.

Barton [1] describes a procedure for updating the finite difference interval \( h \) in the
case when the noise is multiplicative (as is the case of roundoff errors). He assumes
that a bound on the noise is known, and notes that the optimal choice of \( h \) depends
(in the one dimensional case) on \( \frac{|f(x)|}{|f''(x)|} \). Since estimating this ratio can be
expensive, he updates \( h \) by observing how many digits change between \( f(x_k + h) \) and
\( f(x_k) \), beyond the noise level. If this change is too large, \( h \) is decreased at the next
iteration; if it is too small \( h \) is increased. He tested this technique successfully in
conjunction with finite difference quasi-Newton methods. In this paper, we assume
that the noise level is not known and must be estimated, and discuss how to safeguard
against inaccurate estimates of the noise level.

2. Optimization of Smooth Functions. Before embarking on our investiga-
tion of noisy objective functions we consider the case when noise is not present,
and compare the performance of a model based trust region (MB) method and a
straightforward implementation of the L-BFGS method that uses finite differences to
approximate the gradient (FDLM). This will allow us to highlight the strengths of
each approach, and help set the stage for the investigation of the noisy case.

We write the deterministic optimization problem as

\[
\min_{x \in \mathbb{R}^n} f(x),
\]

where \( f : \mathbb{R}^n \to \mathbb{R} \) is twice continuously differentiable. In our numerical investigation,
we employ the MB method of Conn, Scheinberg and Vicente [9]. It begins by evaluat-
ing the function at \( 2n + 1 \) points along the coordinate directions, and as the iteration
progresses, builds a simple quadratic model with minimum norm Hessian. At every
iteration a new function value is computed and stored. Once \( (n + 1)(n + 2)/2 \) func-
tion values are available, a fully quadratic model \( m(x) \) is constructed by interpolation.
Every new iterate \( x_{k+1} \) is given by
\[
x_{k+1} = \arg \min_x \{ m(x) \| x - x_k \|_2 \leq \Delta_k \},
\]
where the trust region radius \( \Delta_k \) is updated using standard rules from derivative-free optimization [9]. We chose the method and software described in [9] because it embodies the state-of-the-art of MB methods and yet is simple enough to allow us to evaluate all its algorithmic components.

The finite difference L-BFGS (FDLM) method is given by
\[
x_{k+1} = x_k - \alpha_k H_k \nabla_h f(x_k),
\]
where \( H_k \) is an approximation to the inverse Hessian, \( \nabla_h f(x_k) \) is a finite difference approximation to the gradient of \( f \), and the steplength \( \alpha_k \) is computed by an Armijo-Wolfe line search; see [34]. We test both forward differences (FD) and central differences (CD)
\[
\nabla_{h,FD} f(x)_i = \frac{f(x + h_{FD} e_i) - f(x)}{h_{FD}}, \quad \text{where} \quad h_{FD} = \max\{1, |x|\} (\epsilon_m)^{1/2},
\]
and central differences (CD)
\[
\nabla_{h,CD} f(x)_i = \frac{f(x + h_{CD} e_i) - f(x - h_{CD} e_i)}{2h_{CD}}, \quad \text{where} \quad h_{CD} = \max\{1, |x|\} (\epsilon_m)^{1/3}.
\]
Here \( \epsilon_m \) is machine precision and \( e_i \in \mathbb{R}^n \) is the \( i \)-th canonical vector.

A sample of results is given in Figure 2.1, which plots the optimality gap \( f(x_k) - f^* \) versus number of function evaluations. For these test problems, the optimal value \( f^* \) is known. For the FDLM method, the number of function evaluations at the \( k \)-th iteration is \( n + t_{1n}^F \) (FD) or \( 2n + t_{1n}^C \) (CD), where \( t_{1n} \) is the number of function evaluations performed by the Armijo-Wolfe line search at the \( k \)-th iteration. The MB method described in [9], which we refer to as DFOtr, normally computes only one new function value per iteration.

**Fig. 2.1.** (Problems without Noise) Performance of the model based trust region method (DFOtr) described in [9], and the finite difference L-BFGS method (FDLM) using forward or central differences, on 4 problems from the Hock-Schittkowski collection [39].

The first problem in Figure 2.1 is quadratic; the MB method will generally have better performance in this case because it has finite termination while the FDLM does not. The rest of the plots in Figure 2.1 illustrate other behavior of the methods observed in our tests. Performance profiles are reported in Appendix A.1. We do not report CPU times because the MB code of Conn, Scheinberg and Vicente [9] is not designed to be efficient in this respect, requiring \( O(n^6) \) flops per iteration, and is thus much slower than the FDLM method as \( n \) increases. There exist, much faster MB
codes (albeit much more complex) such as that of Powell [37], whose linear algebra
cost is only $O(n^4)$. Regardless of the implementation, scalability remains one of the
main limitations of MB methods. To show that the FDLM approach can deal with
problems that are out of reach for MB methods, we report in Table 2.1 results on the
extended Rosenbrock function of various dimensions (as a reference, DFOtr requires
more than 1,800 seconds for $n = 100$).

**Table 2.1**

<table>
<thead>
<tr>
<th>n</th>
<th>10</th>
<th>50</th>
<th>100</th>
<th>1000</th>
<th>2000</th>
<th>5000</th>
</tr>
</thead>
<tbody>
<tr>
<td>FD</td>
<td>$1.8 \times 10^{-4}$</td>
<td>$3.1 \times 10^{-1}$</td>
<td>$7.6 \times 10^{-4}$</td>
<td>$3.3 \times 10^{-2}$</td>
<td>$2.9 \times 10^{-3}$</td>
<td>$5.5 \times 10^{-4}$</td>
</tr>
<tr>
<td>CD</td>
<td>$2.0 \times 10^{-4}$</td>
<td>$4.0 \times 10^{-1}$</td>
<td>1.2</td>
<td>$5.6 \times 10^{-2}$</td>
<td>$5.9 \times 10^{-3}$</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Overall, our numerical results suggest that FDLM is a very competitive method
for (non-noisy) derivative-free optimization, particularly for large problems. Conclu-
sive remarks about the relative performance of the MB and FDLM approaches are,
however, difficult to make because there are a variety of MB methods that follow sig-
nificantly different approaches than the method tested here. For example, the codes
by Powell [36, 37] include two trust region radii and employ a different procedure for
placing the interpolation points. Some implementations of MB methods start with
$O(n^2)$ function values in order to build a quadratic model; other implementations
only require $O(n)$ function values to start.

**2.1. Discussion.** One of the appealing features of the MB method is that it can
move after only 1 function evaluation, as opposed to the $O(n)$ function evaluations
required per iteration by the FDLM approach. However, if the model is not accurate
(or the trust region is too large) and results in an unsuccessful step, the MB approach
may require many function evaluations before the model is corrected (or the trust
region is properly adjusted); this can be seen in the second, third, and fourth plots in
Figure 2.1. On the other hand, finite difference approximations to the gradients (2.3)-
(2.4) carry some risks, as discussed in Section 3.4. We did not encounter difficulties in
our tests on smooth functions, but this is an issue that requires careful considera-
in general.

The MB and FDLM methods both construct quadratic models of the objective
function, and compute a step as the minimizer of the model, which distinguishes
them from most direct and pattern search methods. But the two methods differ
significantly in nature. MB methods define the quadratic model by interpolating
previously evaluated function values and (in some variants) by imposing a minimum-
norm change with respect to the previous model. The estimation of the gradient
and Hessian is done simultaneously, and no special effort is made to approximate the
gradient accurately; it is the overall quality of the model that matters. The location
of the sampling points is determined by the movement of the MB algorithm. These
points tend to lie along a subspace of $\mathbb{R}^n$, which can be harmful to the interpolation
process. To guard against this, many MB methods include a procedure (a geometry
phase) for spreading the sample points in $\mathbb{R}^n$ so that the interpolation problem is not
badly conditioned.

In contrast to MB methods, the finite difference BFGS method invests significant
computation in the estimation of the gradient \((n\) or \(2n\) function evaluations) and de-
egates the construction of the model to BFGS updating. The function evaluations
used in the estimation of the gradient parallelize easily, and the linear algebra costs
are quite modest, as updating the model and computing a step can be performed in a
small multiple of \(n\) using the limited memory BFGS approach \cite{34}. Practical experi-
ence indicates that BFGS and L-BFGS give rise to well-scaled search directions that
typically require little or no extra cost during the line search. Placement of the sample
points is along a linearly independent set of directions (during finite differencing) and
in this sense the method has some resemblance with pattern search methods – but
their similarities stop there.

