Derivative-free optimization for parameter estimation in computational nuclear physics

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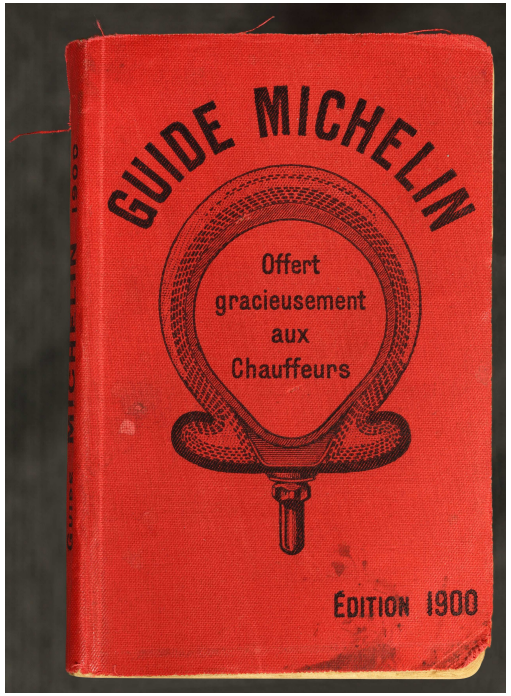
Joint work with Jorge Moré, Todd Munson, and Jason Sarich
and grateful to many physicist collaborators:
A. Ekström, C. Forssén, G. Hagen, M. Hjorth-Jensen, G.R. Jansen, M. Kortelainen, T. Lesinski, R. Machleidt, J. McDonnell, W. Nazarewicz, E. Olsen, T. Papenbrock, P.-G. Reinhardt, N. Schunck, M. Stoitsov, J. Vary, K. Wendt, and others

November 24, 2014

Roadmap

- → Simulation-based optimization problems
- → Calibration of EDFs
- → The POUNDERS algorithm and software
- → Revisit Optimization and Uncertainties from UNEDF
- → Optimization with the new Argonne Masses



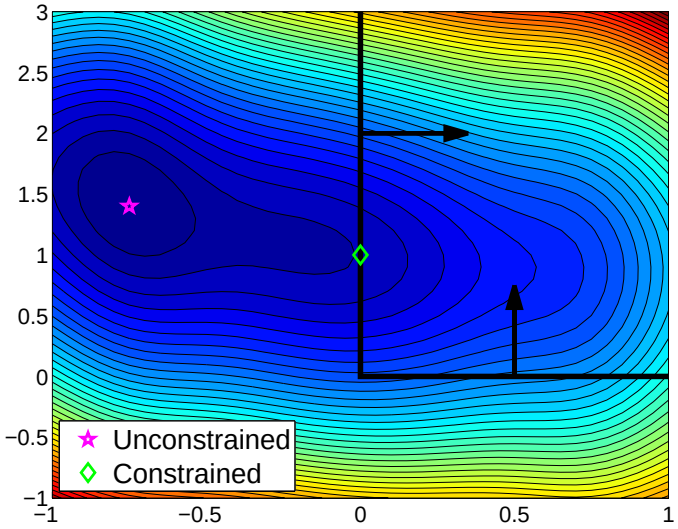
Mathematical/Numerical Nonlinear Optimization

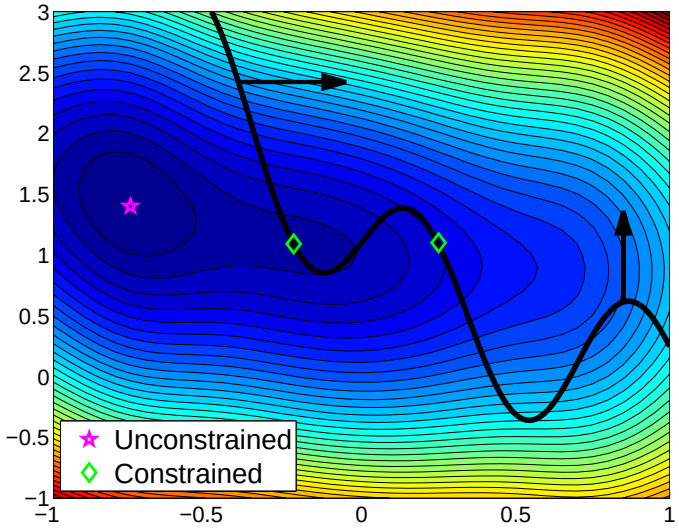
Optimization is the *"science of better"*

Find parameters (controls) $x = (x_1, \ldots, x_n)$ in domain Ω to improve objective f

$$\min \{ f(x) : x \in \Omega \subseteq \mathbb{R}^n \}$$

- (Unless Ω is very special) Need to evaluate f at many x to find a good $\hat{x}_*$
- Focus on local solutions: $f(\hat{x}_*) \leq f(x) \; \forall x \in \mathcal{N}(\hat{x}_*) \cap \Omega$



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$\min_{x \in \mathbb{R}^n} \{ f(x) = F[x, S(x)] : c_S(x) = 0, x \in \Omega \}$

