

Thesis Proposal

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Literature Review and Framework

- Data-Consistent Inversion (DCI)
- Optimization Methods for Solving Inverse Problems
- Dimension Reduction
- Derivative-Free Optimization (DFO)

Research Questions

- Data-Consistent Deregularization for Nonlinear f
- Impact of Noise on MAP Point and Updated Prior
- Learning from Sampling
- Using the Active Subspace
- Application: Callibrated Anomolous Diffusion in Tokamak Plasmas
- Application: Magnetic Equilibria in Tokamaks

Preliminary Results and Research Plan

- Learning from Sampling
- Using the Active Subspace
- Data-Consistent Deregularization for Nonlinear f
- Impact of Noise on MAP Point and Updated Prior
- From Model Problems to Fusion Applications
- Software Dissemination

Timeline

References



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 $f : \Lambda \rightarrow \mathcal{D}$,
 - 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 $\lambda \in \Lambda$.



The Stochastic Inverse Problem (SIP)¹²³

Given:

- » the *prior distribution*, $\pi_{\Lambda}^{\text{prior}}(\lambda)$: the prior or initial knowledge of the parameter space Λ
- » the *observed distribution*, $\pi_{\mathcal{D}}(d)$: the uncertain state of knowledge of the observed data in \mathcal{D} .

The SIP is obtaining an *updated probability distribution*, $\pi_{\Lambda}^{\text{update}}(\lambda)$ combining the given prior information and the observed data.

¹T. Butler et al, *Combining Pushforward Measures and Bayes' Rule to Construct Consistent Solutions to SIPs*

²Tarantola, Albert, *Inverse Problem Theory and Methods for Model Parameter Estimation*

³Stuart, Andrew., *Inverse problems: A Bayesian perspective*



The Forward Uncertainty Quantification (UQ) Problem

Given a probability distribution which is nonzero for every $\lambda \in \Lambda$, the *forward UQ problem* is finding the probability distribution of $f(\Lambda)$.

- » The forward UQ problem is, in its own right, a nontrivial and important problem in UQ.
- » The *classical Bayesian* or *statistical Bayesian* solution to the inverse problem is generally *not consistent*; i.e., it is not a *pull-back probability measure*.
 - This means the distribution of points drawn from the updated distribution $\pi_{\Lambda}^{\text{update}}$ and mapped through f , called the *push-forward* of $\pi_{\Lambda}^{\text{update}}$, is not equal to the observed probability distribution, $\pi_{\mathcal{D}}$.



- » Data-Consistent Inversion (DCI) seeks an updated solution $\pi_{\Lambda}^{\text{update}}$ for which the push-forward exactly equals $\pi_{\mathcal{D}}$.
- » To obtain such a solution, we must solve the forward UQ problem.
- » We denote the solution to the forward UQ problem with $\pi_{\mathcal{D}}^{f(\Lambda)}(d)$.
- » We present the data-consistent solution,

Data-Consistent Solution to the SIP¹

$$\pi_{\Lambda}^{\text{update}}(\lambda) = \pi_{\Lambda}^{\text{prior}}(\lambda) \frac{\pi_{\mathcal{D}}(f(\lambda))}{\pi_{\mathcal{D}}^{f(\Lambda)}(f(\lambda))}. \quad (1)$$

¹T. Butler et al, *Combining Pushforward Measures and Bayes' Rule to Construct Consistent Solutions to SIPs*

- » Approximately solving the forward UQ problem needed to form (1) generally requires density estimation, which converges at best like Monte Carlo, $\sim \mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$, where n represents the number of samples of f .
- » In the case that f is a linear operator and the prior and observed densities are Gaussians, the solution to the SIP can be obtained exactly, and its mean is equivalent to the solution of a deterministic convex optimization problem.
 - The form of the objective function is different for statistical Bayesian inversion and DCI.



