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Recent Developments in Parameter Estimation for Complex Simulations

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Joint work with Jason Sarich and Stefan Wild

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Complex Simulations

Parameter estimation problem are of the form

$$\min \{ f(x) : x_L \le x \le x_U \}, \qquad f(x) = \mathcal{F}[s(x)],$$

where the mapping $s : \mathbb{R}^n \mapsto \mathbb{R}^m$ describes the simulation as a function of the parameters (or controls) x.

Examples

- Nuclear fission
- Modeling subsurface flow in the Hanford area
- Rietveld refinement of powder diffraction data
- Pumping rates for the de-contamination of groundwater

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Parameter Estimation Problems in Nuclear Fission

- $x \in \mathbb{R}^n$ is the vector of parameters
- m is the number of nuclei.
- $f_k(x)$ is the vector of observables for the k-th nucleus.
- y_k is the data vector associated with the k-th nucleus.

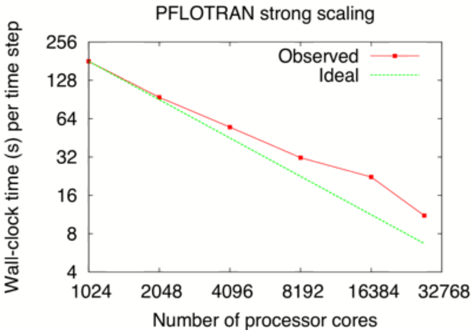
$$x \Longrightarrow \boxed{\text{HFBTHO, MFD, \ldots}} \Longrightarrow f_k(x)$$

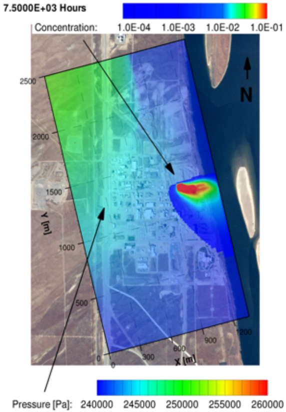
The least-squares approach (χ^2) requires the minimization of

$$f(x) = \frac{1}{2} \sum_{k=1}^{m} \sigma_k \| f_k(x) - y_k \|^2$$

where $\|\cdot\|$ is the l_2 norm and σ_k is a set of weights.

Subsurface Flow in the Hanford Area





- PFLOTRAN (1024 processors, Cray XT3) requires 2.3 hours
- Three layers and about two parameters per layer

Challenges of Complex Simulations

- Expensive evaluations of $f(x)$
- Large memory requirements
- Noisy function evaluations
- Lack of derivatives with respect to parameters
- Possibly several minima
- Limited computational budget

In a complex simulation, we need to obtain acceptable solutions in a small multiple of n function evalutions.

Derivative-Free Optimization Algorithms

Direct Search Methods

- Nelder-Mead (nmsmax, nelder, fminsearch)
- Pattern search (appspack, mdsmax, sid-psm, nomad)

Model-Based Methods

- Quadratic models (uobyqa, newuoa, dfo)
- Radial-basis models (orbit, boosters)
- Quasi-Newton models(imfil, . . .)

Numerical Recipes only mentions the Nelder-Mead method

Model-Based Derivative-Free Algorithms

For $k = 0, \ldots$

- ◇ Compute the model q_k.
- ◇ Check the fidelity of the model.
- ◇ Compute a step s_k in the trust-region $\|s\| \le \Delta_k$.
- ◇ Update x_k and the trust-region radius Δ_k.

Two possible classes of models

- ◇ Quadratic (full, partial, linear)
- ◇ Adaptive models

Quadratic Models

Quadratic models in $\mathbb{R}^n$

$$q(x) = c + g^T(x - x_0) + \tfrac{1}{2}(x - x_0)^T G(x - x_0)$$

are obtained by interpolating f at $\frac{1}{2}(n+1)(n+2)$ points.

Cost of computing a full quadratic model of f in $\mathbb{R}^n$

n	5	10	20	30	40	50
evaluations of f	21	66	231	496	861	1326

Minimal Norm (Frobenius) Quadratics

Least-change (partial) quadratic models determine a new quadratic q_+ for any $m \geq n+1$ points $x_1, \ldots x_m$ by requiring that

$$\min \left\{ \|\nabla^2 q_+ - \nabla^2 q\|_F^2 : q_+(x_k) = f(x_k), \quad 1 \leq k \leq m \right\}$$

where q is the current model.

- Existence of the model is not guaranteed
- There is at most one model that satisfies these conditions
- Computing the model requires order $(m+n)^3$ operations
- Model fidelity depends on the geometry of the sample points

Extensions

In least-squares problems where

$$f(x) = \frac{1}{2} \sum_{k=1}^{m} f_k(x)^2,$$

we can construct quadratic models $q_1, \ldots q_m$, and consider the (non-quadratic) model

$$f_M(x) = \frac{1}{2} \sum_{k=1}^{m} q_k(x)^2.$$

⚠ See Stefan Wild's talk for computational results.

Benchmarking

A **benchmark** is defined by

- ◇ $\mathcal{P}$ – Benchmark problems
- ◇ $\mathcal{T}$ – Convergence test
- ◇ $\mathcal{S}$ – Set of solvers

For each solver $s \in \mathcal{S}$, record the number of function evaluations required to *solve* each problem $p \in \mathcal{P}$.