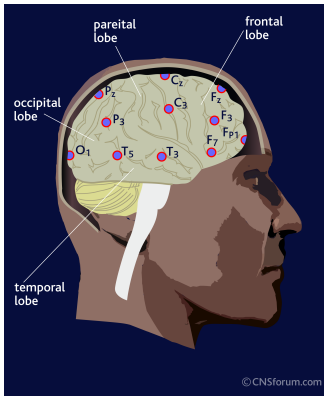
Optimize expensive, nonlinear functions arising in science & engineering

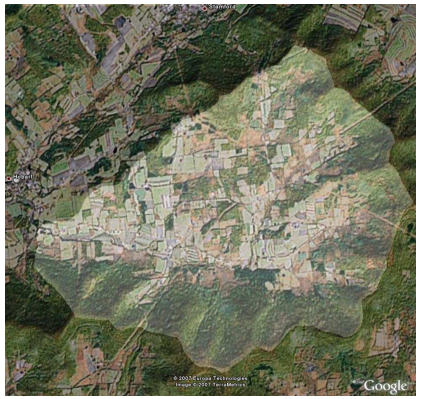
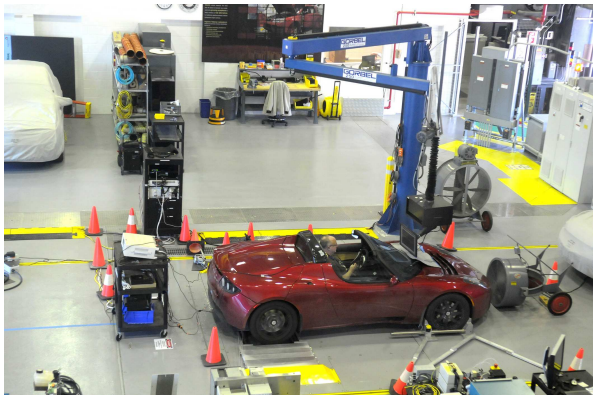
"parameter estimation", "model calibration", "design optimization", ...

- $f : \mathbb{R}^n \to \mathbb{R}$ objective, c constraints, $S : \mathbb{R}^n \to \mathbb{R}^p$ numerical simulation,
- Evaluating S means running a simulation modeling some (smooth) process

  Ex- S = solving PDEs via finite elements
  - Here: assume f is from a deterministic computer simulation
- S can contribute to objective and/or constraints, possibly noisy
- S (could/must be parallelized) takes secs/mins/hrs for 1 x

Evaluation is a bottleneck for optimization

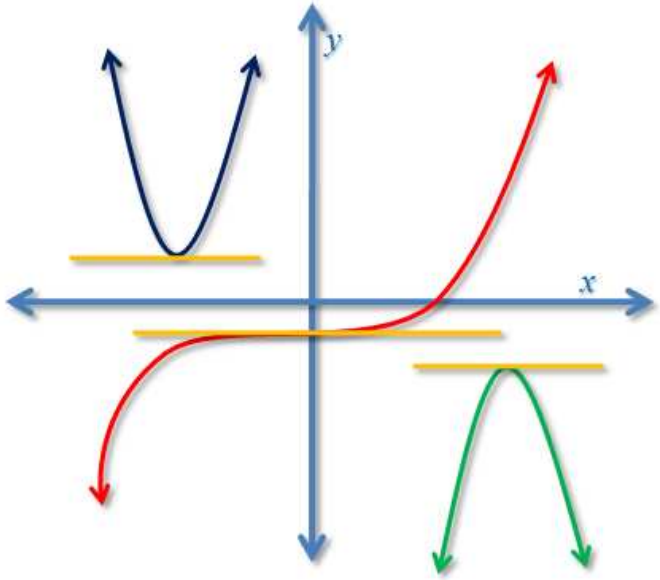


Optimization Tightly Coupled With Derivatives

Typical optimality (no noise, smooth functions)