- » Assume $\pi_{\Lambda}^{\text{prior}}$ and $\pi_{\mathcal{D}}$ are Gaussians with means λ_{prior} and d_{obs} and covariance matrices C_{Λ} and $C_{\mathcal{D}}$, respectively. If f is linear, then $f(\lambda) = A\lambda$. We define

The Classical Misfit Function ¹

$$S(\lambda) = \frac{1}{2} \left(\left\| C_{\mathcal{D}}^{-1/2}(A\lambda - d_{\text{obs}}) \right\|_2^2 + \left\| C_{\Lambda}^{-1/2}(\lambda - \lambda_{\text{prior}}) \right\|_2^2 \right). \quad (2)$$

Comments

- » The statistical mode of the posterior is called the maximum a posteriori point, or *MAP point*.
- » The λ value that minimizes S is the MAP, λ_S^* , and the classical solution to the (linear) SIP is $\pi_{\Lambda}^{\text{post}}(\lambda) = c \cdot \exp(-S(\lambda))$.

¹Tarantola, Albert, *Inverse Problem Theory and Methods for Model Parameter Estimation*



- » S is reformulated so it is an objective function with a minimizer corresponding to the *data-consistent* MAP point.
- » A *deregularization* term is appended so that if A is invertible, the regularization will be canceled. We define

The Data-Consistent Misfit Function ¹

$$T(\lambda) = \frac{1}{2} \left(\left\| C_{\mathcal{D}}^{-1/2} (A\lambda - d_{\text{obs}}) \right\|_2^2 + \left\| C_{\Lambda}^{-1/2} (\lambda - \lambda_{\text{prior}}) \right\|_2^2 \right) - \frac{1}{2} \left(\left\| C_A^{-1/2} (A(\lambda - \lambda_{\text{prior}})) \right\|_2^2 \right), \quad (3)$$

where $C_A = AC_{\Lambda}A^T$.

¹Wildey et al, *A Consistent Bayesian Approach for SIPs Based on Push-forward Measures*

Comments

- » If π_{Λ} and $\pi_{\mathcal{D}}$ are Gaussian, the data-consistent solution to our inverse problem is given exactly by $\pi_{\Lambda}^{\text{update}}(\lambda) = c \cdot \exp(-T(\lambda))$ or, in a more useful form, a Gaussian with mean λ_T^* and covariance matrix

$$C_{\Lambda}^U = (A^{\top} C_{\mathcal{D}}^{-1} A + C_{\Lambda}^{-1} - A^{\top} (C_A)^{-1} A)^{-1}$$

- » The deregularization term in (3) ensures the updated distribution on Λ will only be regularized in directions uninformed by data.



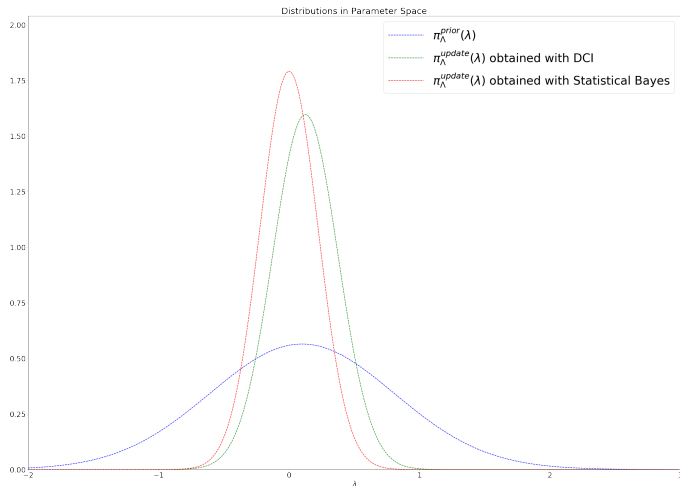
Example 1.

