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Optimization Strategies for Complex UNEDF Simulations

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Complex Simulations

Simulation-based optimization problems are of the form

$$\min\left\{\mathcal{F}[s(x)] : x_L \leq x \leq x_U\right\},$$

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

Challenges

- Expensive evaluations of $f(x) = \mathcal{F}[s(x)]$
- Noisy function evaluations
- Lack of derivatives with respect to parameters
- Possibly several minima
- Limited computational budget

Parameter Estimation Problems in UNEDF

- $x \in \mathbb{R}^n$ 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.

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

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.

Research Issues

- What is the best algorithm for optimization?
- How do we recognize a minimizer?
- What is the sensitivity of the solution?
- Can we find a global minimizer?
- How do we validate the model?

Derivative-Free Optimization Algorithms

Stochastic Methods

- ◇ Simulated annealing algorithms
- ◇ Genetic algorithms
- ◇ Particle swarm algorithms

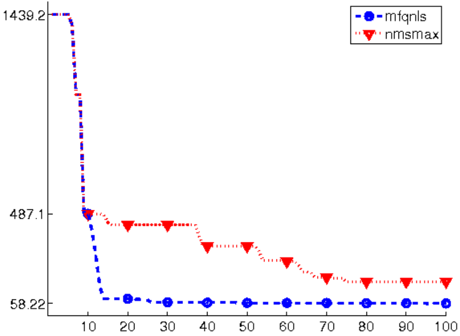
Direct Search Methods

- ◇ 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, . . .)

Parameter Estimation with HFBTHO Code



HFBTHO code

63 nuclei

64 processors

$\mathrm{cost}\{f(x)\} = 12$ minutes

MFQNLS produces acceptable solutions after 2.6 hours, while the Nelder-Mead code NMSMAX has not converged after 20 hours.

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How do we recognize a minimizer?

The standard answer requires $\|\nabla f(x)\|$.

Standard Options

- Hand-coded gradients
- Difference approximations
- Automatic differentiation

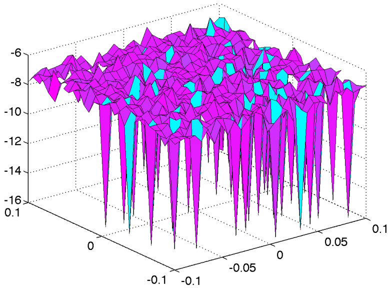
Approximating gradients can be difficult if f is noisy

Noisy Computations

The computed function $f : \mathbb{R}^n \mapsto \mathbb{R}^n$ is of the form

$$f(x) = f_s(x) + \varepsilon(x), \qquad x \in \Omega,$$

where $f_s : \mathbb{R}^n \mapsto \mathbb{R}^n$ is smooth and $\varepsilon : \mathbb{R}^n \mapsto \mathbb{R}^n$ is the noise.



Noise ε

Leading causes of noise

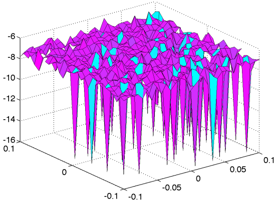
- Petaflops
- Iterative calculations
- Single precision

Partial Trace Eigenvalue Problem

Let A be a symmetric matrix, and define

$$f(x) = \sum_{i=1}^{k} \lambda_i(x)$$

where $\lambda(x)$ are the eigenvalues of $A + \mathrm{diag}(x)$ in increasing order.



Relative error when f is computed with **eigs** and $tol = 10^{-3}$

$n = 243$ and $k = 5$

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Computing Gradient Norms of Noisy Functions

Choose $t > 0$ and a random direction p.

Compute the directional derivative

$$\frac{f(x+tp) - f(x)}{t} \approx \langle \nabla f(x), p \rangle$$

Use the result that with high probability

$$|\langle \nabla f(x), p \rangle| \approx \|\nabla f(x)\|$$

⚠ The choise of t is delicate

Noisy Functions

Assume that the computed function $f : \mathbb{R} \mapsto \mathbb{R}$ is of the form

$$f(t) = f_s(t) + \varepsilon(t), \qquad t \in [t_a, t_b],$$

where $f : \mathbb{R} \mapsto \mathbb{R}$ is a smooth function, and $\varepsilon : \mathbb{R} \mapsto \mathbb{R}$ is the noise.

Assumption. The random variables $\{\varepsilon(t) : t \in [t_a, t_b]\}$ are independent and identically distributed.

Definition. The *noise level* of f is

$$\varepsilon_f = \left(\mathrm{Var}\{\varepsilon(t)\}\right)^{1/2}.$$

The Main Results

We have algorithms for the following problems:

- Determine the noise with a few function evaluations
- Determine optimal approximations to $\langle \nabla f(x), p \rangle$
- Determine $\|\nabla f(x)\|$

Theorem. If f_s is continuous at t, then

$$\lim_{h \to 0} \mathrm{Var}\left\{ \Delta f(t) \right\} = 2\, \varepsilon_f^2.$$

Computational Results

Case 1. $f(x) = x^T x(1 + \sigma \, \mathrm{randn})$ with $\sigma = 10^{-3}$

n_f	$\mathrm{mean}(\varepsilon_f)$
7	9.780e-04
9	1.024e-03
11	1.001e-03
13	9.888e-04
15	9.923e-04

