Arnoldi-based Sampling for High-dimensional Optimization using Imperfect Data

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We present a sampling strategy suitable for optimization problems characterized by high-dimensional design spaces and imperfect data — objective values and derivatives with numerical errors that cannot be eliminated in practice. Such errors can arise, for example, in time-averaged objectives that depend on chaotic states and in optimization under uncertainty. The proposed sampling method is based on a generalization of Arnoldi’s method used in Krylov iterative methods. We show how this Arnoldi-sampling strategy can be combined with regression to construct reduced-order models for optimization. In the presence of inaccurate high-dimensional data, the proposed optimization algorithm shows significant potential relative to conventional derivative-based and derivative-free algorithms.

I. Introduction

Large-scale numerical simulations play a central role in contemporary aircraft design, and, increasingly, this role goes beyond the use of simulations as proxies for experiments. This trend is exemplified by differential-equation-constrained optimization (DECO), which couples simulations with numerical optimization. DECO has been used to optimize highly-refined aircraft where small improvements translate into significant economic and environmental benefits. Moreover, DECO has the potential to enable the design of unprecedented aircraft configurations where empirical data is sparse and intuition is lacking.

Clearly, DECO has enormous value and potential for aerospace engineers; however, while DECO algorithms for steady and periodic deterministic systems are maturing, there remains a broad class of problems that cannot be optimized with conventional algorithms. These problems exhibit

1. a high-dimensional design space,
2. complex physics that must be modeled using large-scale simulations, and
3. simulation outputs, e.g. lift force or total energy, that are “imperfect”.

In this context, imperfect outputs are quantities of interest whose numerical errors cannot be eliminated, at least in practice; consequently, such outputs fail to meet the underlying assumptions of conventional gradient-based optimization algorithms. The word imperfect is intentionally chosen to distinguish the anticipated errors from more traditional numerical errors that can, usually, be estimated and effectively reduced. In the following sections, we briefly elaborate on two such sources of imperfect data.

A. Time-averaged Outputs from Chaotic Systems

The outputs of interest in many engineering systems are time-averages of chaotic solutions. Relevant examples include the lift and drag on aerodynamic bodies [2], the energy produced by a fusion reactor [3], and the (phase-averaged) pressure in an internal-combustion engine [4].

Chaotic systems are characterized by a sensitive dependence on initial conditions; the distance between two states that are “close” initially will exponentially increase with time. This is illustrated in Figure 1(a) using the Lorenz DE [5] and two initial conditions that satisfy $\|\Delta x_0\| \leq 10^{-10}$.

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For example, a 1% reduction in the fuel consumed by the worldwide fleet would result in 7 million fewer tonnes of CO2 emitted per year [1].
In addition to the initial conditions, chaotic systems are sensitive to other parameters. This has significant implications for time-averaged outputs, which we illustrate using the Lorenz system and the objective function

$$J_T(\rho) = \frac{1}{2T} \int_0^T (z(t, \rho) - z_{\text{targ}})^2 \, dt,$$

where $z(t, \rho)$ is one of the Lorenz state variables, $z_{\text{targ}} = 35$, and $T > 0$ is the period of integration. The design variable here is $\rho$, a parameter in the Lorenz DE.

Figure 1(b) plots the Lorenz objective $J_T$ versus the parameter $\rho$ for an averaging period of $T = 400$. High-frequency oscillations can be observed in the objective function $J_T$. In theory, we could eliminate these fluctuations by integrating over an infinite time horizon, but, in practice, we must truncate the simulation at a finite $T$. The oscillations in $J_T$ reflect the sensitivity of the Lorenz DE to changes in $\rho$, and they hint at the difficulties of using gradient-based optimization. Indeed, as $T \to \infty$ the gradient of $J_T$ diverges [6] despite the fact that the objective itself converges.

Researchers have proposed methods to compute derivatives of objectives that depend on chaotic systems, such as the ensemble adjoint [6–8] and least-squares adjoint [9]. These methods share one shortcoming: they produce estimates of the derivatives only. Figure 1(b) illustrates some derivatives estimated using the ensemble adjoint. Although the derivatives capture the general slope of the objective, errors are clearly visible. Such errors are incompatible with conventional gradient-based optimization.