Let $f(\lambda) = 2\lambda$, $\lambda_{\text{prior}} = 0.1$, $C_{\Lambda} = [0.5]$, $d_{\text{obs}} = 0.25$, and $C_{\mathcal{D}} = [0.25]$; note, $N = M = 1$. We find

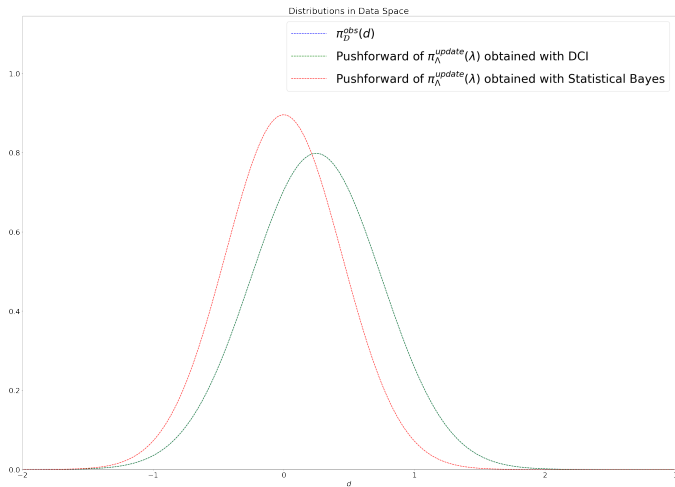
$$S(\lambda) = 2((2\lambda - 0.25)^2 + (\lambda - 0.1)^2) \quad \text{and} \quad T(\lambda) = 2(2\lambda - 0.25)^2.$$

- » S is minimized by $\lambda_S^* = 3/25$.
- » With Gaussian assumptions on the prior and data, we have $\pi_{\Lambda}^{\text{post}} \sim \exp(-S(\lambda))$ which is a $N(\lambda_S^*, 1/18)$.
- » Notice $f(\lambda_S^*) = 6/25 \neq d_{\text{obs}}$.
- » T is minimized by $\lambda_T^* = 1/8$.
- » With Gaussian assumptions on the prior and data, we have $\pi_{\Lambda}^{\text{update}} \sim \exp(-T(\lambda))$ which is a $N(\lambda_T^*, 1/16)$.
- » Notice $f(\lambda_T^*) = d_{\text{obs}}$.





Distributions in parameter space from Example 1.



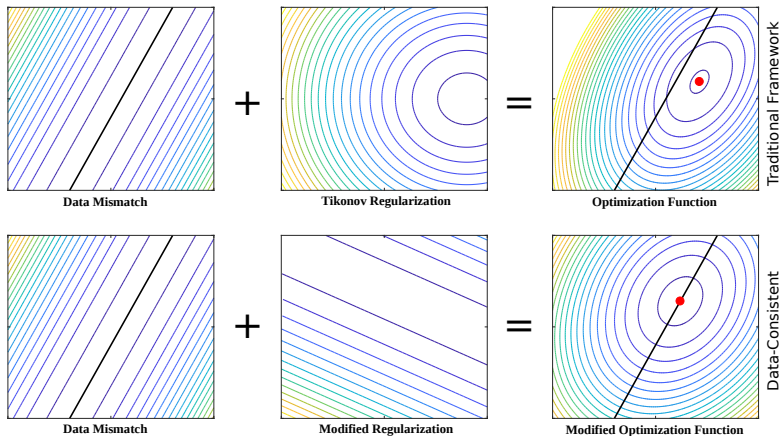
Distributions in data space from Example 1.

Example 2. ¹

Let $f(\lambda) = 2\lambda_1 - \lambda_2$, $\lambda_{\text{prior}} = (0.1 \quad 0.2)^\top$, $C_\Lambda = \text{diag}[0.5, 0.25]$, $d_{\text{obs}} = 0.1$, and $C_{\mathcal{D}} = [0.25]$. ($N = 2$ and $M = 1$.)

