Optimizing Noisy Functions with Machine Learning

Jordan R. Hall

Department of Mathematical and Statistical Sciences
University of Colorado Denver

Friday, February 1, 2019

Notation

- We define a model parameter space Λ with dimension N and a data space $\mathcal{D}$ with dimension M.
  - In most settings, Λ will be of higher dimension than $\mathcal{D}$.
- We define a parameter-to-data map $f : \Lambda \to \mathcal{D}$,
  - f may be polluted by noise.
  - ∇f may be inaccessible.
- We write $d = f(\lambda) \in \mathcal{D}$ to denote a particular datum corresponding to the evaluation of a point $\lambda \in \Lambda$.

- We consider functions $f : \Lambda \to \mathcal{D}$ where $\dim(\Lambda) = N$ is large and $\dim(\mathcal{D}) = M$ is such that $M < N$ or $M << N$.
  - Functions of interest may represent postprocessed quantities from the solution of complex physical models.
- It is not often that every parameter has equal impact on function values – usually some parameters matter more than others.
- The dimension reduction techniques considered seek to explain outputs $f(\Lambda)$ in an *active subspace* $\mathcal{A} \subset \Lambda$ for which $\dim(\mathcal{A}) < N$.
  - Many common uses (e.g., statistics) of f involve integration over Λ and are subject to the *curse of dimensionality*.
  - This forces the use of Monte Carlo or Quasi-Monte Carlo methods.
  - A lower-dimensional representation of f may enable faster methods.

- $\nabla f(\lambda) \in \Lambda$ is a column vector containing the N partial derivatives of f, which for this discussion we assume exist, and are square integrable in Λ equipped with some probability density that is positive everywhere in Λ and 0 otherwise.
  - We consider $\pi_\Lambda^{\text{prior}}(\lambda)$, the density describing our prior state of knowledge, which we abbreviate as π_Λ.
- For convenience, one transforms inputs λ to the origin with some fixed variance, typically so that $\lambda \in [-1, 1]^N$. We define

Covariance in Gradient Space [1]

$$W = \int_\Lambda \nabla f(\lambda) \nabla f(\lambda)^\top \pi_\Lambda(\lambda) d\lambda, \tag{1}$$

which is an $N \times N$ symmetric positive semi-definite matrix.

[1] Constantine, *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*

- Interpreting W as a certain covariance structure over Λ leads one to the idea of computing the Singular Value Decomposition of W,

Singular Value Decomposition (SVD) of W

$$W = U \Sigma V^*, \tag{2}$$

where U is $N \times N$ unitary, Σ is $N \times N$ diagonal with the singular values of W along its diagonal, and V^* is $N \times N$ unitary.

- We plot the singular values, $\{\sigma_i\}_{i=1}^n$ and seek a drop-off in magnitude between some pair of singular values, σ_j and σ_{j+1}. The active subspace is the span of $u_1, \ldots, u_j$, which are the first j columns of U, the left singular vectors of W.

» For a point $\lambda \in \Lambda$, we define

Projection into $\mathcal{A}$, *active variables*

$$\mathcal{P}_{\mathcal{A}}(\lambda) = \sum_{i=1}^{j} \left(u_i^T \lambda\right) u_i, \tag{3}$$

which is the projection of λ in the active directions of f.

» We have arrived at the property that

Resolution of f in $\mathcal{A}$

$$f\left(\mathcal{P}_{\mathcal{A}}(\lambda)\right) \approx f(\lambda). \tag{4}$$

- Finding an active subspace requires forming an approximation to W via Monte Carlo. Here we consider techniques in [1] [2].
- We let $D_S = \{(\lambda_i, f(\lambda_i))\}_{i=1}^{S}$, which is a set of S pairs of samples $\lambda_i \in \Lambda$ and their function values.
- One may use D_S to approximate ∇f. We denote each estimation to $\nabla f(\lambda_i) \approx \widehat{\nabla f}(\lambda_i)$.
- We form the $N \times S$ matrix $\tilde{W}$ (which we present as $\tilde{W}^\top$)

Monte Carlo Approximation to W [1]

$$\tilde{W}^\top := \left[\widehat{\nabla f}(\lambda_1) \cdots \widehat{\nabla f}(\lambda_S) \right]. \tag{5}$$