$$\nabla_x f(x_*) + \lambda^T \nabla_x c_E(x_*) = 0, c_E(x_*) = 0$$

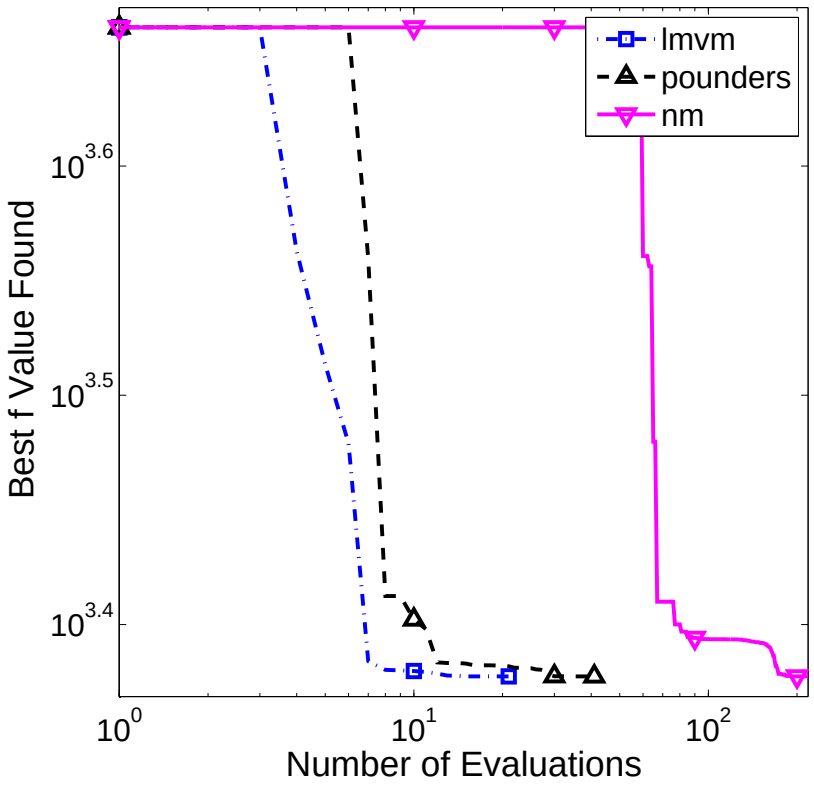


(sub)gradients $\nabla_x f$, $\nabla_x c$ enable:

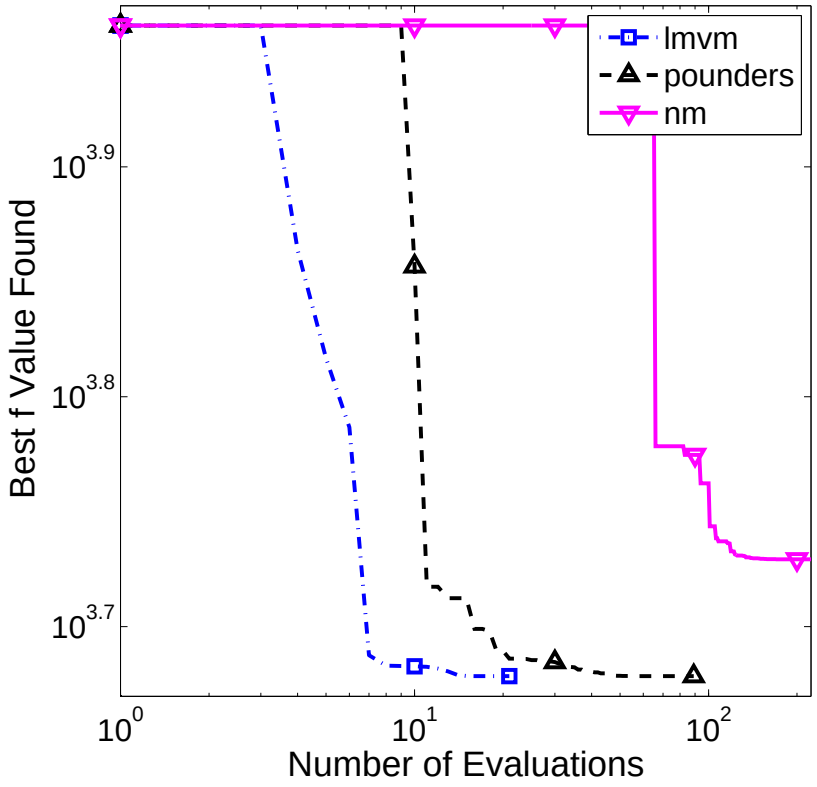
- Faster feasibility
- Faster convergence
  - Guaranteed descent
  - Approximation of nonlinearities
- Better termination
  - Measure of criticality $\|\nabla_x f\|$ or $\|\mathcal{P}_\Omega(\nabla_x f)\|$

But derivatives $\nabla_x S(x)$ are not always available/do not always exist

The Price of Algorithm Choice (I)



$n = 3$



$n = 6$

lmvm Uses available $\nabla_x f$

nm Assumes $\nabla_x f$ unavailable

pounders Assumes $\nabla_x f$ unavailable, exploits problem structure

Example: Calibration of EDFs ("χ^2 minimization")

$$\min_{x \in \Omega} f(x) = \sum_{i=1}^{p} \left(\frac{s_i(x;\theta_i) - d_i}{w_i} \right)^2$$

$s_i(x;\theta)$ Simulated nucleus observable

e.g., energies, radii, odd-even mass diffs, energy gaps, single particle energies