It is rare to find in the derivative-free optimization (DFO) literature comparisons
between the finite difference BFGS method and direct search or model based trust
region methods, even when testing smooth objective functions without noise. One
reason for this omission may be the perception that finite difference based methods
are inefficient as they require at least \(n\) function evaluations per iteration, whereas
other methods for DFO are more frugal in this respect. In an early paper, Powell \cite{35}
wrote in regards to derivative-free optimization: “I believe that eventually the better
methods will not use derivative approximations.” In this paper, we argue that a finite
difference L-BFGS method is, indeed, an effective technique for the minimization of
certain classes of noisy functions.

These observations are a good starting point for our discussion of stochastic op-
timization problems.

3. Optimization of Noisy Functions. We study problems of the form

\[
\min_{x \in \mathbb{R}^n} f(x) = \phi(x) + \epsilon(x).
\]

We assume that \(\phi : \mathbb{R}^n \to \mathbb{R}\) is a smooth twice continuously differentiable function and
\(\epsilon(x)\) is a random variable whose distribution is independent of \(x\). (The notation \(\epsilon(x)\)
simply means that at any \(x\) we compute the realization of a random variable.) The
model (3.1) covers the case of multiplicative noise, i.e., when \(f(x) = \phi(x)(1 + \hat{\epsilon}(x))\)
and \(\hat{\epsilon}(x)\) is a random variable. To establish convergence results, we will assume that
\(\epsilon(x)\) is i.i.d and bounded, but our algorithm and presentation apply to the general
model (3.1). Specifically, we are also interested in the case when the noise \(\epsilon(x)\) is
deterministic, as is the case of roundoff errors or when adaptive algorithms are part
of the function evaluation.

3.1. The Finite Difference Interval. Our method relies crucially on the com-
putation of an appropriate finite difference parameter \(h\). It has been shown by Moré
and Wild \cite{31} that if one can estimate the level of noise in \(f\), which we denote by \(\sigma_f\),
one can compute a nearly optimal \(h\) for which the error in approximating \(\nabla f(x)\) is
\(O(\sigma_f^{1/2})\) and \(O(\sigma_f^{1/3})\) for forward differences and central differences, respectively.
The noise level \(\sigma_f\) of the function \(f\) given in (3.1) is defined as the standard
deviation of \(\epsilon(x)\), i.e.,

\[
\sigma_f = (\text{Var}\{\epsilon(x)\})^{1/2}.
\]

This quantity can be estimated using the difference table technique proposed by Ham-
ing \cite{14}, as extended and refined by Moré and Wild \cite{30}. We denote our estimate
of the noise level of \(f\) by \(\epsilon_f\).

With \(\epsilon_f\) in hand, we define the finite differencing interval as suggested in \cite{31}.
The \(i\)-th component of the forward difference approximation of the gradient of \(f\) at
and \( \nu_2 \) is an estimate of \( \max_{x \in [x, x + h_{\text{FD}} e_i]} |\nabla^2 f(x)^T e_i| \). The central difference approximation is given by

\[
[\nabla_{h,\text{CD}} f(x)]_i = \frac{f(x + h_{\text{CD}} e_i) - f(x - h_{\text{CD}} e_i)}{2h_{\text{CD}}}, \quad \text{where} \quad h_{\text{CD}} = 3^{1/3} \left( \frac{\epsilon_f}{\nu_3} \right)^{1/3},
\]

and \( \nu_3 \) is an estimate of the third derivative along \( e_i \), in an interval of length \( 2h_{\text{CD}} \) around \( x \). Since estimating 2nd or 3rd derivatives along each coordinate direction is expensive, in our implementation we perform this estimation once along a random direction, as discussed in Section 3.4. In the sequel, we let \( \nabla_h f(x) \) denote (3.3) or (3.4) when the distinction is not important.

### 3.2. Noise Estimation

The noise level \( \sigma_f \) of a function measures the uncertainty in the computed function values, and can be estimated using Hamming’s table of function differences [14]. To generate this table, Moré and Wild [30] first choose a random direction \( v \in \mathbb{R}^n \) of unit norm, evaluate the function at \( q + 1 \) equally spaced points (with spacing \( \delta \)) along that ray, and compute the function differences

\[
\Delta^0 f(x) = f(x),
\]

\[
\Delta^{j+1} f(x) = \Delta^j [\Delta f(x)] = \Delta^j [f(x + \delta v)] - \Delta^j [f(x)], \quad j \geq 0.
\]

Let \( x_i = x + u_i \delta v \), where \( u_i = -q/2 + i \), for \( i = 0, ..., q \), denote the sample points centered around \( x \). Using the computed function differences one can build a table whose entries are

\[
T_{i,j} = \Delta^j f(x_i), \quad 1 \leq j \leq q \quad \text{and} \quad 0 \leq i \leq q - j.
\]

Hamming’s approach relies on the fact that differences in \( \phi \) tend to zero rapidly, while the differences in \( e(x) \) do not [14]. As a result, the noise level \( \sigma_f \) can be estimated from the mean of the squares of the columns of this difference table [30]. Specifically, for each \( j \) (where \( j \) indexes a column of the difference table and also represents the order of differencing) one defines

\[
\gamma_j = \frac{(j!)^2}{(2j)!},
\]

\[
s_j \overset{\text{def}}{=} \gamma_j \frac{q}{q + 1 - j} \sum_{i=0}^{q-j} T_{i,j}^2,
\]

Once an appropriate value of \( j \) is identified, the noise estimate \( \epsilon_f \) is defined as

\[
\epsilon_f \leftarrow s_j.
\]

Moré and Wild [30] propose an efficient and reliable procedure, referred to as ECnoise, for determining the free parameters in this procedure, namely: (i) the order of differencing \( j \); (ii) the number of points \( q \) where the function is evaluated; and (iii) the spacing \( \delta \) between the sample points; see Section 3.4. ECnoise is inexpensive as it typically requires only between 4 – 10 function evaluations to estimate the noise level. It is available at: [http://www.mcs.anl.gov/~wild/cnoise/](http://www.mcs.anl.gov/~wild/cnoise/).
3.3. Specification of the Finite Difference L-BFGS Method. We are now ready to present the algorithm for the minimization of the function (3.1). It invokes two procedures, LineSearch and Recovery, that together produce a new iterate and, if necessary, recompute the estimate of the noise. These two procedures are described in detail after the presentation of the algorithm.

The algorithm stores the smallest function value obtained during the finite difference gradient computation, (3.3) or (3.4). Specifically, for forward differences we define

\[ f_s = \min_{x_i \in S} f(x_i), \quad \text{where} \quad S = \{ x_i : x_i = x + h_{FD}e_i, \; i = 1, \ldots, n \}, \]

and let \( x_s \) denote a point where the minimum is achieved. Since \( S \) is a stencil, we refer to \( x_s \) as the best point on the stencil.