**B. Uncertainty Propagation in High-dimensional Input Spaces**

Numerical simulations contain many sources of uncertainty. For example, turbulence and combustion models introduce errors with respect to the true physics, the operating conditions of a system are not deterministic (e.g. the Reynolds number is not known precisely), and perturbations to the intended design are introduced by the manufacturing process. The field of optimization under uncertainty (OUU), a branch of uncertainty quantification (UQ), seeks to account for such uncertainties during the optimization process. OUU can help ensure good performance over a range of parameters, and it can help reduce the probability of failure.

Typically, at each iteration of an OUU, uncertainties in the input parameters must be propagated through the numerical simulation to deduce uncertainties in the outputs, e.g. the standard deviation in a force or energy. Uncertainty propagation is especially challenging when there are a large (> 100) number of uncertain input parameters. These situations require approximations to cope with the “curse of dimensionality”.

Several parameter-selection and model-reduction strategies have been proposed for the propagation of stochastic, or aleatory, uncertainties in high-dimensional input spaces [10–12]. Methods of propagating epistemic uncertainties, i.e. model errors, in high-dimensional spaces have also been investigated [13, 14]. If these methods are to be used for high-dimensional OUU problems, derivative information will be needed;
however, differentiating these propagation methods accurately is not practical. Therefore, an optimization algorithm must account for the discrepancy between the outputs and their derivatives.

To illustrate why dimension-reduction strategies are difficult to differentiate, consider computing the expected value, \( E[f(x)] \), of the Rosenbrock function

\[
f(x + \xi) = [1 - (x + \xi)]^2 + 100 [(y - \eta) - (x + \xi)^2]^2,
\]

where \( x = (x, y)^T \in \mathbb{R}^2 \) are the design variables and \( \xi, \eta \in \mathcal{N}(0, 0.5^2) \) are Gaussian random variables. In this example, we use the dominant eigenvalue of the Hessian to define a subspace for dimension reduction. Figure 2(a) shows one such subspace defined at \( x = (-0.5, 0)^T \).

Figure 2(b) plots the expected value obtained by (correctly) accounting for changes in the subspace. The figure also plots the expected value obtained by fixing the subspace, which reflects how derivatives would be computed for most dimension-reduction strategies. Fixing the subspace results in a 12% error in the derivative. Note that, to correctly compute the derivative in the present example, we would need to differentiate eigenvectors of the Hessian, which would be impractical for high-dimensional outputs based on simulations.

C. Other Sources of “Imperfect” Outputs

Time-averaging in chaotic systems and uncertainty propagation in high-dimensional spaces are two important examples that produce imperfect data and motivate the current work. However, inconsistencies between the outputs and their derivatives can also arise in other applications of DECO.

1. Cut-cell [15–17] and immersed-boundary methods [18–20] are popular and effective methods for numerically solving DEs on complex, moving geometries. In geometry optimization, these methods produce discontinuities in the design space as the mesh-topology and/or stencil is updated. A similar problem exists when unstructured grids are regenerated during shape optimization.

2. The differentiate-then-discretize [21], or “continuous” [22], adjoint yields derivatives that are inconsistent with the discretized output. See, for example, [23,24].

3. Incomplete sensitivities have been proposed [25, 26] to reduce the computational cost of computing the gradient. The terms that are dropped or estimated in these approaches necessarily result in approximate derivatives.

4. A multi-fidelity approach may be used in which a higher fidelity tool produces the output but a lower fidelity method is used to estimate gradients [27].

The inaccuracies 1 and 2 described above are discretization errors that can be reduced through mesh refinement. However, the mesh refinement needed to sufficiently reduce these errors may not be possible in practice, and in these cases the algorithm proposed below could be helpful.
D. Imperfect Data and the State-of-the-art

The examples above highlight important emerging applications — high-dimensional uncertainty propagation and simulation of chaotic systems — in which outputs of interest and their derivatives exhibit some form of inaccuracy. If we want to optimize these outputs, can we rely on state-of-the-art optimization methods?

For low-dimensional design spaces, derivative-free optimization methods could be effective for the applications described above. These methods include deterministic interpolation/regression-based surrogate models [28–30], the Nelder-Mead simplex method [31], and genetic algorithms [32,33]. However, “it is usually not reasonable to try and optimize problems with more than a few tens of variables...” with derivative-free methods [30].

Derivative-based algorithms are highly scalable, making them ideally suited for optimization of smooth functions in large design spaces. Although the challenge of differentiating the simulation software is a potential drawback, algorithmic differentiation [34] has made this task easier. Unfortunately, derivative-based algorithms are also not suitable for the target applications, because they require sufficient accuracy in the data and consistency between the outputs and their derivatives.