- » For any $\lambda \in \Lambda$, $f(\lambda) = d = 2\lambda_1 - \lambda_2$. Since there is just a single d_{obs} , we have $0.1 = 2\lambda_1 - \lambda_2$.
- » S is minimized by $\lambda_S^* = (7/50, 19/100)$. With Gaussian assumptions, we have $\pi_\Lambda^{\text{post}} \sim \exp(-S(\lambda))$ with mean λ_S^* . Notice $f(\lambda_S^*) = 9/100 \neq d_{\text{obs}}$.
- » In the data-consistent formulation, we have T minimized by $\lambda_T^* = (13/90, 17/90)$. Notice $f(\lambda_T^*) = 9/90 = d_{\text{obs}}$. With Gaussian assumptions, we have $\pi_\Lambda^{\text{update}} \sim \exp(-T(\lambda))$ with mean λ_T^* .

¹Wildey et al, *A Consistent Bayesian Approach for SIPs Based on Push-forward Measures*



This figure ¹ shows the process of obtaining the statistical/classical Bayesian solution and data-consistent solution in Example 2.

¹Wildey et al, *A Consistent Bayesian Approach for SIPs Based on Push-forward Measures*

- » We consider functions $f : \Lambda \rightarrow \mathcal{D}$ where $\dim(\Lambda) = N$ is large and $\dim(\mathcal{D}) = M$ is such that $M < N$ or $M \ll N$.
 - 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

$$W = \int_{\Lambda} \nabla f(\lambda) \nabla f(\lambda)^{\top} \pi_{\Lambda}(\lambda) d\lambda, \quad (4)$$

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

¹Constantine, *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

$$W = U\Sigma V^*, \quad (5)$$

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, \dots, 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*

$$\mathcal{P}_{\mathcal{A}}(\lambda) = \sum_{i=1}^j (u_i^T \lambda) u_i, \quad (6)$$

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}

$$f(\mathcal{P}_{\mathcal{A}}(\lambda)) \approx f(\lambda). \quad (7)$$

- » 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

$$\tilde{W}^\top := \begin{bmatrix} \widehat{\nabla f}(\lambda_1) & \cdots & \widehat{\nabla f}(\lambda_S) \end{bmatrix}. \quad (8)$$

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

²Constantine 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, $\tilde{u}_1, \dots, \tilde{u}_j$.
- » Then we define

Monte Carlo approximation to \mathcal{A}

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

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 $N = \dim \Lambda$ 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 .

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

²Qiqi, *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.**

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

²Jan-Peter Calliess, *Lipschitz optimisation for Lipschitz interpolation*

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



» We consider the problem

Optimization Under Additive Uncertainty ¹

$$\min_{\lambda \in \mathbb{R}^N} \mathbb{E} [f(\lambda) + \nu(\lambda; \epsilon)], \quad (9)$$

» where:

- (i.) $f : \mathbb{R}^N \rightarrow \mathbb{R}$ 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., $\mathbb{E}_\epsilon(\nu(\lambda; \epsilon)) = 0$.

¹Chen 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 $f + \epsilon$ via STARS¹.*

- 1: Define: $(\text{maxit}; \lambda^{(0)}; f_0 := f(\lambda^{(0)}) + \epsilon_0; \mu^*; h)$. Set $i=1$.
- 2: Draw a random $N \times 1$ vector r^i , where $r_j^i \sim N(0, 1)$ for $j = 1, \dots, N$ and draw ϵ_i .
- 3: Evaluate $g_i := f(\lambda_{i-1} + \mu^* u_i) + \epsilon_i$.
- 4: Set $d_i := \frac{g_i - f_{i-1}}{\mu^*} u_i$.
- 5: Set $\lambda_i = \lambda_{i-1} - h \cdot d_i$.
- 6: Evaluate $f_i := f(\lambda_i) + \epsilon_i$; set $i=i+1$; return to 2.
- 7: Terminate when $i=\text{maxit}$.