**Algorithm 3.1** Adaptive Finite Difference L-BFGS (FDLM)

**Inputs:** \( f \) (objective function), \( x_0 \) (initial iterate), \( a_{\max} \) (max number of backtracks), \( k \leftarrow 0 \) (iteration counter), \( t_{\text{count}} \leftarrow 0 \) (function evaluation counter), \( t_{ls} \leftarrow 0 \) (function evaluation counter during LineSearch routine), \( t_{\text{rec}} \leftarrow 0 \) (function evaluation counter during Recovery procedure), \( \zeta \in (0, 1) \) (curvature threshold)

1. Compute \( f_0 = f(x_0) \); set \( t_{\text{count}} = 1 \)
2. Compute an estimate \( \epsilon_f \) of the noise using \texttt{ECnoise} \cite{30}, at the cost of \( t_{\text{ecn}} \) function evaluations
3. Update the function evaluation counter: \( t_{\text{count}} = t_{\text{count}} + t_{\text{ecn}} \)
4. Compute \( h \) via (3.3) (FD) or (3.4) (CD)
5. Compute \( \nabla_h f(x_k) \) using (3.3) or (3.4), and store \( (x_s, f_s) \)
6. \( t_{\text{count}} = t_{\text{count}} + n \) (FD) or \( t_{\text{count}} = t_{\text{count}} + 2n \) (CD)
7. **while** a convergence test is not satisfied **do**
8. Compute \( d_k = -H_k \nabla_h f(x_k) \) using the L-BFGS approach \cite{34}
9. \( (x_+, f_+, \alpha_k, t_{ls}, LS_{\text{flag}}) = \text{LineSearch}(x_k, f_k, \nabla_h f(x_k), d_k, a_{\max}) \)
10. \( t_{\text{count}} = t_{\text{count}} + t_{ls} \)
11. **if** \( LS_{\text{flag}} = 1 \) **then** \( \triangleright \text{Line search failed} \)
12. \( (x_+, f_+, h, t_{\text{rec}}) = \text{Recovery}(f_k, x_k, d_k, h, x_s, f_s) \)
13. \( t_{\text{count}} = t_{\text{count}} + t_{\text{rec}} \)
14. **end if**
15. \( x_{k+1} = x_+ \) and \( f_{k+1} = f_+ \)
16. Compute \( \nabla_h f(x_{k+1}) \) using (3.3) or (3.4), and store \( (x_s, f_s) \)
17. Compute curvature pair: \( s_k = x_{k+1} - x_k \) and \( y_k = \nabla_h f(x_{k+1}) - \nabla_h f(x_k) \)
18. Store \( (s_k, y_k) \) if \( s_k^T y_k \geq \zeta \| s_k \| \| y_k \| \)
19. \( t_{\text{count}} = t_{\text{count}} + n \) (FD) or \( t_{\text{count}} = t_{\text{count}} + 2n \) (CD)
20. \( k = k + 1 \)
21. **end while**

We now discuss the four main components of the algorithm.

3.3.1. Line Search. The LineSearch function (Line 9 of Algorithm 3.1) aims to find a steplength \( \alpha_k \) that satisfies the Armijo-Wolfe conditions,

\[
\begin{align*}
(3.10a) \quad f(x_k + \alpha_k d_k) & \leq f(x_k) + c_1 \alpha_k \nabla_h f(x_k)^T d_k, & \text{(Armijo condition)} \\
(3.10b) \quad \nabla_h f(x_k + \alpha_k d_k)^T d_k & \geq c_2 \nabla_h f(x_k)^T d_k, & \text{(Wolfe condition)}
\end{align*}
\]
for some constants $0 < c_1 < c_2 < 1$. In the deterministic setting, when the gradient is exact and the objective function $f$ is bounded below, there exist intervals of steplengths $\alpha_k$ that satisfy the Armijo-Wolfe conditions [34, Lemma 3.1]. However, when $f$ is noisy, satisfying (3.10a)-(3.10b) can be problematic. To start, $d_k$ may not be a descent direction for the smooth underlying function $\phi$ in (3.1), and even if it is, the noise in the objective may cause the line search routine to make incorrect decisions. Therefore, we allow only a small number ($a_{\text{max}}$) of line search iterations while attempting to satisfy (3.10a)-(3.10b). We also introduce the following relaxation: if (3.10a)-(3.10b) is not satisfied at the first trial point of the line search ($\alpha_k = 1$), we relax the Armijo condition (3.10a) for subsequent trial values as follows:

$$f(x_k + \alpha_k d_k) \leq f(x_k) + c_1 \alpha_k \nabla^T d_k + 2\epsilon f.$$  

There are three possible outcomes of the LineSearch function: (i) a steplength $\alpha_k$ is found that satisfies the Armijo-Wolfe conditions, where the Armijo condition may have been relaxed as in (3.11); (ii) after $a_{\text{max}}$ line search iterations, the line search is able to find a steplength $\alpha_k$ that only satisfies the relaxed Armijo condition (3.11) but not the Wolfe condition; (iii) after $a_{\text{max}}$ line search iterations the previous two outcomes are not achieved; we regard this as a line search failure, set $LS_{\text{flag}} = 1$, and call the Recovery function to determine the cause of the failure and take corrective action.

### 3.3.2. Recovery Mechanism

As mentioned above, the Recovery subroutine is the mechanism by which action is taken when the line search fails to return an acceptable point. This can occur due to the confusing effect of noisy function evaluations, a poor gradient approximation, or high nonlinearity of the objective function (the least likely case). The procedure is described in Algorithm 3.2.

The input to the Recovery subroutine is the current iterate $x_k$ and function value $f_k$, the search direction $d_k$, the current finite difference interval $h$, and the best point $x_\ast$ in the finite difference stencil together with the corresponding function value $f_\ast$.

The Recovery routine can take three actions:

1. Return a new estimate of the differencing interval $h$ and leave the current iterate $x_k$ unchanged. In this case, a new noise estimate is computed along the current search direction $d_k$.
2. Generate a new iterate $x_{k+1}$ without changing the differencing interval $h$. The new iterate is given by a small perturbation of $x_k$ or by the best point in the stencil $x_\ast$.
3. Leave the current iterate unchanged and compute a new estimate of the noise level, along a random direction, and a new finite difference interval $h$.

To start, the Recovery routine invokes the ECnoise procedure to compute a new noise estimate $\epsilon_k^f$ along the current search direction $d_k$, and the corresponding differencing interval $\hat{h}$ using formula (3.3) or (3.4). We estimate the noise along $d_k$ because the Recovery procedure may compute a new iterate along $d_k$, and it thus seem natural to explore the function in that direction.

If the current differencing interval $h$ differs significantly from the new estimate $\hat{h}$, then we suspect that our current noise estimate is not reliable, and return $\hat{h}$ without changing the current iterate (Case 1). This feature is especially important when the noise is multiplicative since in this case the noise level changes over the course of optimization, and the finite difference interval may need to be updated frequently.

On the other hand (Line 5), if the two differencing intervals, $h$ and $\hat{h}$, are similar, we regard them as reliable and assume that the line search procedure failed due to the
Algorithm 3.2 Recovery Routine

**Inputs:** $x_k$ (current iterate), $f_k = f(x_k)$ (current function value), $h$ (current finite difference interval), $d_k$ (search direction), $(x_s, f_s = f(x_s))$ (best point on the stencil), $t_{rec} \leftarrow 0$ (function evaluation counter for this routine)

1. Compute new noise estimate $\epsilon_{d_k}^k$ in direction $d_k$, and new $\bar{h}$ via (3.3) or (3.4).
2. Update function evaluation counter: $t_{rec} = t_{rec} + 1$
3. if $\bar{h} < 0.7h$ OR $\bar{h} > 1.5h$ then
4. \hspace{1em} $x_h = x_k$ and $x_+ = x_k$, $f_+ = f_k$ \hspace{1em} $\triangleright$ Case 1
5. else
6. \hspace{1em} Compute small perturbation of $x_k$ \hspace{1em} $\triangleright$ Compute small perturbation of $x_k$
7. \hspace{2em} $t_{rec} = t_{rec} + 1$
8. \hspace{1em} if $x_h$ satisfies the Armijo condition (3.10a) then
9. \hspace{2em} \hspace{1em} $x_+ = x_h$, $f_+ = f_h$, $h = h$ \hspace{1em} $\triangleright$ Case 2
10. \hspace{1em} else if $f_h \leq f_s$ AND $f_h \leq f_k$ then
11. \hspace{3em} $x_+ = x_h$, $f_+ = f_h$, $h = h$ \hspace{1em} $\triangleright$ Case 3
12. \hspace{1em} else if $f_k > f_s$ AND $f_h > f_s$ then
13. \hspace{2em} $x_+ = x_s$, $f_+ = f_s$, $h = h$ \hspace{1em} $\triangleright$ Case 4
14. \hspace{1em} else
15. \hspace{2em} Compute new noise estimate $\epsilon_{v_k}^k$ along random direction $v_k$ and new $\bar{h}$
16. \hspace{3em} $h = \bar{h}$
17. \hspace{2em} $t_{rec} = t_{rec} + f_{ecn}$
18. \hspace{1em} $\triangleright$ Case 5
19. \hspace{1em} end if
20. \hspace{1em} end if
21. \hspace{1em} end if
22. \hspace{1em} end if
23. Output: $x_+, f_+, h, t_{rec}$

confusing effects of noise. We must therefore generate a new iterate by other means.