Case 2. f is the partial trace eigenvalue problem

$$\varepsilon_f = 1.5 \, 10^{-8}$$

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Isomerization of α-pinene

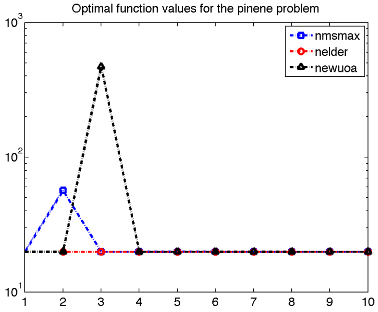
Determine the reaction coefficients in the thermal isomerization of α-pinene from measurements $z_1, \ldots z_8$ by minimizing

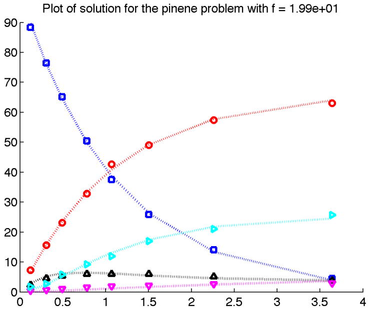
$$\sum_{j=1}^{8} \|y(\tau_j;\theta) - z_j\|^2$$

where $y(\cdot, \theta)$ satisfies

$$\begin{aligned} y_1' &= -(\theta_1 + \theta_2) y_1 \\ y_2' &= \theta_1 y_1 \\ y_3' &= \theta_2 y_1 - (\theta_3 + \theta_4) y_3 + \theta_5 y_5 \\ y_4' &= \theta_3 y_3 \\ y_5' &= \theta_4 y_3 - \theta_5 y_5 \end{aligned}$$

Isomerization of α-pinene





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Incompressible Elastic Rods

The shape of a rod, clamped at the origin and acted on by a vertical force α, a horizontal force β, and torque γ is described by

$$
\begin{aligned}
x_1'(s) &= \cos[\theta(s)] \\
x_2'(s) &= \sin[\theta(s)] \\
\theta'(s) &= \alpha x_1(s) - \beta x_2(s) + \gamma,
\end{aligned}
$$

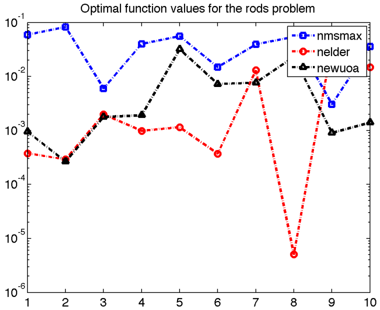
subject to the boundary conditions $x_1(0) = x_2(0) = \theta(0) = 0$, where θ is the angle of inclination, and s is arc length.

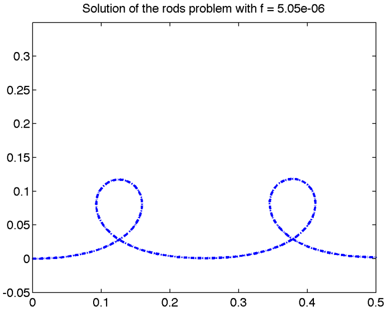
Determine the shape of the rod such that

$$x_1(1) = a, \quad x_2(1) = b, \quad \theta(1) = c,$$

for specified values of a, b and c.

Incompressible Elastic Rods





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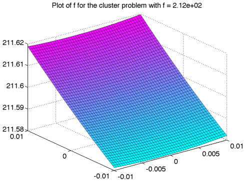
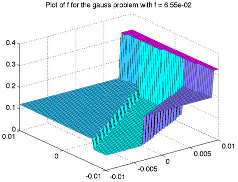
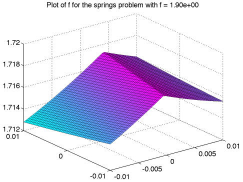
Slices



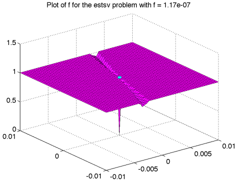
Plot of f for the cluster problem with f = 2.12e+02
211.62
211.61
211.6
211.59
211.58
0.01
0
-0.01
-0.01
-0.005
0
0.005
0.01



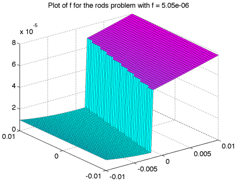
Plot of f for the gauss problem with f = 6.55e-02
0.4
0.3
0.2
0.1
0
0.01
0
-0.01
-0.01
-0.005
0
0.005
0.01



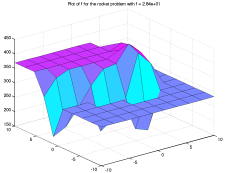
Plot of f for the springs problem with f = 1.90e+00
1.72
1.718
1.716
1.714
1.712
0.01
0
-0.01
-0.01
-0.005
0
0.005
0.01



Plot of f for the estsv problem with f = 1.17e-07
1.5
1
0.5
0
0.01
0
-0.01
-0.01
-0.005
0
0.005
0.01



Plot of f for the rods problem with f = 5.05e-06
x 10^-5
8
6
4
2
0
0.01
0
-0.01
-0.01
-0.005
0
0.005
0.01



Plot of f for the rocket problem with f = 2.84e+01
450
400
350
300
250
200
150
10
5
0
-5
-10
-10
-5
0
5
10

Future Work

Year 4

- Model and geometry-based optimization algorithms
- Open-source implementation of model-based algorithms
- Investigation of performance on new UNEDF functionals

Year 5

- Performance, evaluation, and validation of DFT functional
- Algorithms for noisy and constrained calculations
- Fission pathways