[1] Russi, *UQ with Experimental Data and Complex System Models*

[2] Constantine et al, *Computing Active Subspaces Efficiently with Gradient Sketching*

- Forming the SVD of $\tilde{W}$, $\tilde{W} = \tilde{U}\tilde{\Sigma}\tilde{V}^*$, we search for a drop off in the magnitude of the singular values $\{\tilde{\sigma}_i\}_{i=1}^S$. Assuming such a drop off occurs for an index $j : 1 < j < S$, we have the j corresponding left singular vectors,$\tilde{u}_1, \ldots, \tilde{u}_j$.
- Then we define

Monte Carlo approximation to $\mathcal{A}$

$$\mathcal{A}\,(f; D_S) := \text{span}\{\tilde{u}_1, \ldots, \tilde{u}_j\},$$

the active subspace of f with respect to the samples D_S.

- For low dimensional $\mathcal{A}$, we may check $f(\mathcal{P}_{\mathcal{A}}(\lambda)) \approx f(\lambda)$ in a *sufficient summary plot*, where we plot active variables against function values.

- Many important physical systems possess turbulent or chaotic behavior.
- The physical state of the system $u(x, \lambda)$ and the corresponding parameter to observable map $f(u(x, \lambda))$ may be modeled as a stochastic process, or as a deterministic function with additive or multiplicative noise.
  - In this setting, the efficient extraction of accurate gradients of f in parameter space is a challenging undertaking, as popular techniques based on linearization, including adjoint methods, are inaccurate [1] [2].
  - The finite-difference approximation of ∇f_Λ involve $N = \text{dim}\Lambda$ additional, usually nonlinear model solves for the physical system state $u(x, \lambda_i + \delta\lambda_i)$, and may be greatly polluted by the noise in f.

[1] Lea, *Sensitivity analysis of the climate of a chaotic system*

[2] Qiqi, *Least Squares Shadowing sensitivity analysis of chaotic limit cycle oscillations*

- We are interested in derivative-free optimization (DFO) algorithms suited for additive and multiplicative noise. These techniques only require evaluations of the noisy model and random draws from a normal distribution.
  - In particular, we consider the STep-size Approximation in Randomized Search (STARS) algorithm [1].
- The smoothing factor and step size in STARS depend on scale factors of the L_1 Lipschitz constant of f. It is of interest to obtain estimates of L_1, which is not straightforward in a gradient-free setting. We refer to [2] [3] for Lipschitz constant learning.
- We note that **the convergence of STARS is dimension dependent.**

---

[1] Chen and Wild, *Randomized DFO of Noisy Convex Functions*

[2] Jan-Peter Calliess, *Lipschitz optimisation for Lipscitz interpolation*

[3] Kvasov and Sergeyev, *Lipschitz gradients for global optimization in a one-point-based partitioning scheme*

» We consider the problem

Optimization Under Additive Uncertainty [1]

$$\min_{\lambda \in \mathbb{R}^N} \quad \mathbb{E}\left[f(\lambda) + \nu(\lambda; \epsilon)\right], \tag{6}$$

» where:

(i.) $f : \mathbb{R}^N \to \mathbb{R}$ is convex;
(ii.) ϵ is a random variable with probability density $P(\epsilon)$;
(iii.) for all λ the additive noise model ν is independent and identically distributed, has bounded variance σ_a^2, and is unbiased; i.e., $\mathbb{E}_\epsilon(\nu(\lambda; \epsilon)) = 0$.

[1] Chen and Wild, *Randomized DFO of Noisy Convex Functions*

Stepsize h

$$h = (4L_1(N+4))^{-1}$$

where N is the dimension and L_1 is the global Lipschitz constant for $\|\nabla f\|$.

Smoothing factor μ^*

$$\mu^* = \left[\frac{8\sigma_a^2 N}{L_1^2(N+6)^3}\right]^{\frac{1}{4}}$$

where σ_a^2 is the variance of the additive noise.

Algorithm 1: *Minimization of f via STARS*[1].

1: Define: $\left(\texttt{maxit}; \lambda^{(0)}; f_0 := f(\lambda^{(0)}); \mu^*; h\right)$. Set `i=1`.

2: Draw a random $N \times 1$ vector r^i, where $r^i_j \sim N(0,1)$ for $j = 1, \dots, N$ and draw ϵ_i.