We compute a small perturbation of $x_k$, of size $h$, along the current search direction $d_k$ (Line 6); if this point $x_h$ satisfies the Armijo condition (3.10a), it is accepted, and the procedure terminates on Line 10 (Case 2). Otherwise we make use of the best point $x_s$ on the stencil. If the function value $f_h$ at the trial point is less than both the current function value $f_k$ and $f_s$, then $x_h$ is accepted and the procedure ends on Line 13 (Case 3). Else, if $f_s$ is smaller than both $f_k$ and $f_h$, we let $x_s$ be the new iterate and terminate on Line 15 (Case 4). These two cases are inspired by the global convergence properties of pattern search methods, and do not require additional function evaluations.

If none of the conditions above are satisfied, then the noise is re-estimated along a random direction ($v_k \in \mathbb{R}^n$) using \texttt{ECnoise}, a new differencing interval is computed, and the \texttt{Recovery} procedure terminates without changing the iterate (Case 5). An additional action that could be taken in this last case is to switch to higher-order differences if this point of the algorithm is ever reached, as discussed in Section 5.

### 3.3.3. Hessian approximation

Step 8 of Algorithm 3.1 computes the L-BFGS search direction. The inverse Hessian approximation $H_k$ is updated using standard
rules [34] based on the pairs \( \{ s_j, y_j \} \), where

\[
(3.12) \quad s_k = x_{k+1} - x_k, \quad y_k = \nabla_h f(x_{k+1}) - \nabla_h f(x_k).
\]

When the line search is able to satisfy the Armijo condition but not the Wolfe condition, there is no guarantee that the product \( s_k^T y_k \) is positive. In this case the pair \((s_k, y_k)\) is discarded if the curvature condition \( s_k^T y_k \geq \zeta \|s_k\|\|y_k\|\) is not satisfied for some \( \zeta \in (0, 1) \).

### 3.3.4. Stopping Tests

A variety of stopping tests have been proposed in the derivative-free optimization literature; see e.g., [9, 17, 19, 22, 23, 37]. Here we discuss two approaches that can be employed in isolation or in combination, as no single test is best suited for all situations.

**Gradient Based Stopping Test.** One could terminate the algorithm as soon as

\[
(3.13) \quad \|\nabla_h f(x_k)\|_\infty \leq \text{tol},
\]

where \( \text{tol} \) is a user-specified parameter. When using forward differences, the best one can hope for is the norm of the gradient approximation to be \( \tau(\epsilon_f)^{1/2} \), where \( \tau \) depends on the norm of the second derivative. For central differences, the best accuracy is \( \bar{\tau}(\epsilon_f)^{2/3} \), where \( \bar{\tau} \) depends on the norm of the third derivative.

**Function Value Based Stopping Test.** One could also terminate the algorithm when

\[
(3.14) \quad |f(x_k) - f(x_{k-1})| \leq \hat{\tau}\epsilon_f,
\]

for \( \hat{\tau} > 1 \). This test is reasonable because the ECnoise procedure that estimates \( \epsilon_f \) is scale invariant. However, there is a risk that (3.14) will trigger termination too early, and to address this one could employ a moving average. The test can have the form

\[
\frac{|f_{\text{MA}}(x_k) - f(x_k)|}{|f_{\text{MA}}(x_k)|} \leq \text{tol} \quad \text{or} \quad \frac{|f_{\text{MA}}(x_k) - f(x_k)|}{\max(1, |f_{\text{MA}}(x_k)|)} \leq \text{tol},
\]

where \( f_{\text{MA}}(x_k) \) is a moving average of function values, of length \( M \), calculated as follows. Let \( f_k = f(x_k) \) and let \( F^k = [f_{k-j+1}, \ldots, f_{k-1}, f_k] \) be the vector formed by the most recent function values, where \( j = \min\{k + 1, M\} \). We define

\[
(3.15) \quad f_{\text{MA}}(x_k) = \frac{1}{j} \sum_{i=1}^{j} F^k_i.
\]

An alternative, is to formulate the stop test as

\[
|f_{\text{MA}}(x_k) - f(x_k)| \leq \tau(\epsilon_f)^{1/2} \quad \text{for FD}, \quad \text{or} \quad |f_{\text{MA}}(x_k) - f(x_k)| \leq \tau(\epsilon_f)^{2/3} \quad \text{for CD}.
\]

### 3.4. Implementation of the Noise Estimation Procedure

ECnoise has three parameters that if not appropriately chosen can cause ECnoise to fail to return a reliable estimate of the noise level: (i) the order of differencing \( j \); see (3.8); (ii) the number of points \( q \) used in the noise estimation, and (iii) the spacing \( \delta \) between the points.

We have found the strategy proposed by Moré and Wild [30] to be effective in deciding the order of differencing \( j \). It determines that \( j \) is appropriate if the values of \( \sigma_i \) surrounding \( \sigma_j \) are close to each other and if there are changes in sign among
elements of the $j$-th column of the difference table $T_{i,j}$; the latter is a clear indication that the entries of the $j$-th column are due to noise.

Concerning the number $q$ of sample points, we found that the values employed by ECnoise [30] are reliable, namely $4 - 8$ function evaluations for stochastic noise and $6 - 10$ for deterministic noise. However, our experience suggests that those settings may be conservative, and in our implementation use only 4 function evaluations for stochastic noise and 6 function evaluations for deterministic noise.

The finite difference approximations (3.3) and (3.4) require a coarse estimate of the second or third derivatives ($\nu_2$, $\nu_3$), and are often fairly insensitive to these estimates. However, in some difficult cases poor estimates may prevent the algorithm from reaching the desired accuracy. In our implementation we estimate $\nu_2$ using the heuristic proposed in [31, Section 5, Algorithm 5.1] at the cost of 2 - 4 function evaluations. If this heuristic fails to provide a reasonable estimate of $\nu_2$, we employ the finite difference table (3.6) as a back-up to construct a rough approximation of the norm of the second derivative. In our experiments this back-up mechanism has proved to be adequate. When computing central difference approximations to the gradient, we simply set $\nu_3 \leftarrow \nu_2$, for simplicity.

4. Convergence Analysis. In this section, we present two sets of convergence results for the minimization of the noisy function (3.1) under the assumption that $\phi$ is strongly convex. First, we analyze a method that uses a fixed steplength, and then consider a more sophisticated version that employs a line search to compute the steplength. The main contribution of our analysis is the inclusion of this line search and the fact that we do not assume that the errors in objective function or gradient go to zero, in any deterministic or probabilistic sense; we only assume a bound on these errors. To focus on these issues, we assume that $H_k = I$, because the proof for a general positive definite matrix $H_k$ with bounded eigenvalues is essentially the same, but is longer and more cluttered as it involves additional constants.

4.1. Fixed Steplength Analysis. We consider the method

$$x_{k+1} = x_k - \alpha g_k,$$

(4.1)

where $g_k$ stands for a finite difference approximation to the gradient, $g_k = \nabla_h f(x_k)$, or some other approximation; our treatment is general. We define $e(x)$ to be the error in the gradient approximation, i.e.,

$$g_k = \nabla \phi(x_k) + e(x_k).$$

(4.2)

We should note the distinction between $e(x)$ and $\epsilon(x)$; the latter denotes the noise in the objective function (3.1).

We introduce the following assumptions to establish the first convergence result.

A.1 (Strong Convexity of $\phi$) The function $\phi$ (see (3.1)) is twice continuously differentiable and there exist positive constants $\mu$ and $L$ such that $\mu I \preceq \nabla^2 \phi(x) \preceq LI$ for all $x \in \mathbb{R}^n$. (We write $\phi^* = \phi(x^*)$, where $x^*$ is the minimizer of $\phi$.)

A.2 (Boundedness of Noise in the Gradient) There is a constant $\bar{\epsilon}_g > 0$ such that

$$\|e(x)\| \leq \bar{\epsilon}_g$$

(4.3)

for all $x \in \mathbb{R}^n$. 


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Assumption A.2 is satisfied if the approximate gradient is given by forward or central differences with the value of $h$ given in (3.3) or (3.4), provided that the error $\epsilon(x)$ in the evaluation of the objection function value is bounded; see (4.30).