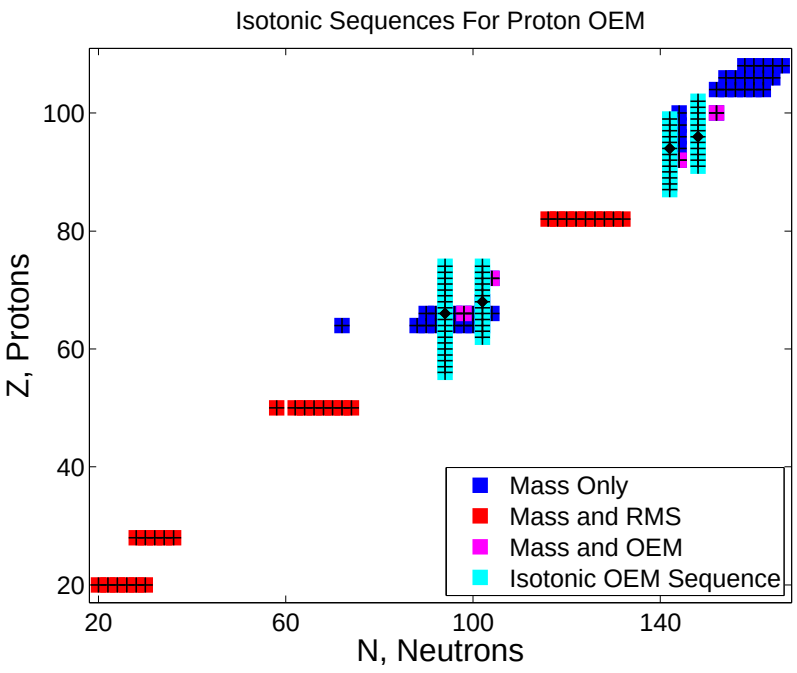
$\rightarrow$ HFBTHO code output

d_i Observable i (exp.) data

w_i Weight/error for data type i

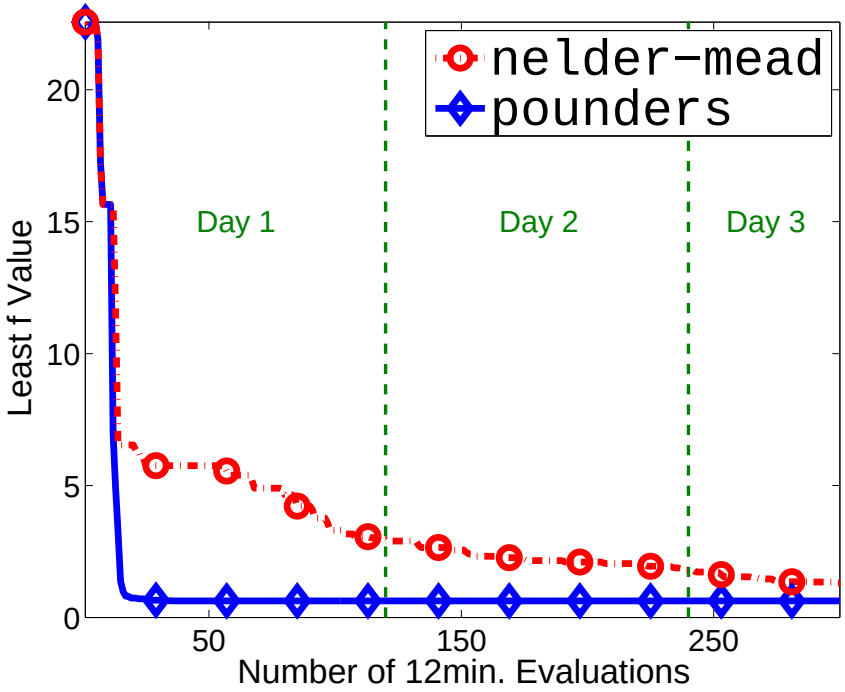
x Free parameters (coupling constants)

Ω Bound constraints

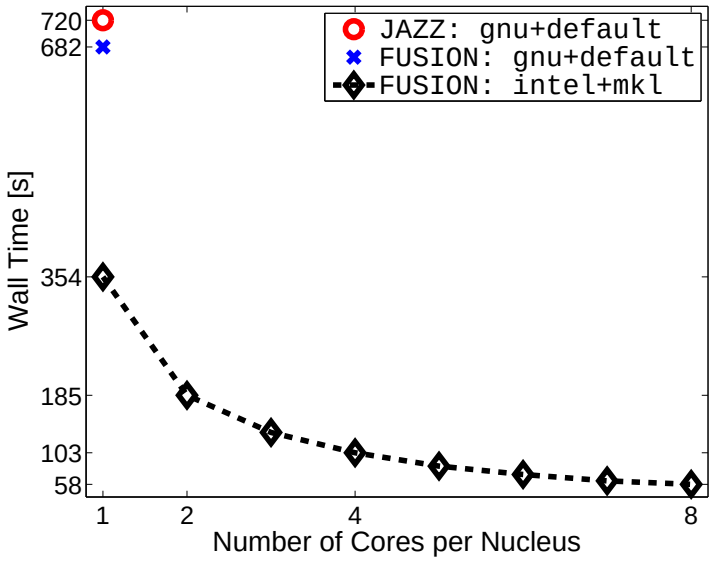


Observables in UNEDF0

The Price of Algorithm Choice (II)