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

- » Recall for a linear f where $f(\lambda) = A\lambda$, the deregularization term in (3) is

Deregularization Term

$$\left\| C_A^{-1/2} (A(\lambda - \lambda_{\text{prior}})) \right\|_2^2, \quad (10)$$

where $C_A = AC_\Lambda A^\top$.

Research Question

For a nonlinear f , inversion via convex optimization may be performed if f is linearized and Gaussian assumptions are met.

- What form should the deregularization term take to roughly preserve data consistency?
- Can we construct error bounds based on local linearization error?



For a linear map f and Gaussian knowledge state, the optimization solution of a SIP will be exact.

Research Questions

- » To what extent does additive or multiplicative noise alter DCI via optimization?
- » We investigate how using DFO to solve for a data-consistent MAP point compares to standard DCI methods (density estimation) in this setting.



We are interested in several problems that involve sampling Λ and evaluating f including solving the forward problem, finding an active subspace via Monte Carlo, and performing DFO.

Research Questions

- » We are interested in comparing active subspaces obtained from sampling f with few samples, or with samples generated from some other process, such as a DFO algorithm.
- » We are interested in learning Lipschitz constants ^{1 2} from sampling, where samples are few and potentially generated by DFO.

¹Jan-Peter Calliess, *Lipschitz optimisation for Lipschitz interpolation*

²Kvasov and Sergeyev, *Lipschitz gradients for global optimization in a one-point-based partitioning scheme*



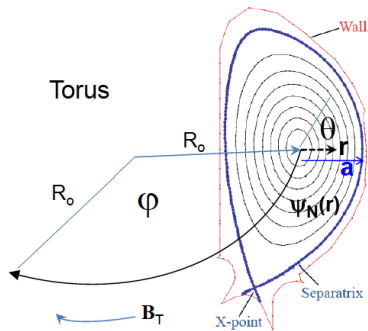
- » We are interested in investigating the effectiveness of only optimizing f in its active variables.
- » The most compelling approach we have observed is to modify the DFO algorithm discussed above to only take random walks in directions lying in \mathcal{A} .

Modified DFO Algorithm

- Obtain the first j singular unit vectors u_1, \dots, u_j corresponding to the SVD of \hat{W} .
 - Take j draws from a specified normal distribution, which we denote with $s_i \sim N(\mu, \sigma^2)$.
 - Form the random vector v for the k -th step in a DFO algorithm as
$$v^{(k)} = \sum_{i=1}^j s_i u_i.$$
- » Other weighting schemes on the u_i 's could be considered, such as weights given by singular values.



Tokamak Geometry

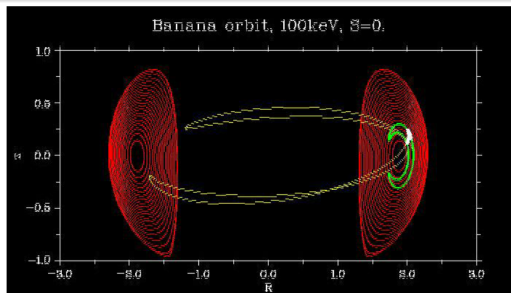


Poloidal cross section at a constant toroidal angle

- » Normalized flux coordinate ψ_N : 0 at r , 1 at $\frac{r}{a} = 1$.

Transport in Tokamaks

Transport in tokamak plasmas can be strongly driven by a combination of *neoclassical* effects and plasma *microturbulence*.



Neoclassical theory predicts complex particle motion

- » Neoclassical transport: simplified Vlasov-Boltzman equation coupled with Maxwell's equations ¹.