3: Evaluate $g_i := f(\lambda_{i-1} + \mu^* u_i)$.

4: Set $d_i := \dfrac{g_i - f_{i-1}}{\mu^*} u_i$.

5: Set $\lambda_i = \lambda_{i-1} - h \cdot d_i$.

6: Evaluate $f_i := f(\lambda_i)$; set `i=i+1`; return to 2.

7: Terminate when `i=maxit`.

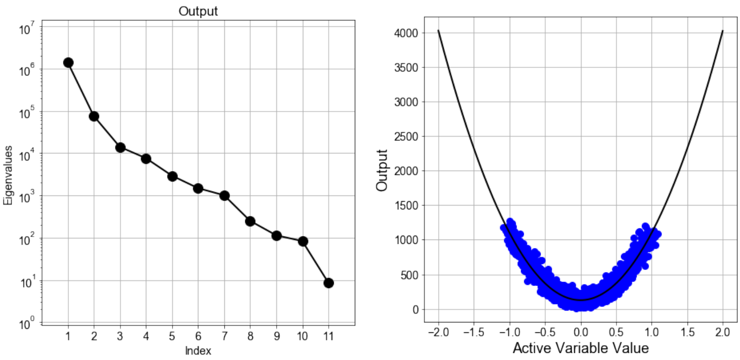
[1] Chen and Wild, *Randomized DFO of Noisy Convex Functions*

Example 3.

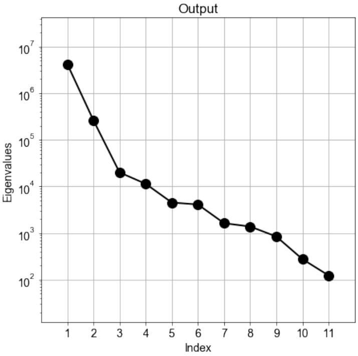
Let $\Lambda = [-1, 1]^{11}$ and define

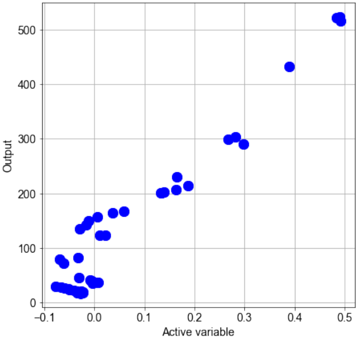
$$f(\lambda) = \sum_{i=0}^{10} 2^{(-1)^i i} \lambda_i^2 + \epsilon(\lambda),$$

where $\epsilon(\lambda)$ is a draw of additive noise corresponding to the input λ; here, we take draws of ϵ of order 10^{-4}. We see that $\mathcal{D} = [0, 2^{10}]$ and $N = 11$, $M = 1$. Note that the minimum of f is given by $0 \in \Lambda$. Here, as i increases, terms in f become either more important or less important, depending on whether i is even or odd.

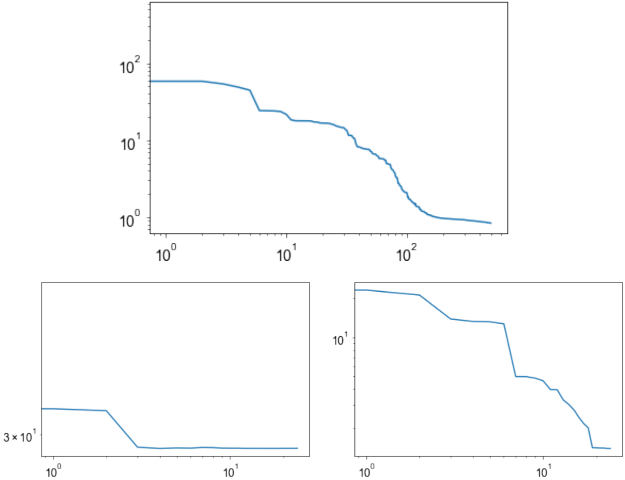


Left: A plot of the eigenvalues of the matrix $\hat{W}$ formed from 1000 Monte Carlo samples in Λ. We see one dominant eigenvalue on the order of 10^6. Right: A sufficient summary plot where all 1000 samples are projected into $\mathcal{A}$ and plotted against their function values; a quadratic surrogate fits the projected data with $R^2 \approx 0.9$.