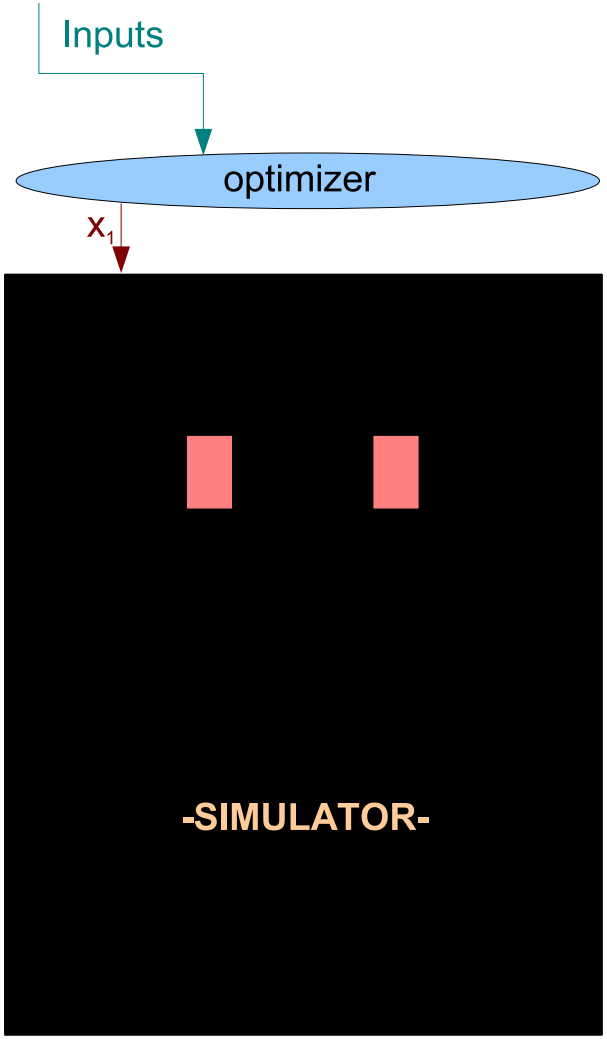
Significantly reduced the number of DFT simulations required



- UNEDF0: [Kortelainen et al., PRC 2010]
- UNEDF1: [Kortelainen et al., PRC 2012]
- UNEDF2: [Kortelainen et al., PRC 2014]

Algorithms

"Simplest" Formulation: Blackbox f



Optimizer gives x, physicist provides $f(x)$

- f can be a blackbox (executable only or proprietary/legacy codes)
- Only give a single output
  - no derivatives with respect to x: $\nabla_x S(x), \nabla^2_{x,x} S(x)$
  - no problem structure

Good solutions guaranteed in the limit, but:

- Usually have computational budget (due to scheduling, finances, deadlines)
- Limited number of evaluations

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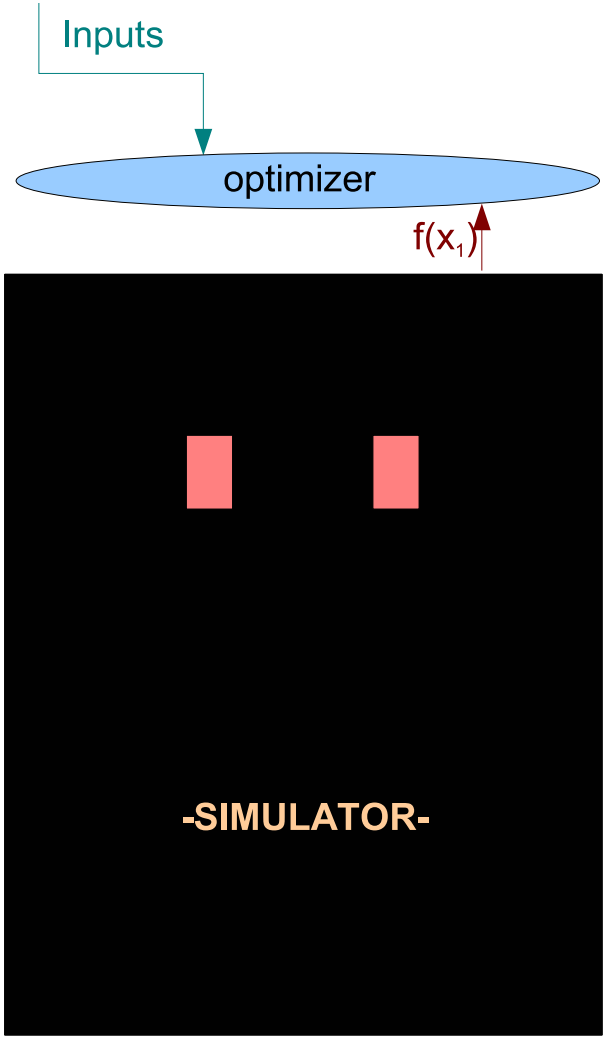

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Derivative-Free, Local Algorithms

Solve general problems $\min\{f(x) : x \in \mathbb{R}^n\}$:

- Only require function values (no $\nabla f(x)$)
- Don't rely on finite-difference approximations to $\nabla f(x)$
  - Can be misleading due to noise
  - Can be inefficient (each set of $n+1$ evaluations useful for a single step only)
- Seek greedy and rapid decrease of function value