- ◇ What is an appropriate set of benchmark problems?
- ◇ What is an appropriate convergence test?

J. Moré and S. Wild, *Benchmarking derivative-free optimization algorithms*, www.mcs.anl.gov/~more/dfo

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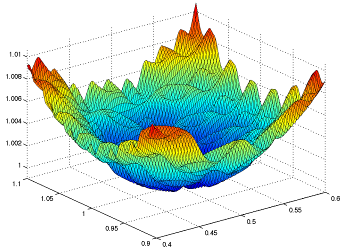
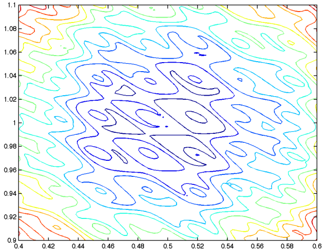
Example: Noisy Quadratics

Given a noise function $\phi : \mathbb{R}^n \mapsto [-1, 1]$, consider

$$f(x) = (1 + \tfrac{1}{2}\|x - e\|^2)(1 + \varepsilon_f \phi(x)),$$

where $\varepsilon_f = 10^{-3}$ is the noise level, and e is the vector of all ones.





Simulation-Based Optimization Problems

⚠ What kind of simulation do you have?

Problem	Simulation
Gaussian elimination	GE with row pivoting
Singular value estimation	condition number estimator
The non-negative svd	svd of a projection of a matrix
Particles with springs	eigenvalues of a symmetric matrix
Satellite orbit	ode23
Isomerization of α-pinene	ode45
Incompressible elastic rods	ode45

Joint work with J. Reed (UCSD)

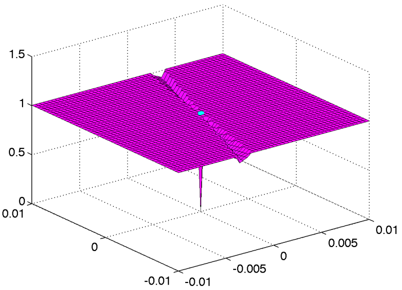
Simulation Slices: Singular Value Estimation

Find an upper triangular matrices $A \in \mathbb{R}^{d \times d}$ that minimize

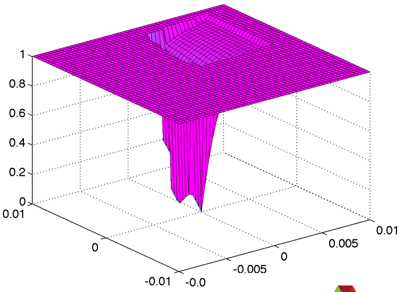
$$f(A) = \frac{\sigma_1(A)}{\text{estsv}(A)}$$

where $\text{estsv}(\cdot)$ is an estimate of σ_1.

Plot of f for the estsv problem with f = 1.17e-07



Plot of f for the estsv problem with f = 1.04e-03



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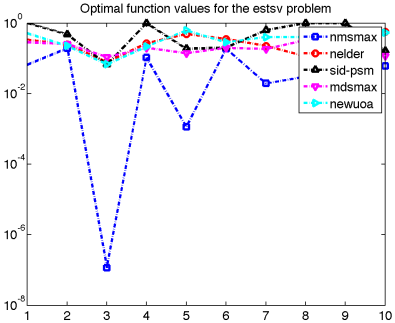
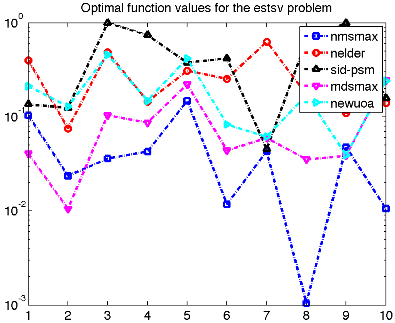
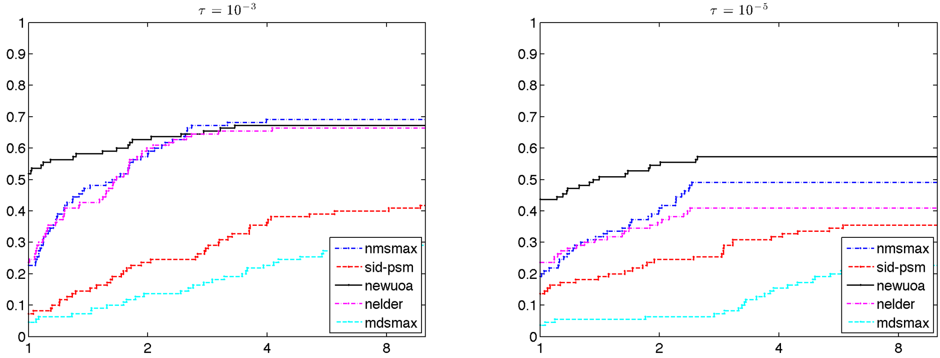
Performance of Optimization Solvers: Singular Value Estimation





Performance Profiles for SBO Problems



Concluding Remarks

- Parameter estimation of complex simulations will require (extremely) advanced architectures
- Our benchmarking results show that model-based solvers generally perform best on complex simulations
- See Stefan Wild's talk for computational results on a nuclear fission (SciDAC UNEDF) application
- Talk to us for your optimization needs