Stochastic approximation (SA) algorithms [35–38] can be used to optimize functions whose evaluation contains noise. Some forms of SA also permit the use of noisy gradients [35,39]. There are both theoretical and practical issues with applying SA to the applications described earlier. Theoretically, the “noise” must be unbiased and independent of the design space [38], and these assumptions are not met by the target applications. From a practical perspective, SA algorithms tend to use many “low quality” iterations to ensure (probabilistic) convergence, so function and gradient evaluations must be inexpensive. This requirement is also not fulfilled by the DE-constrained optimization problems under consideration.

Reduced-order models (ROM) offer a distinct approach from derivative-free and derivative-based optimization. Rather than tackling the DE-based optimization directly, ROM methods first seek a simplified, and presumably less expensive, model for the DE simulation. Subsequently, the optimization is performed using the ROM as a surrogate for the full DE model. Methods in this class include projection-based approaches like proper-orthogonal decomposition [40–44]. These approaches typically fix the design parameters while constructing the ROM, although a method that accounts for parameter dependence was recently proposed by Lieberman et al. [45] in the case of steady, linear DEs. However, building parametric ROMs for nonlinear and/or unsteady DEs remains an active and challenging area of research.

II. Arnoldi Sampling and Regression Models

The presence of errors in the data suggests the use of a regression-based model of the objective. Thus, our approach is to sample the function and its gradient and then apply regression to this data to build surrogate models for optimization. The idea of including derivative information in a surrogate model is not new; see, for example, the review [46]. The contribution of this work is the sampling procedure, which is critical in a high-dimensional setting.

A. Arnoldi Sampling

Many sampling strategies are available for surrogate modeling, such as the popular Latin-hypercube sampling method [47]. While many sampling techniques are effective for low-dimensional design spaces, they become increasingly impractical as the number of variables grows. Moreover, conventional sampling methods were developed for interpolation or regression of function values and do not account for derivative information. To address these short-comings, we propose a sampling procedure based on Arnoldi’s method.

Arnoldi’s method is found in Krylov subspace methods for spectral analysis and solving linear systems; see, for example, [48] and [49] and the references therein. In those applications, Arnoldi’s method is used to construct an orthogonal basis for the Krylov subspace \( K_m(z) \equiv \text{span}\{z, Az, A^2z, \ldots, A^{m-1}z\} \).

A version of Arnoldi’s method based on modified Gram-Schmidt is provided in Algorithm 1 for reference. An important feature of Arnoldi’s method is that the matrix \( A \) is not required explicitly: only matrix-vector products of the form \( Az \) are needed. We exploit this aspect of the algorithm in the proposed sampling procedure.

To understand the origins of the proposed sampling procedure, it is helpful to review how Arnoldi’s method is traditionally used in the context of optimization. Efficient optimization algorithms for \( C^2 \) objectives apply Newton’s method, or a quasi-Newton method, to the first-order optimality conditions. For
unconstrained convex problems, Newton’s method produces systems of the form

$$Wp = -g,$$

where $p$ is a trial step, $g = \nabla f$ is the gradient of the objective, and $W = \nabla^2 f$ is the Hessian, or an approximation to it. When Algorithm 1 is used in this setting, $A$ becomes $W$ and Arnoldi’s method reduces to the symmetric Lanczos algorithm that appears in the conjugate gradient method.

When applied to optimization problems, Arnoldi’s method requires Hessian-vector products. These products can be computed in several ways, including algorithmic differentiation [34] and, when PDEs are involved, second-order adjoints [50–52]. The products can also be computed using a finite-difference approximation applied to the gradient, since

$$[\nabla^2 f] z_j = \lim_{\epsilon \to 0} \frac{g(x + \epsilon z_j) - g(x)}{\epsilon}. \quad (1)$$

What does this have to do with sampling? Arnoldi’s method can be transformed into a sampling method by recognizing that the Hessian-vector products selected by the algorithm represent an infinitesimal sampling procedure. If these infinitesimal perturbations are made finite, they can be used as a sampling procedure. In other words, the sample locations are defined by

$$x_j = x_0 + \alpha z_j,$$

where $\alpha > 0$ is the sample radius, and the $z_j$ are defined by Arnoldi’s method with $Az_j$ replaced with $[g(x_0 + \alpha z_j) - g(x_0)] / \alpha$. This Arnoldi sampling procedure is listed in Algorithm 2.