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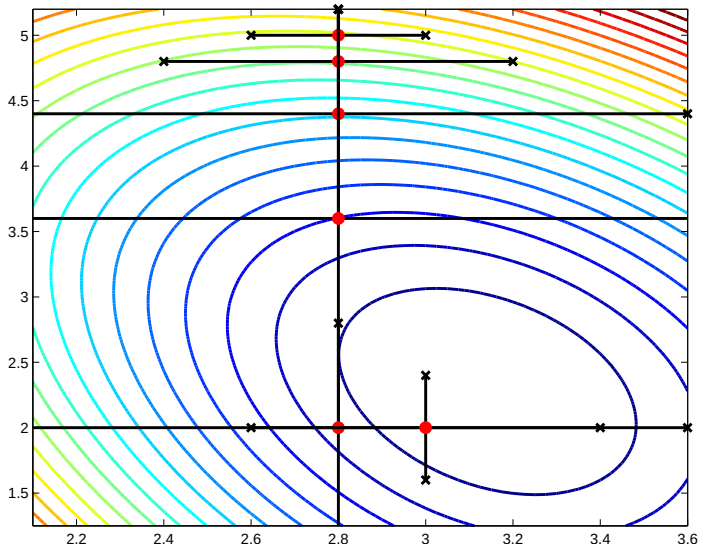
Two main styles of local DFO algorithms

- Direct search methods (pattern search, Nelder-Mead, ...)
- Model-based methods (quadratics, radial basis functions, ...)

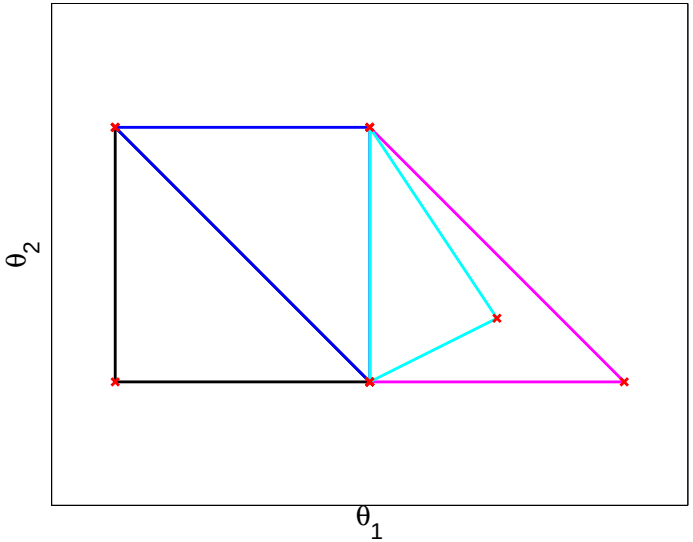
Algorithms: Direct Search Methods

Pattern Search



Easy to parallelize f evaluations

Nelder-Mead



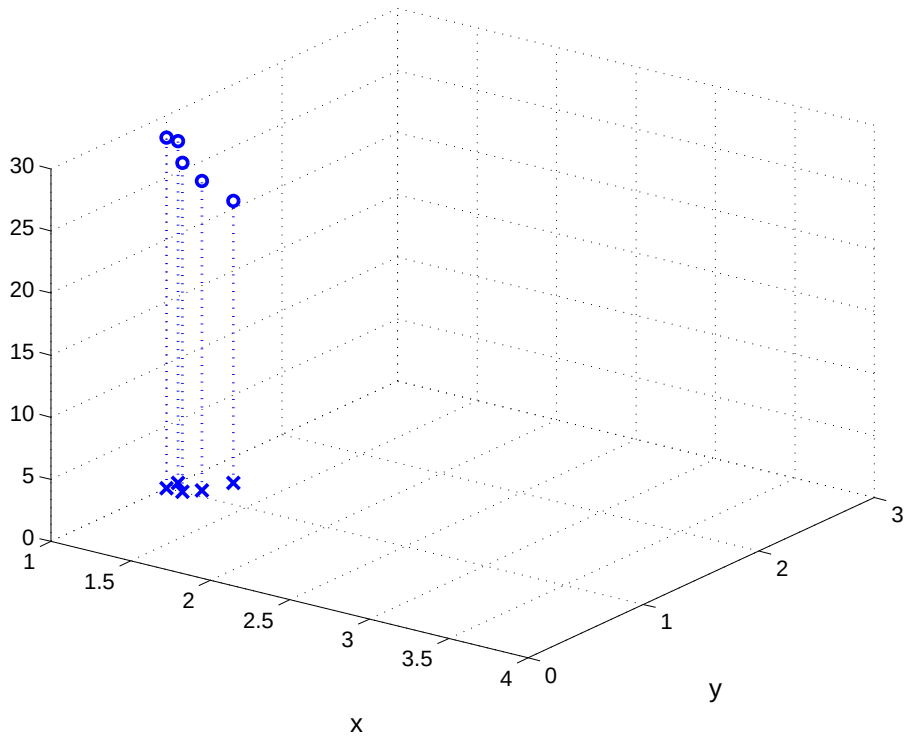
Popularized by *Numerical Recipes*

- Rely on indicator functions: $[f(x_k + s) <^? f(x_k)]$
- Work with **black-box** $f(x)$, do not exploit structure $F[x, S(x)]$

$\longrightarrow$[Kolda, Lewis, Torczon, SIREV 2003]

Making the Most of Little Information on f

- f is expensive $\Rightarrow$ can afford to make better use of points
- Overhead of the optimization routine is negligible relative to the cost of evaluating the simulation.