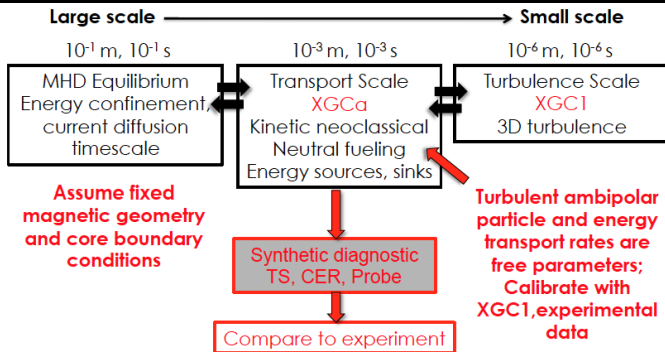
¹Wesson, *Tokamaks*

Simulating the microturbulence in the plasma involves very expensive kinetic simulations, especially when simulating the plasma edge ¹.

- » An alternate approach to simulate microturbulence is by fitting an anomalous diffusion model.
 - Fit using experimental data
 - Direct Numerical Simulation (DNS) approach: Fit using high-fidelity simulation data.
 - Deterministic efforts in this setting include ².
- » This approach is similar to common modeling techniques in parameterizing micro-scale effects in macro/meso-scale systems (e.g., turbulence models, sub-grid models).

¹S. Ku et al, *A new hybrid-Lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma*

²Battaglia et al, *Kinetic neoclassical transport in the H-mode pedestal*



Research Question

We propose to investigate the data-consistent calibration of an anomalous diffusion model in an axisymmetric setting (XGCa) to high-fidelity experimental or simulation data (XGC1) ¹.

¹S. Ku et al, *A new hybrid-Lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma*

- » The dimensionless, axisymmetric Grad-Shafranov equation:

The Grad-Shafranov Equation ¹

$$r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial \psi_n}{\partial r} \right) + \frac{\partial^2 \psi_n}{\partial z^2} = -\frac{\alpha^2}{2} \frac{df^2}{d\psi_n} - r^2 \alpha^2 \frac{dp}{d\psi_n}. \quad (11)$$

- » In equilibrium fitting to data ²: p and f^2 are expanded as basis functions in ψ_n , with the constraint that p and f^2 vanish at the boundary.

Research Question

The updated PDF π_{Λ}^u is important to prediction of plasma profiles.

DCI problem: Find the updated PDF of the uncertain parameters in the expansions of p and f^2 .

¹Takeda, T. and Tokuda, S., *Computation of MHD equilibrium of tokamak plasma*

²Lao et al, *Reconstruction of current profile parameters and plasma shape in tokamaks*



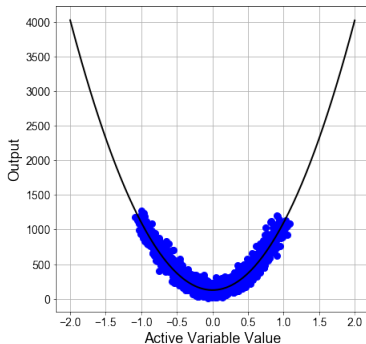
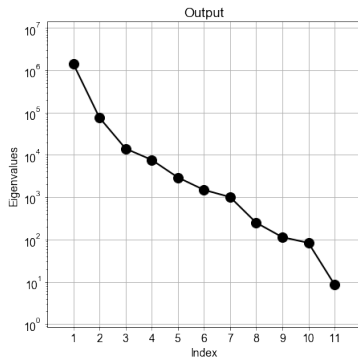
Example 3.

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

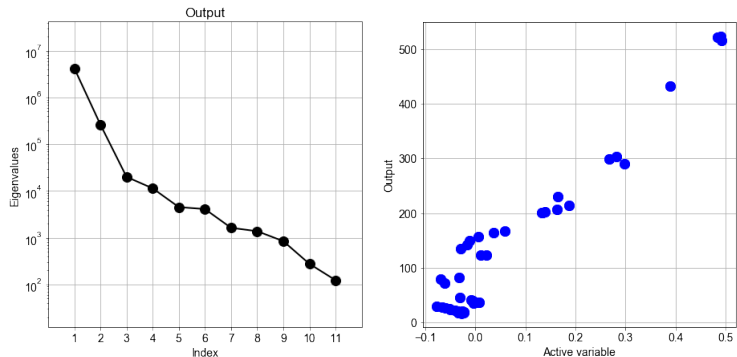
$$f(\lambda) = \sum_{i=0}^{10} 2^{(-1)^i i} \lambda_i^2 + \epsilon(\lambda),$$

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.