We now establish linear convergence to a neighborhood of the solution. Afterwards, we comment on the extension of this result to the case when a quasi-Newton iteration of the form $x_{k+1} = x_k - \alpha H_k g_k$ is used.

**Theorem 4.1.** Suppose that Assumptions A.1-A.2 hold. Let $\{x_k\}$ be the iterates generated by iteration (4.1), where $g_k$ is given by (4.2), and the steplength satisfies

$$\alpha \leq 1/L.$$  

Then for all $k$,

$$\phi(x_{k+1}) - \left[ \phi^* + \frac{\epsilon_g^2}{2\mu} \right] \leq (1 - \alpha\mu) \left[ \phi(x_k) - \left[ \phi^* + \frac{\epsilon_g^2}{2\mu} \right] \right],$$

where $\epsilon_g$ is defined in (4.3).

**Proof.** Since $\phi$ satisfies Assumption A.1, we have by (4.2),

$$\phi(x_{k+1}) \leq \phi(x_k) - \alpha \nabla \phi(x_k)^T g_k + \frac{\alpha^2 L}{2} \|g_k\|^2$$

$$= \phi(x_k) - \alpha \nabla \phi(x_k)^T (\nabla \phi(x_k) + e(x_k)) + \frac{\alpha^2 L}{2} \|\nabla \phi(x_k) + e(x_k)\|^2$$

$$= \phi(x_k) - \alpha \left(1 - \frac{\alpha L}{2}\right) \|\nabla \phi(x_k)\|^2 + \frac{\alpha^2 L}{2} \|\nabla \phi(x_k)\|^2 + \frac{\alpha^2 L}{2} \|e(x_k)\|^2$$

$$\leq \phi(x_k) - \alpha \left(1 - \frac{\alpha L}{2}\right) \|\nabla \phi(x_k)\|^2 + \alpha \left(1 - \alpha L\right) \|\nabla \phi(x_k)\| \|e(x_k)\| + \frac{\alpha^2 L}{2} \|e(x_k)\|^2.$$

where the last inequality follows from the fact that $(\frac{1}{\sqrt{2}} \|\nabla \phi(x_k)\| - \frac{1}{\sqrt{2}} \|e(x_k)\|)^2 \geq 0$

and the assumption $\alpha L < 1$. Simplifying this expression, we have, for all $k$,

$$\phi(x_{k+1}) \leq \phi(x_k) - \frac{\alpha}{2} \|\nabla \phi(x_k)\|^2 + \frac{\alpha}{2} \|e(x_k)\|^2.$$  

(4.6)

Since $\phi$ is $\mu$-strongly convex, we can use the following relationship between the norm of the gradient squared, and the distance of the $k$-th iterate from the optimal solution,

$$\|\nabla \phi(x_k)\|^2 \geq 2\mu(\phi(x_k) - \phi^*),$$

which together with (4.6) yields

$$\phi(x_{k+1}) \leq \phi(x_k) - \alpha \mu (\phi(x_k) - \phi^*) + \frac{\alpha}{2} \|e(x_k)\|^2,$$

and by (4.3),

$$\phi(x_{k+1}) - \phi^* \leq (1 - \alpha \mu)(\phi(x_k) - \phi^*) + \frac{\alpha \epsilon_g^2}{2}.$$
Hence,
\[
\phi(x_{k+1}) - \phi^* - \frac{\epsilon_g^2}{2\mu} \leq (1 - \alpha\mu)(\phi(x_k) - \phi^*) + \frac{\alpha x^2 g^2 - \epsilon_g^2}{2\mu}
\]
\[
= (1 - \alpha\mu)(\phi(x_k) - \phi^*) + (\alpha\mu - 1)\frac{\epsilon_g^2}{2\mu}
\]
\[
= (1 - \alpha\mu) \left( \phi(x_k) - \phi^* - \frac{\epsilon_g^2}{2\mu} \right).
\]

We interpret the term \(\phi^* + \frac{\epsilon_g^2}{2\mu}\) in (4.5) as the best value of the objective that can be achieved in the presence of noise. Theorem 4.1 therefore establishes a \(Q\)-linear rate of convergence of \(\{\phi(x_k)\}\) to that value.

Another way of stating the convergence result embodied in Theorem 4.1 is by applying the recursion to (4.5), i.e.,
\[
\phi(x_k) - \left[ \phi^* + \frac{\epsilon_g^2}{2\mu} \right] \leq (1 - \alpha\mu)^k \left( \phi(x_0) - \left[ \phi^* + \frac{\epsilon_g^2}{2\mu} \right] \right),
\]
so that
\[
\phi(x_k) - \phi^* \leq (1 - \alpha\mu)^k \left( \phi(x_0) - \left[ \phi^* + \frac{\epsilon_g^2}{2\mu} \right] \right) + \frac{\epsilon_g^2}{2\mu}.
\]

This convergence result has a similar flavor to that presented in [32] for the incremental gradient method using a fixed steplength; see also [4, Section 4]. Note that (4.8) is an \(R\)-linear convergence result and as such is weaker than (4.5).

It is possible to prove a similar result to Theorem 4.1 for a general positive definite \(H_k\), assuming bounds on \(\|H_k\|\) and \(\|H_k^{-1}\|\), as would be the case with a limited memory BFGS update. However, the provable convergence rate in this case would be closer to 1, and the provable asymptotic objective value would be no smaller than the value in (4.5). This is similar to the situation in optimization without noise, where the provable convergence rate for L-BFGS is no better than for steepest descent, even though L-BFGS is superior in practice. Since this more general analysis does not provide additional insights on the main topic of this paper, we have not included them here.

4.2. Line Search Analysis. In the literature of optimization of noisy functions, a number of convergence results have been established for algorithms that employ a fixed steplength strategy [2, 4, 32], but there has been little analysis of methods that use a line search.

In this section, we present a convergence result for the iteration
\[
x_{k+1} = x_k - \alpha_k g_k,
\]
where the steplength \(\alpha_k\) is computed by a backtracking line search governed by the relaxed Armijo condition
\[
f(x_k - \alpha_k g_k) \leq f(x_k) - c_1\alpha_k g_k^T g_k + 2\epsilon_A.
\]
Here \(c_1 \in (0, 1)\) and \(\epsilon_A > 0\) is a user specified parameter whose choice is discussed later on. If a trial value \(\alpha_k\) does not satisfy (4.10), the new value is set to a (fixed) fraction \(\tau < 1\) of the previous value, i.e., \(\alpha_k \leftarrow \tau \alpha_k\).
Our analysis relies on the following additional assumption on the error in the objective function.

A.3 (Boundedness of Noise in the Function) There is a constant \( \bar{\epsilon}_f > 0 \) such that

\[
|f(x) - \phi(x)| = |\epsilon(x)| \leq \bar{\epsilon}_f \quad \text{for all } x \in \mathbb{R}^n.
\]

The following result establishes linear convergence to a neighborhood of the solution.

**Theorem 4.2.** Suppose that Assumptions A.1-A.3 hold. Let \( \{x_k\} \) be the iterates generated by iteration (4.9), where \( g_k \) is given by (4.2) and the step length \( \alpha_k \) is the maximum value in \( \{\tau^{-j} : j = 0, 1, \ldots\} \) satisfying the relaxed Armijo condition (4.10) with \( \epsilon_A > \bar{\epsilon}_f \) and \( 0 < c_1 < 1/2 \). Then, for any \( \beta \in \left(0, \frac{1-2c_1}{1+2c_1}\right) \), we have that

\[
\phi(x_{k+1}) - [\phi^* + \bar{\eta}] \leq \rho (\phi(x_k) - [\phi^* + \bar{\eta}]), \quad k = 0, 1, \ldots,
\]

where

\[
\rho = 1 - \frac{2\mu c_1 \tau (1 - \beta^2)}{L}, \quad \bar{\eta} = \frac{1}{2\mu \beta^2} \epsilon_g^2 + \frac{L}{\mu c_1 \tau (1 - \beta^2)} (\epsilon_A + \bar{\epsilon}_f),
\]

and \( \epsilon_g \) and \( \bar{\epsilon}_f \) are defined in (4.3) and (4.11). Additionally, if \( c_1 < 1/4 \), we can choose \( \beta = 1 - 4c_1 \), in which case,

\[
\rho = 1 - \frac{32\mu c_1^3}{L}, \quad \bar{\eta} = \frac{1}{2\mu (1 - 4c_1)^2} \epsilon_g^2 + \frac{L}{16\mu c_1^3} (\epsilon_A + \bar{\epsilon}_f).
\]

**Proof.** By equation (4.6) in the proof of Theorem 4.1, if \( \alpha \leq 1/L \), we have

\[
\phi(x_k - \alpha g_k) \leq \phi(x_k) - \frac{\alpha}{2} \|\nabla \phi(x_k)\|^2 + \frac{\alpha}{2} \|\epsilon(x_k)\|^2,
\]

which given assumption A.3 implies

\[
f(x_k - \alpha g_k) \leq f(x_k) - \frac{\alpha}{2} (\|\nabla \phi(x_k)\|^2 - \|\epsilon(x_k)\|^2) + 2\bar{\epsilon}_f.
\]

Since we assume \( \epsilon_A > \bar{\epsilon}_f \), it is clear from comparing (4.10) and (4.16) that (4.10) will be satisfied for sufficiently small \( \alpha \). Thus, we have shown that the line search always finds a value of \( \alpha_k \) such that (4.10) is satisfied.