In addition to providing the sample locations and sampled data, Algorithm 2 also produces approximations to the eigenvectors of the Hessian; see lines 16 and 17. This approximation is based on iterative eigenvalue methods [48]. While Arnoldi sampling can also be used to find the approximate eigenvalues, we leave the determination of the eigenvalues to the regression, described later.

The eigen-decomposition in Arnoldi sampling uses the symmetric part of $H_m$, the $m \times m$ upper Hessenberg matrix composed of the $h_{i,j}$. In contrast, the conventional Arnoldi’s method for spectral analysis uses the matrix $H_m$ itself. We use the symmetric part, because $H_m$ reduces to a symmetric matrix when the gradients are accurate and $\alpha \to 0$.

When the gradients are accurate and $\alpha$ is chosen suitably, Arnoldi sampling reduces to a Arnoldi’s method with finite-difference approximations for the Hessian-vector products. Like finite-difference approximations, $\alpha$ must be chosen carefully to achieve optimal performance. Unlike finite-difference approximations, our proposed method benefits from a relatively large sampling radius, one that would normally cause undesirable truncation errors in a finite-difference approximation. In particular, larger $\alpha$ values improve the conditioning of the regression, described next.
Algorithm 2: Arnoldi Sampling.

Data: \( \alpha > 0 \), \( x_0, f_0 = f(x_0) \) and \( g_0 = g(x_0) \)

Result: sample locations \( X = [x_0, x_1, x_2, \ldots, x_m] \), sampled function values \( F = [f_0, f_1, \ldots, f_m] \), sampled gradient values \( G = [g_0, g_1, \ldots, g_m] \), and approximate eigenvectors of the Hessian \( V = [v_1, v_2, \ldots, v_m] \)

1. set \( z_1 = -g_0/\|g_0\| \)
2. for \( j = 1, 2, \ldots, m \) do
   3. set \( x_j = x_0 + \alpha z_j \)
   4. sample \( f_j = f(x_j) \) and \( g_j = g(x_j) \)
   5. compute \( z_{j+1} = (g_j - g_0)/\alpha \)
   6. for \( i = 1, \ldots, j \) do (Modified Gram-Schmidt)
      7. \( h_{i,j} = z_{j+1}^T z_j \)
      8. \( z_{j+1} \leftarrow z_{j+1} - h_{i,j} z_j \)
   9. end
10. compute \( h_{j+1,j} = \|z_{j+1}\| \)
11. if \( \|h_{j+1,j}\| = 0 \) then (check for breakdown)
12. set \( m = j \) and break
13. end
14. \( z_{j+1} \leftarrow z_{j+1}/h_{j+1,j} \)
15. end
16. compute eigen-decomposition of the symmetric part of \( H_m \), i.e. \( \frac{1}{2} [H_m + H_m^T] \tilde{V}_m = \tilde{V}_m \tilde{\Lambda}_m \).
17. compute the approximate eigenvectors \( V_m = Z_m \tilde{V}_m \)

B. Regression Models

The data produced by Arnoldi sampling can be used to construct a variety of different surrogate models. In the present work we focus on quadratic models of the form

\[
q(x) = \tilde{f} + \tilde{g}^T (x - x_0) + \frac{1}{2}(x - x_0)^T \tilde{\Lambda} V^T (x - x_0),
\]

where \( \tilde{f} \in \mathbb{R} \) and \( \tilde{g} \in \mathbb{R}^n \) are the model value and gradient, respectively. The Hessian is approximated by the low-rank matrix \( \tilde{V} \tilde{\Lambda} V^T \) where \( \tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_k) \) holds estimates of the largest \( k \leq m \) eigenvalues and \( V \in \mathbb{R}^{n \times k} \) are the corresponding estimates of the eigenvectors produced by Arnoldi sampling. Here, \( m \) is the number of iterations used in Arnoldi sampling, and \( V \) are the first \( k \) vectors from \( V_m \).

The parameters in the model (2) are \( \tilde{f}, \tilde{g} \), and the \( \tilde{\lambda}_j \), providing \( 1 + n + k \) degrees of freedom. In general, one could also allow the \( V \) to be parameters, but this would produce a nonlinear least-squares regression that is highly multimodal and ill-conditioned. By using the \( V \) from Arnoldi sampling, the least-squares regression reduces to a linear problem.