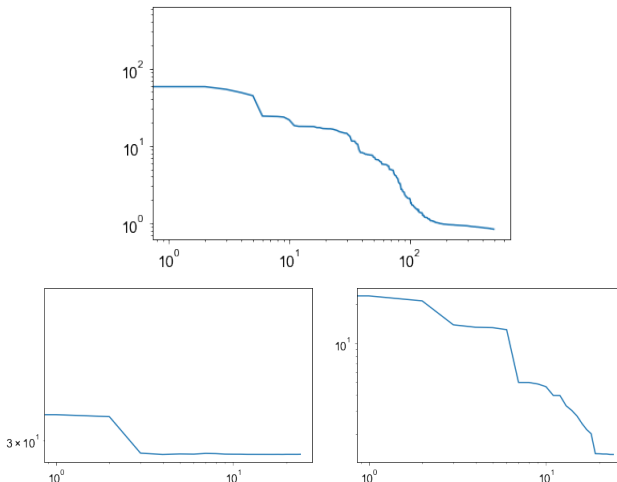




Left: A plot of the eigenvalues of the matrix \hat{W} formed from 1000 Monte Carlo samples in Λ . We see one dominant eigenvalue on the order of 10^6 . Right: A sufficient summary plot where all 1000 samples are projected into \mathcal{A} and plotted against their function values; a quadratic surrogate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

We must consider ways to express the data-consistent deregularization for nonlinear f . This is a theoretical task which will require a closer literature review and heavy collaboration with advisers.

Research Plan

- » Reformulate problem as minimization of the statistical Bayesian misfit constrained by data-consistency, which will impose a nonlinear equality constraint.



Under assumptions of Gaussian priors and data and a linear f , the solution of our SIP is exactly determined by optimization methods. How do multiplicative or additive noise models on f perturb the solution of the SIP?

Research Plan

- » We propose to analyze additive and multiplicative noise in the context of optimization methods for DCI.
- » We consider the impact of this noise on MAP points and updated priors, especially when optimization is performed in a derivative-free setting.



We propose to investigate the approximate solution of data-consistent inverse problems in tokamak plasma modeling via optimization approaches.

Derivative Free Optimization

- » Initial model functions + noise
- » DCI of a subgrid large eddy simulation(LES) model for isotropic turbulent flow.
- » DCI of an anomalous diffusion model for gyrokinetic turbulence in XGCa.

Gradient-based methods

- » Approximate DCI for a model elliptic problem with a parameterized forcing function, with parameter gradients obtained via adjoint methods.
- » Data-consistent MHD equilibria (Grad-Shafranov)



- » 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}.
- » 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.

¹T. Butler et al



²Constantine et al












We outline a rough timeline for the remaining 2 years in a 5.5 year plan.

- » Clean existing algorithms and examples, generate richer research results related to DFO and active subspaces, and build a model inverse problem for investigation. (Dec 2018/Jan 2019)
- » On RA for Spring 2019. (Jan 2019-May 2019)
- » Write and present MS-level results. (Feb/Mar 2019)
- » Work on theoretical formulation of deregularization for nonlinear f . Work on generating notebooks and examples. (Ongoing/Spring and Summer 2019)
- » Summer research; begin writing thesis; summer school/internship/conferences. (Jun/Jul/Aug 2019)
- » Fall 2019 - Writing phase, revisions.
- » Spring 2020 - Final revisions, software, documentation.
- » Summer 2020 Internship/collaborations, publishing, formatting.
- » Defend thesis Summer 2020 or early Fall 2020.



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