Bank of data, $\{x_i, f(x_i)\}_{i=1}^{k}$:

= Points (& function values) evaluated so far

= Everything known about f

Goal:

- Make use of growing Bank as optimization progresses

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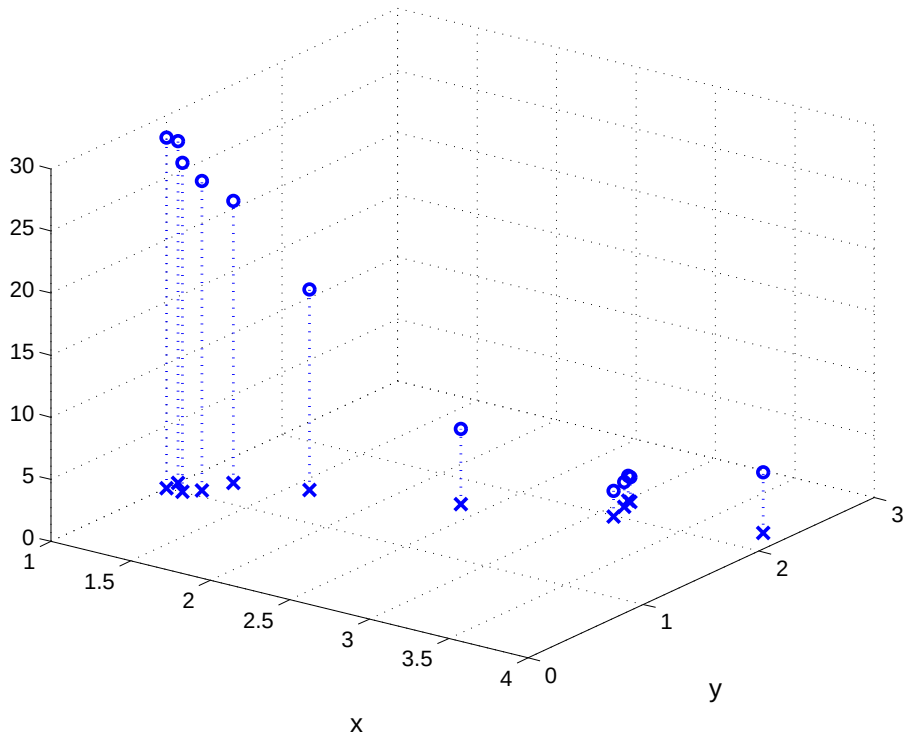

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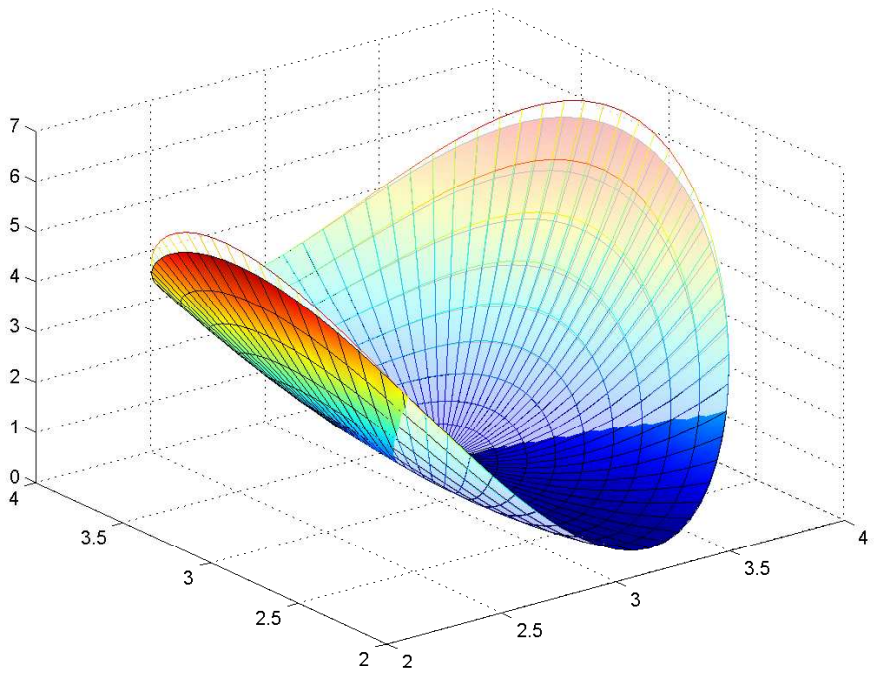
Trust-Region Methods Use Models Instead of f

To reduce the number of expensive f evaluations
$\rightarrow$ Replace difficult optimization problem $\min f(x)$ with a much simpler one
$\min \{\mathbf{m}(\mathbf{x}) : \mathbf{x} \in \mathcal{B}\}$