In addition, we need to ensure that \( \alpha_k \) is not too small when the iterates are far from \( x^* \). To this end we define

\[
\beta_k = \frac{\|\epsilon(x_k)\|}{\|\nabla \phi(x_k)\|},
\]

which together with (4.2) gives

\[
(1 - \beta_k) \|\nabla \phi(x_k)\| \leq \|g_k\| \leq (1 + \beta_k) \|\nabla \phi(x_k)\|.
\]

Now, using (4.17) and (4.18) in (4.16) we have

\[
f(x_k - \alpha g_k) \leq f(x_k) - \frac{\alpha}{2} (1 - \beta_k^2) \|\nabla \phi(x_k)\|^2 + 2\bar{\epsilon}_f
\]

\[
\leq f(x_k) - \frac{\alpha (1 - \beta_k^2)}{2(1 + \beta_k)^2} \|g_k\|^2 + 2\bar{\epsilon}_f
\]

\[
= f(x_k) - \frac{\alpha (1 - \beta_k)}{2(1 + \beta_k)} \|g_k\|^2 + 2\bar{\epsilon}_f.
\]
Since we assume that $\epsilon_A > \epsilon_f$ and $c_1 < 1/2$, it is then clear that the Armijo condition (4.10) is satisfied for any $\alpha \leq 1/L$ if $(1 - \beta_k)/(1 + \beta_k) \geq 2c_1$. This is equivalent to requiring that

$$
\beta_k \leq \beta \leq \frac{1 - 2c_1}{1 + 2c_1} < 1,
$$

where $\beta$ is an arbitrary positive constant satisfying (4.19).

**Case 1.** We now select such a value $\beta$ and refer to iterates such that $\beta_k \leq \beta$ as Case 1 iterates. Thus, for these iterates any $\alpha \leq 1/L$ satisfies the relaxed Armijo condition (4.10), and since we find $\alpha_k$ using a constant backtracking factor of $\tau < 1$, we have that $\alpha_k > \tau/L$. Therefore, using Assumption A.3 and (4.18) we have

$$
\phi(x_k - \alpha_k g_k) \leq \phi(x_k) - c_1 \alpha_k \|g_k\|^2 + 2\epsilon_A + 2\epsilon_f
$$

(4.20)

Expression (4.20) measures the reduction in $\phi$ at iterates belonging to Case 1.

**Case 2.** We now consider iterates that do not satisfy the conditions of Case 1, namely, iterates for which $\beta_k > \beta$, or equivalently,

$$
\|e(x_k)\| > \beta \|\nabla \phi(x_k)\|.
$$

(4.21)

We have shown that the relaxed Armijo condition (4.10) is satisfied at every iteration of the algorithm. Using as before Assumption A.3, we deduce from (4.10) that

$$
\phi(x_k - \alpha_k g_k) \leq \phi(x_k) - c_1 \alpha_k \|g_k\|^2 + 2\epsilon_A + 2\epsilon_f
$$

(4.22)

We now add and subtract $c_1(\tau/L)(1 - \beta)^2\|\nabla \phi(x_k)\|^2$ from the right hand side of this relation and recall (4.21), to obtain

$$
\phi(x_k - \alpha_k g_k) \leq \phi(x_k) - \frac{c_1 \tau (1 - \beta)^2}{L} \|\nabla \phi(x_k)\|^2 + \frac{c_1 \tau (1 - \beta)^2}{L} \|\nabla \phi(x_k)\|^2 + 2\epsilon_A + 2\epsilon_f
$$

(4.23)

where

$$
\eta = \frac{c_1 \tau (1 - \beta)^2}{L^2} \epsilon_g^2 + 2\epsilon_A + 2\epsilon_f.
$$

(4.24)

Equation (4.23) establishes a recursion in $\phi$ for the iterates in Case 2.

Now we combine the results from the two cases: (4.20) and (4.23). Since the term multiplying $\|\nabla \phi(x_k)\|^2$ is the same in the two cases, and since $\eta \geq 2\epsilon_A + 2\epsilon_f$, we have that for all $k$

$$
\phi(x_{k+1}) \leq \phi(x_k) - \frac{c_1 \tau (1 - \beta)^2}{L} \|\nabla \phi(x_k)\|^2 + \eta.
$$

(4.25)
Subtracting $\phi^*$ from both sides of (4.25), and using the strong convexity condition (4.7), gives

$$
\phi(x_{k+1}) - \phi^* \leq \left(1 - \frac{2\mu c_1 \tau (1 - \beta)^2}{L}\right)(\phi(x_k) - \phi^*) + \eta.
$$

Clearly $0 < \rho < 1$, since the quantities $2c_1, \mu/L, \tau$ and $1 - \beta$ are all less than one. We have thus shown that for all $k$

$$
\phi(x_{k+1}) - \phi^* \leq \rho(\phi(x_k) - \phi^*) + \eta.
$$

Subtracting $\eta/(1 - \rho)$ from both sides, it follows that

$$
\phi(x_{k+1}) - \phi^* - \frac{\eta}{1 - \rho} \leq \rho(\phi(x_k) - \phi^*) - \frac{\rho \eta}{1 - \rho}
$$

$$
= \rho\left(\phi(x_k) - \phi^* - \frac{\eta}{1 - \rho}\right),
$$

and thus

$$
\phi(x_{k+1}) - \phi^* - \bar{\eta} \leq \rho(\phi(x_k) - \phi^* - \bar{\eta}), \quad k = 0, 1, \ldots,
$$

where $\bar{\eta} = \eta/(1 - \rho)$. From (4.24), (4.26), we have that

$$
\bar{\eta} = \frac{L}{2\mu c_1 \tau (1 - \beta)^2} \left(\frac{c_1 \tau (1 - \beta)^2 \bar{e}_g^2}{L \beta^2} + 2\varepsilon_A + 2\bar{e}_f\right)
$$

$$
= \frac{1}{2\mu \beta^2 \bar{e}_g^2} + \frac{L}{\mu c_1 \tau (1 - \beta)^2} \left(\varepsilon_A + \bar{e}_f\right).
$$

This establishes (4.12) and (4.13).