To determine the parameter values in (2), we seek to minimize the least-squares error between a) the model and the sampled function values and b) the model derivative and the sampled gradients. Thus, the first set of \( m + 1 \) residuals are given by

\[
r_j = q(x_j) - f_j, \quad j = 0, 1, 2, \ldots, m.
\]

Adopting a Matlab-style notation, the second set of (vector) residuals can be expressed as

\[
r_{m+n+1:m+(j+1)n} = (\nabla q)_j - g_j, \quad j = 0, 1, 2, \ldots, m,
\]

where the model gradient is given by

\[
(\nabla q)_j = \tilde{g} + \tilde{\Lambda} V^T (x_j - x_0).
\]

The least-squares problem is to find \( \tilde{f}, \tilde{g}, \) and \( \tilde{\Lambda} \) that minimizes \( \frac{1}{2} r^T r \). More generally, a weighted least-squares objective can be adopted when the error in the sampled gradients is larger than the error in the sampled function, or vice versa.
C. Optimization Framework

We adopt a trust-region framework for this work, because it has proven effective for both quadratic models [53] as well as more general models [54]. Algorithm 3 lists the particular framework we have adopted for this work. Each iteration begins by constructing the quadratic model from the Arnoldi samples. Subsequently, convergence is assessed by comparing the model’s gradient norm to the desired tolerance, \( \tau \). If the algorithm has not converged, the quadratic model is minimized over a trust region of radius \( \Delta \). This constrained optimization problem is solved using the algorithm of Moré and Sorensen [55].

Once the trail step, \( p \), has been found, Algorithm 3 follows a standard trust-radius update based on the ratio, \( \rho \), of the actual objective reduction to the model’s prediction of the reduction. One departure from conventional trust-region methods arises if the step is rejected: in this case the proposed method evaluates the objective and gradient at a perturbation of the current solution estimate. This perturbation is performed in case the step was rejected because the current “imperfect” objective was lower than the true value. We use \( \epsilon = 10^{-8} \) for the perturbation factor.

Finally, while trust-region algorithms are well studied for accurate and even inexact\(^b\) function evaluations, their use with imperfect data is less developed. We plan a careful study of the theoretical properties of Algorithm 3 in future work, but make no guarantees regarding its convergence at present.

Algorithm 3: Arnoldi Sampling in a Trust-region Framework.

**Data:** \( x_0, k \) (approximate-Hessian rank), \( m \) (Arnoldi iterations), \( \alpha \) (sample radius), \( \Delta \) (initial trust radius), and \( \tau \) (convergence tolerance)

**Result:** approximate minimum, \( x \)

1. set \( x \leftarrow x_0 \), and compute \( F_{1,1} = f(x) \) and \( G_{:,1} = g(x) \)
2. use Arnoldi sampling (Algorithm 2) to obtain samples, \( X, F, G \), and approximate eigenvectors, \( V \)
3. for \( l = 1, 2, \ldots \) do
   4. Use linear regression to find parameters \( \bar{f}, \bar{g} \), and the \( \bar{\lambda}_j \) in quadratic model
   5. if \( \| \bar{g} \| \leq \tau \) then (check convergence)
      6. return
   7. end
   8. Solve a trust-region optimization problem based on the quadratic model:
      \[
      \min_p q(p), \quad \text{subject to } \| p \| \leq \Delta.
      \]
   9. compute \( f_l = f(x + p) \) and \( g_l = g(x + p) \)
10. compute \( \rho = \text{ared/pred} = -(f_{l-1} - f_l)/q(p) \)
11. if \( \rho < 0.1 \) then
12.  \( \Delta \leftarrow \Delta/4 \)
13. else
14.  if \( \rho > 3/4 \) and \( \| p \| < \Delta \) then
15.  \( \Delta \leftarrow \min(2\Delta, \Delta_{\text{max}}) \)
16.  end
17.  end
18. if \( \rho > 10^{-4} \) then
19.  set \( x \leftarrow x + p \), and update \( F_{:,1} = f_l \) and \( G_{:,1} = g_l \)
20. else
21.  set \( x \leftarrow x + \epsilon p \), and update \( F_{:,1} = f(x) \) and \( G_{:,1} = g(x) \)
22. end
23. use Arnoldi sampling (Algorithm 2) to update \( X, F, G \), and \( V_{:,1:k} \)
24. end

\(^b\)Inexact refers to errors that can be reduced, e.g. errors due to incomplete convergence of a solver.
III. Results

A. Objective with Synthetic Errors

We begin by investigating Arnoldi sampling applied to a nonlinear convex objective with synthetic errors introduced in the function and gradient evaluations. The objective is defined by

\[ F(x) = \left(2^{-4p+2}\right)\hat{x}^T D \left[I + 2\,\text{diag} \left(\hat{x}^2\right)\right] \hat{x}, \]

where \( D = \text{diag} \left(1, \left(\sqrt{2}\right)^{-1}, \ldots, \left(\sqrt{2p}\right)^{-1}\right), \) \( \hat{x} = Hx, \)

and \( H \) is the \( 2p \times 2p \) Hadamard matrix formed using Sylvester’s construction. The design variable \( x \) is of dimension \( n = 2p \); for the following results, we have selected a problem size of \( n = 2^8 = 256 \).