Left: A plot of the eigenvalues of the matrix $\hat{W}$ formed from using 100 DFO iterates as samples in Λ. We again see one dominant eigenvalue between orders 10^6 and 10^7. Right: A sufficient summary plot where all 100 samples are projected into $\mathcal{A}$ and plotted against their function values.



Top: 500 iterations of standard DFO; Bottom Left: 25 iterations of minimizing f with DFO along the λ_8 axis; Bottom Right: 25 iterations of minimizing f with DFO along the λ_6 axis.

- Currently, only some of the software used to produce results in this paper are publicly available on GitHub.com.
- Some of the algorithms used here and other algorithms that are of interest are within open-source packages available online [1] [2].
- Special thanks to Michael Pilosov for bringing Active Subspace package into Python 3
- Other schemes considered here make modifications to given algorithms and remain under development.
- A major goal of this thesis proposal will be producing well-documented, open-source software complete with python Jupyter Notebooks containing illustrative, replicable examples.

[1] T. Butler et al
[2] Constantine et al

- Battaglia, D. J. and Burrell, K. H. and Chang, C. S. and Ku, S. and deGrassie, J. S. and Grierson, B. A. “Kinetic neoclassical transport in the H-mode pedestal." Physics of Plasmas,Volume 21, No. 7. 2014.
- T. Butler and J. Jakeman and T. Wildey. “Combining Push-Forward Measures and Bayes’ Rule to Construct Consistent Solutions to Stochastic Inverse Problems." SIAM Journal on Scientific Computing, Volume 40, No. 2, pp. A984-A1011, 2018.
- Jan-Peter Calliess. “Lipschitz optimisation for Lipschitz interpolation." In 2017 American Control Conference (ACC 2017), Seattle, WA, USA, May 2017.
- Chen and Wild. “Randomized Derivative-Free Optimization of Noisy Convex Functions." Funded by the Department of Energy. 2015.
- Constantine, Paul G. “Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies." SIAM, 2015.
- Constantine, Eftekhari, Wakin. “Computing Active Subspaces Efficiently with Gradient Sketching." Conference paper, 2015 IEEE 6th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP).
- Kvasov and Sergeyev. “Lipschitz gradients for global optimization in a one-point-based partitioning scheme." Journal of Computational and Applied Mathematics. Volume 236, Issue 16, pp. 4042-4054. 2012.
- S. Ku and R. Hager and C.S. Chang and J.M. Kwon and S.E. Parker. “A new hybrid-Lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma." Journal of Computational Physics, Volume 315, pp. 467-475. 2016.
- Lao, L.L, St. John, H, R.D. Stambaugh, A.G. Kellman, and Pfeiffer, W.,“Reconstruction of current profile parameters and plasma shapes in tokamaks”, Nuclear Fusion, Volume 25,No. 11,pp. 1611,1985.

- Lea, Daniel J. and Allen, Myles R. and Haine, Thomas W. N. “Sensitivity analysis of the climate of a chaotic system." Tellus A, Volume 52, No. 5, pp. 523-532. 2000.
- Russi, Trent M. “Uncertainty Quantification with Experimental Data and Complex System Models." Dissertation, University of California Berkeley. 2010.
- Smith, Ralph.“Uncertainty Quantification: Theory, Implementation, and Applications.” SIAM, 2013.
- Stuart, Andrew. “Inverse problems: A Bayesian perspective." Acta Numerica, volume 19, pp. 451-559. 2010.
- Tarantola, Albert. “Inverse Problem Theory and Methods for Model Parameter Estimation." SIAM. 2005.
- Takeda, T. and Tokuda S.,“Computation of MHD equilibrium of tokamak plasma”, Journal of Computational Physics,93,1,1 - 107,1991.
- Qiqi Wang and Rui Hu and Patrick Blonigan. “Least Squares Shadowing sensitivity analysis of chaotic limit cycle oscillations." Journal of Computational Physics, Volume 267, pp. 210-224. 2014.
- Wesson, J. “Tokamaks." “Oxford University Press, 4th edition." 2011.
- Wildey, T., Butler, T., Jakeman, J., Walsh, S. " A Consistent Bayesian Approach for Stochastic Inverse Problems Based on Push-forward Measures." SAND2017-3436PE. 2017.