We can obtain simpler expressions for $\rho$ and $\bar{\eta}$ by making a particular selection of $\beta$. Recall that this parameter is required to satisfy (4.19) so that (4.28) holds for all $k$. In the case when $c_1 \in (0, 1/4]$, the choice $\beta = 1 - 4c_1$ will satisfy (4.19) since

$$
1 - 4c_1 - \frac{1 - 2c_1}{1 + 2c_1} = \frac{1 - 4c_1 + 2c_1 - 8c_1^2 - (1 - 2c_1)}{1 + 2c_1} < 0.
$$

Substituting this value of $\beta$ in the definition of $\rho$ (see (4.26)) and in (4.29) gives

$$
\rho = 1 - \frac{2\mu c_1 \tau (1 - \beta)^2}{L} = 1 - \frac{32\mu c_1^3}{L},
$$

and

$$
\bar{\eta} = \frac{1}{2\mu \beta^2 \bar{e}_g^2} + \frac{L}{\mu c_1 \tau (1 - \beta)^2} \left(\varepsilon_A + \bar{e}_f\right) = \frac{1}{2\mu (1 - 4c_1)^2 \bar{e}_g^2} + \frac{L}{\mu \tau 16 c_1} \left(\varepsilon_A + \bar{e}_f\right),
$$

which gives (4.14).
As with \((4.8)\) there is a different way of stating the convergence result. Applying \((4.28)\) recursively and then moving the constant term to the right-hand-side of the expression yields
\[
\phi(x_k) - \phi^* \leq \rho^k (\phi(x_0) - [\phi^* + \bar{\eta}]) + \bar{\eta}.
\]

Application of Theorem 4.2 requires a choice of the parameter \(\beta\) that affects the convergence constant \(\rho\) and the level of accuracy \(\bar{\eta}\). One of the most intuitive expressions we could find was \((4.14)\), which was obtained by assuming that \(c_1 < 1/4\) and choosing \(\beta = 1 - 4c_1\). This value is reasonable provided \(c_1\) is not too small. There are other ways of choosing \(\beta\) when \(c_1\) is very small; in general the theorem is stronger if \(\beta\) is not chosen close to zero.

In the case where \(\nabla \phi(x)\) is estimated by a forward difference approximation we can further distill our error estimate, since \(\bar{\epsilon}_f\) is the source of all noise. Using A.3, it is easy to show that
\[
\|\epsilon(x_k)\| = \|g_k - \nabla \phi(x_k)\| \leq \frac{Lh}{2} + 2\bar{\epsilon}_f/h
\]
where the equality follows by substituting \(h = 2\sqrt{\bar{\epsilon}_f/L}\), which is the value that minimizes the right hand side of the inequality. Therefore, by \((4.3)\) we can assume that \(\epsilon_g = 2\sqrt{L\bar{\epsilon}_f}\), and the asymptotic accuracy can be estimated as
\[
\bar{\eta} = \frac{1}{2\mu\beta^2} \epsilon_g^2 + \frac{L}{\mu c_1 \tau (1 - \beta)^2} (\epsilon_A + \bar{\epsilon}_f)
\]
\[
= \frac{2L}{\mu \beta^2 \bar{\epsilon}_f} + \frac{L}{\mu c_1 \tau (1 - \beta)^2} (\epsilon_A + \bar{\epsilon}_f)
\]
\[
= \frac{L\bar{\epsilon}_f}{\mu} \left( \frac{2}{\beta^2} + \frac{1 + \theta}{c_1 \tau (1 - \beta)^2} \right),
\]
where in the last line we have written \(\epsilon_A = \theta \bar{\epsilon}_f\), for some \(\theta > 1\). If we choose \(\beta = 1 - 4c_1\) when \(c_1 < 1/4\), then
\[
\bar{\eta} = \frac{L\bar{\epsilon}_f}{\mu} \left( \frac{2}{(1 - 4c_1)^2} + \frac{1 + \theta}{16c_1 \tau} \right).
\]

Equations \((4.32)\) and \((4.33)\) show that the asymptotic accuracy level \(\bar{\eta}\) is proportional to the bound in the error in the objective function \((4.11)\) times the condition number. Note also that \((4.31)\) is comparable (but larger) than the accuracy level \(\epsilon_g^2/2\mu\) in Theorem 4.1. This is not surprising as it reflects the fact that, although the line search method can take steps that are much larger than \(1/L\), the theory only uses the fact that \(\alpha\) cannot be much smaller than \(1/L\).

In the analysis presented in this section, we have chosen to analyze a backtracking line search rather than one satisfying the Armijo-Wolfe conditions \((3.10a)-(3.10b)\) because in the strongly convex case, the curvature condition \((3.10b)\) is less critical, and because this simplifies the analysis. It would, however, be possible to do a similar analysis for the Armijo-Wolfe conditions, but the algorithm and analysis would be more complex. (We should also mention that we could remove the parameter \(\epsilon_A\) from the relaxed Armijo condition \((4.10)\) at the cost of making the analysis more complex.)

An extension of Theorem 4.2 to a quasi-Newton iteration with positive definite \(H_k\) could be proved, but for the reasons discussed above, we have limited our analysis to the case \(H_k = I\).
5. Numerical Experiments on Noisy Functions. In this section we present numerical results comparing the performance of the finite difference L-BFGS method (FDLM, Algorithm 3.1) and the model based trust region method (MB) described in [9], which we denote by DF0tr. We selected 49 nonlinear optimization test problems from the Hock and Schittkowski collection [39]. The distribution of problems, in terms of their dimension \( n \), is given in Table 5.1.

\[
\begin{array}{|c|c|c|c|c|c|c|c|c|c|c|c|}
\hline
n & 2 & 3 & 4 & 5 & 6 & 9 & 10 & 20 & 30 & 50 & 100 \\
\hline
\text{Number of Problems} & 15 & 6 & 5 & 2 & 5 & 1 & 4 & 3 & 3 & 2 & \text{ } \\
\hline
\end{array}
\]

A limit of \( 100 \times n \) function evaluations and 30 minutes of CPU time is given to each method. The FDLM method also terminates if one of the following two conditions holds: i) \(|f_{\text{MA}}(x_k) - f(x_k)| \leq 10^{-8} \max\{1,|f_{\text{MA}}(x_k)|\}\), where \( f_{\text{MA}}(x_k) \) is defined in (3.15); or ii) \( \|\nabla_h f(x_k)\| \leq 10^{-8} \). The MB method terminates if the trust region radius satisfies \( \Delta_k \leq 10^{-8} \). The very small tolerance \( 10^{-8} \) was chosen to display the complete evolution of the runs.

We consider 4 different types of noise: (i) stochastic additive, (ii) stochastic multiplicative, (iii) deterministic additive, and (iv) deterministic multiplicative, and for each type of noise we consider 4 different noise levels. Below, we show a small sample of results for the first two types of noise; a larger sample can be found in Appendix A.

Stochastic Additive Noise. The objective function has the form \( f(x) = \phi(x) + \epsilon(x) \), where \( \phi \) is a smooth function and \( \epsilon(x) \) is a uniform random variable, i.e.,

\[
\epsilon(x) \sim U(-\xi, \xi).
\]

We investigate the behavior of the methods for noise levels corresponding to \( \xi \in \{10^{-8}, 10^{-6}, 10^{-4}, 10^{-2}\} \). In Figure 5.1 we report results for the 4 problems studied in Section 2, namely \( s271, s334, s293 \) and \( s289 \), for 2 different noise levels \( (10^{-8} \text{ and } 10^{-2}) \). The figure plots the optimality gap \( (f(x_k) - \phi^*) \) versus the number of function evaluations. (For all test problems, \( \phi^* \) is known.) We note that \( \phi^* = 0 \) for problems \( s271, s293, s289 \). The first problem, \( s271 \) is quadratic, which is benign for DF0tr, which terminates as soon as a fully quadratic model is constructed.

Stochastic Multiplicative Noise. The objective has the form \( f(x) = \phi(x)(1 + \epsilon(x)) \), where \( \phi \) is smooth and \( \epsilon(x) \) is the stochastic noise defined in (5.1). We can write the objective in the additive form \( f(x) = \phi(x) + \epsilon(x) \), where \( \epsilon(x) = \phi(x)\epsilon(x) \) varies with \( x \), and since \( \phi^* = 0 \) for problems \( s271, s293 \) and \( s289 \), the noise term \( \epsilon(x) \) decays to zero as \( x_k \) approaches the solution; this is not the case for problem \( s334 \). The results are given in Figure 5.2.

Performance Profiles. Figure 5.3 shows performance profiles [11] for all 49 problems, for the 4 different types of noise mentioned above, and for 2 different noise levels \( (10^{-8} \text{ and } 10^{-2}) \), giving a total of 392 problems. Deterministic noise was generated using the procedure proposed by Moré and Wild [29], which is described in Appendix A.3. For these tests, we follow [28, 29] and terminate the runs as soon as

\[
f(x_0) - f(x_k) \leq (1 - \tau) (f(x_0) - f_L),
\]

where \( \tau = 10^{-5} \), \( x_0 \) is the starting point, and \( f_L \) is the smallest value of \( f \) obtained by any solver within a given budget of \( 100 \times n \) function evaluations.