To mimic the errors encountered in the target applications, Gaussian perturbations are added to the function and gradient after each evaluation of the data. The standard deviation of the perturbations is set to 5% of the initial value of the function and initial max-norm of the gradient.

At each optimization iteration, Arnoldi sampling is limited to 4 samples resulting in 4 + 4(2p) = 1028 datum for the regression. The sampling radius is fixed at \( \alpha = 0.1 \) and the initial trust radius is set to \( \Delta = 10 \).

For the quadratic regression model, we use \( k = 2 \) eigenvalue estimates; i.e., a rank-2 Hessian approximation. The regression model has \( 1 + 2p + 2 = 259 \) parameters.

Figure 3 plots two sets of convergence histories that compare the Arnoldi-based algorithm with the (derivative-based) BFGS [56] quasi-Newton method and the (derivative-free) Nelder-Mead algorithm [31]. The figures plot, in a log-log scale, the objective value \( F \) versus the computational cost measured in function evaluations. The BFGS and Arnoldi-based algorithms are initialized with \( x_0 = [1, 1, \ldots, 1]^T \), and, in the absence of synthetic errors, \( F(x_0) = 0.25 \). The Nelder-Mead algorithm uses \( x_0 \) as one of vertices for the initial simplex, and perturbs each variable value by 5% (independently) to find the remaining \( n \) vertices.

From the two samples, we see that the behavior of BFGS is inconsistent. In one case it makes excellent progress, while in the other case errors in the data cause the line search to stall during the first iteration. The Nelder-Mead simplex fails in both cases. Its failure is the result of the relatively large problem dimension. In contrast, the quadratic regression with Arnoldi sampling performs consistently well, reducing \( F \) by more than 2-orders of magnitude.

To investigate the average performance of the algorithms, statistics were gathered over 100 independent runs. These results are listed in Table 1. The statistics confirm the anecdotal trends inferred from Figure 3. Note that the mean minimum objective for BFGS reflects this method’s inconsistent behavior not its typical performance: it either converges well or not at all. The statistics for the Nelder-Mead simplex algorithm indicate that it consistently fails on this problem. Finally, as observed in Figure 3, the Arnoldi-sampling-based algorithm is both consistent and effective.

| Algorithm                | Mean min F | Std. min F   |
|-------------------------|------------|--------------|
| BFGS (derivative-based) | 0.1151     | 1.227 x 10^{-1} |
| Nelder-Mead (derivative-free) | 0.2502 | 6.860 x 10^{-6} |
| Arnoldi-based           | 0.0019     | 8.399 x 10^{-4} |

IV. Conclusions

Numerical optimization has helped engineers in numerous fields; however, there remain important applications that cannot use conventional optimization algorithms. In this work, we have targeted applications that have large-dimensional design spaces and whose outputs are imperfect, i.e., their outputs and derivatives contain irreducible errors that are incompatible with most gradient-based algorithms. To enable optimization for these applications, we have developed a high-dimensional sampling method based on Arnoldi’s method.
Arnoldi sampling adaptively selects new sample points and tends to capture the dominant eigenmodes of the (spatially averaged) Hessian. The sampling strategy can be used in conjunction with regression to build reduced-order models for optimization when errors are present in the objective and its derivatives. To illustrate this, a trust-region framework was presented in which quadratic models were regressed using data provided by Arnoldi sampling.

The trust-region algorithm was used to minimize a convex, nonlinear objective with synthetic errors introduced in the evaluation of the objective and its gradient. The performance of the algorithm on this problem was promising relative to derivative-based (BFGS) and derivative-free (Nelder-Mead) algorithms. In particular, whereas BFGS had inconsistent convergence and Nelder-Mead failed to converge, the Arnoldi-based algorithm consistently reduced the objective by 2-orders of magnitude.

In the final paper we will investigate the performance of the proposed algorithm applied to a chaotic system.

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