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Fig. 5.1. **Stochastic Additive Noise.** Performance of the model based trust region method (DFOtr) described in [9], and the finite difference L-BFGS (FDLM) method using forward or central differences. The figure plots results for 4 problems from the Hock-Schittkowski collection, for 2 different noise levels. Each column represents a different problem and each row a different noise level.

Fig. 5.2. **Stochastic Multiplicative Noise.** Performance of the model based trust region method (DFOtr) and the finite difference L-BFGS (FDLM) method on the four problems displayed in Figure 5.1.

**Observations.** Even though there is some variability, our tests indicate that overall the performance of the MB and FDLM methods is roughly comparable in terms of function evaluations—but not in terms of computing time, which is much higher for the MB method as \(n\) grows. Contrary to conventional wisdom, the high per-iteration cost of finite differences is offset by the faster convergence of the FDLM method, and the potential instability of finite differences is generally not harmful in our tests. As expected, forward differences are more efficient for low levels of noise, and central differences give rise to a more robust algorithm for high noise levels (e.g. \(10^{-2}\)); this suggests that using even higher order gradient approximations would be useful for more difficult problems.

**5.1. The Recovery Mechanism.** We investigate the effect of the Recovery mechanism, and whether it improves the robustness of our approach. We run the FDLM method with and without the Recovery procedure; the latter amounts to terminating as soon as the LineSearch procedure fails (Line 11, Algorithm 3.1). In Figure 5.4 we present the result for two problems s271 and s293 with stochastic ad-
Deterministic Multiplicative Noise: $10^{-0.8}$

Stochastic Multiplicative Noise: $10^{-0.8}$

Deterministic Additive Noise: $10^{-0.2}$

Stochastic Additive Noise: $10^{-0.2}$

$\text{No noise and two noise levels.}$

Recovery (noise levels $10^{-5}$, $10^{-1}$).

Recovery from the optimal solution.

The first two plots show results for stochastic additive noise, and the last two plots show results for stochastic multiplicative noise.

To further illustrate the importance of the Recovery mechanism, Table 5.2 shows the number of problems for which FDLM without the Recovery mechanism was unable to reach, within an order of magnitude, the optimal function value achieved by the FDLM method.

<table>
<thead>
<tr>
<th>Noise Type</th>
<th>Noise Level</th>
<th>FD</th>
<th>CD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic</td>
<td>$10^{-5}$</td>
<td>19</td>
<td>4</td>
</tr>
<tr>
<td>Additive</td>
<td>$10^{-2}$</td>
<td>12</td>
<td>4</td>
</tr>
<tr>
<td>Stochastic</td>
<td>$10^{-5}$</td>
<td>26</td>
<td>5</td>
</tr>
<tr>
<td>Multiplicative</td>
<td>$10^{-2}$</td>
<td>29</td>
<td>13</td>
</tr>
</tbody>
</table>

Table 5.2

Number of problems (from the complete set of 49 problems) for which the FDLM method without the Recovery mechanism is unable to reach, within an order of magnitude, the function value achieved by the FDLM method with the Recovery mechanism, for two types of noise and two noise levels.

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Fig. 5.5. Performance of a hybrid variant of the FDLM method is allowed to switch from forward to central differences.

Our complete set of experiments show that the Recovery procedure is invoked more often when the noise level is high or when forward differences are employed, as expected. It plays an important role for problems with multiplicative noise where the noise level changes during the course of the iteration and our approach relies on the Recovery mechanism to adjust the finite difference interval. For most problems, the Recovery procedure is never invoked, but in the most difficult cases it plays a crucial role.

5.2. Combining Forward and Central Differences. Our experiments (see e.g., Figures 5.1-5.2) show that the FDLM method with forward differences is more efficient than the central difference variant in the initial stages of the optimization, but the latter is able to achieve more accurate solutions within the given budget. It is therefore natural, to consider a method that starts with forward differences and switches to central differences. In our framework we employ the Recovery procedure to decide when to make the transition, which occurs the first time that Recovery reaches Case 2, 3, 4 or 5 of Algorithm 3.2. Figure 5.5 reports the results on 4 problems were the benefit of this approach is apparent. Nevertheless, the design of a well-crafted algorithm that uses mixed precision is complex and will be addressed in a future study.

6. Final Remarks. We presented a finite difference quasi-Newton method for the optimization of noisy black-box functions. It relies on the observation that when the level of noise (i.e., its standard deviation) can be estimated, it is possible to choose finite difference intervals that yield reliable forward or central difference approximations to the gradient. To estimate the noise level, we employ the ECnoise procedure of Moré and Wild [30]. Since this procedure may not always be reliable, or since the noise level may change during the course of the minimization, our algorithm includes a Recovery procedure that adjusts the finite difference interval, as needed. This procedure operates in conjunction with a backtracking Armijo line search.

Our numerical experiments indicate that our approach is robust and efficient. Therefore, performing $O(n)$ function evaluations at every iteration to estimate the gradient is not prohibitively expensive and has the advantage that the construction of the model of the objective can be delegated to the highly scalable L-BFGS updating technique. We present a convergence analysis of our method using an Armijo-type backtracking line search that does not assume that the error in the function evaluations tends to zero.

Appendix A. Extended Numerical Results.

In this section, we present extended numerical results.

A.1. Extended Numerical Results – Smooth Functions. In this section, we present extended numerical results for smooth deterministic functions. Figure A.1 shows performance profiles for different $\tau$ values (see equation (5.2)).
A.2. Extended Numerical Results – Summary of Noisy Problems.

A.2.1. Stochastic Additive Noise. In this section, we present extended numerical results for problems with stochastic additive noise. Figure A.2 shows the optimality gap $f(x_k) - \phi^*$ versus number of function evaluations.

![Stochastic Additive Noise](image)

**Fig. A.2.** *Stochastic Additive Noise.* Performance of the model based trust region method (MB) implemented in [9], and the finite difference L-BFGS (FDLM) method using forward or central differences. Each row represents a different problem and each column a different noise level.
A.2.2. Stochastic Multiplicative Noise. In this section, we present extended numerical results for problems with stochastic multiplicative noise. Figures A.3 shows the optimality gap $f(x_k) - \phi^*$ versus number of function evaluations.

Fig. A.3. Stochastic Multiplicative Noise. Performance of the model based trust region method (MB) implemented in [9], and the finite difference L-BFGS (FDLM) method using forward or central differences. Each row represents a different problem and each column a different noise level.

A.3. Deterministic Noise. In this section, we describe the deterministic noise (additive and multiplicative) we considered in this paper. Deterministic noise was generated using the procedure described by Moré and Wild [29]. Namely,

(A.1) \[ \epsilon(x) = \xi \psi(x), \]

where $\xi \in \{10^{-8}, 10^{-6}, 10^{-4}, 10^{-2}\}$, and $\psi: \mathbb{R}^n \to [-1, 1]$ is defined in terms of the cubic Chebyshev polynomial $T_3(\alpha) = \alpha(4\alpha^2 - 3)$, as follows:

(A.2) \[ \psi(x) = T_3(\psi_0(x)), \quad \psi_0(x) = 0.9 \sin(100\|x\|_1) \cos(100\|x\|_\infty) + 0.1 \cos(\|x\|_2). \]
A.3.1. Deterministic Additive Noise. In this section, we present extended numerical results for problems with deterministic additive noise. Figures A.4 shows the optimality gap $f(x_k) - \phi^*$ versus number of function evaluations.

Fig. A.4. Deterministic Additive Noise. Performance of the model based trust region method (MB) implemented in [9], and the finite difference L-BFGS (FDLM) method using forward or central differences. Each row represents a different problem and each column a different noise level.
A.3.2. Deterministic Multiplicative Noise. In this section, we present extended numerical results for problems with deterministic multiplicative noise. Figures A.5 shows the optimality gap $f(x_k) - \phi^*$ versus number of function evaluations.

![Graph showing performance of different methods with deterministic multiplicative noise](image)

**Fig. A.5. Deterministic Multiplicative Noise.** Performance of the model based trust region method (MB) implemented in [9], and the finite difference L-BFGS (FDLM) method using forward or central differences. Each row represents a different problem and each column a different noise level.
Acknowledgments. We thank Jorge Moré and Stefan Wild for many useful suggestions and insights on noise estimation and derivative-free optimization.

References.