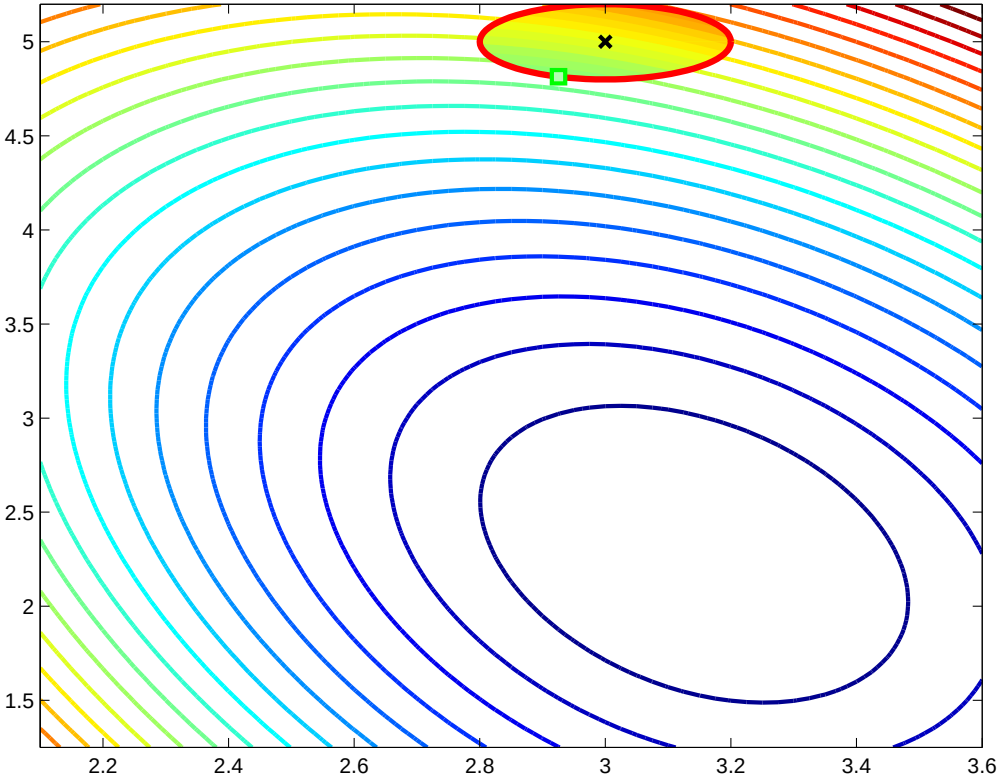


Classic NLP Technique:

- f Original function: computationally expensive, no derivatives
- m Surrogate model: computationally attractive, analytic derivatives

Basic Trust-Region Idea

Use a surrogate $\mathbf{m}(\mathbf{x})$ in place of the unwieldy $f(x)$



Optimize over $\mathbf{m}$ to avoid expense of f:

- Trust m to approximate f within $\mathcal{B} = \{x \in \mathbb{R}^n : \|x - x_k\| \leq \Delta_k\}$,
- Obtain next point from $\min\{m(x) : x \in \mathcal{B}\}$,
- Evaluate function and update (x_k, Δ_k) based on how good the model's prediction was.

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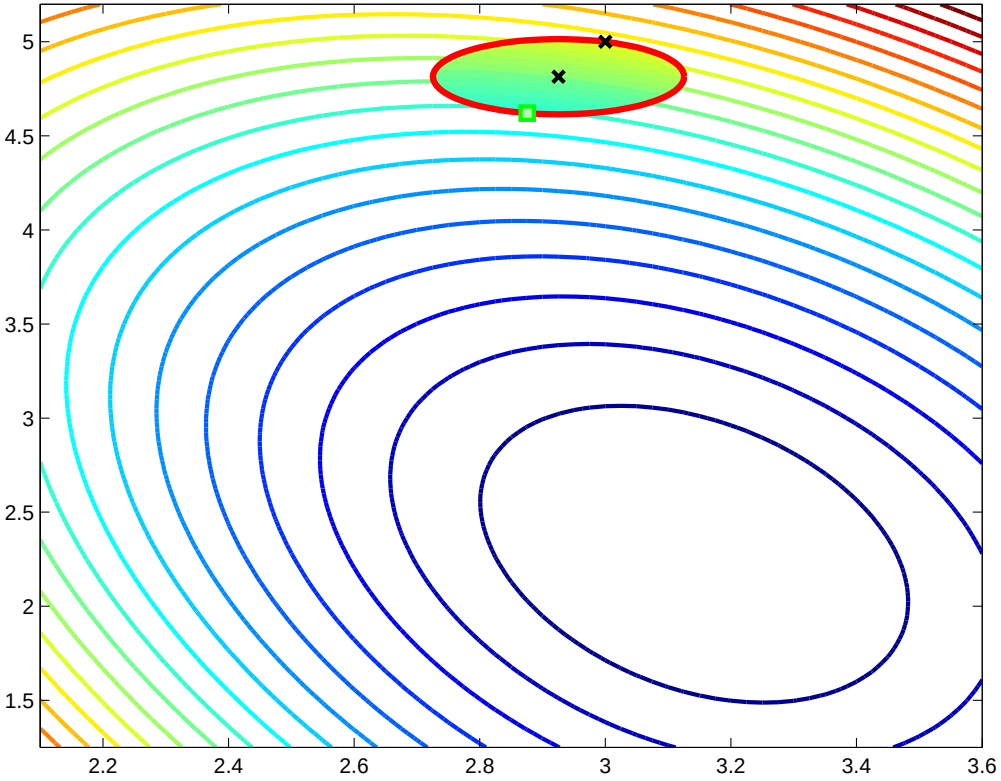

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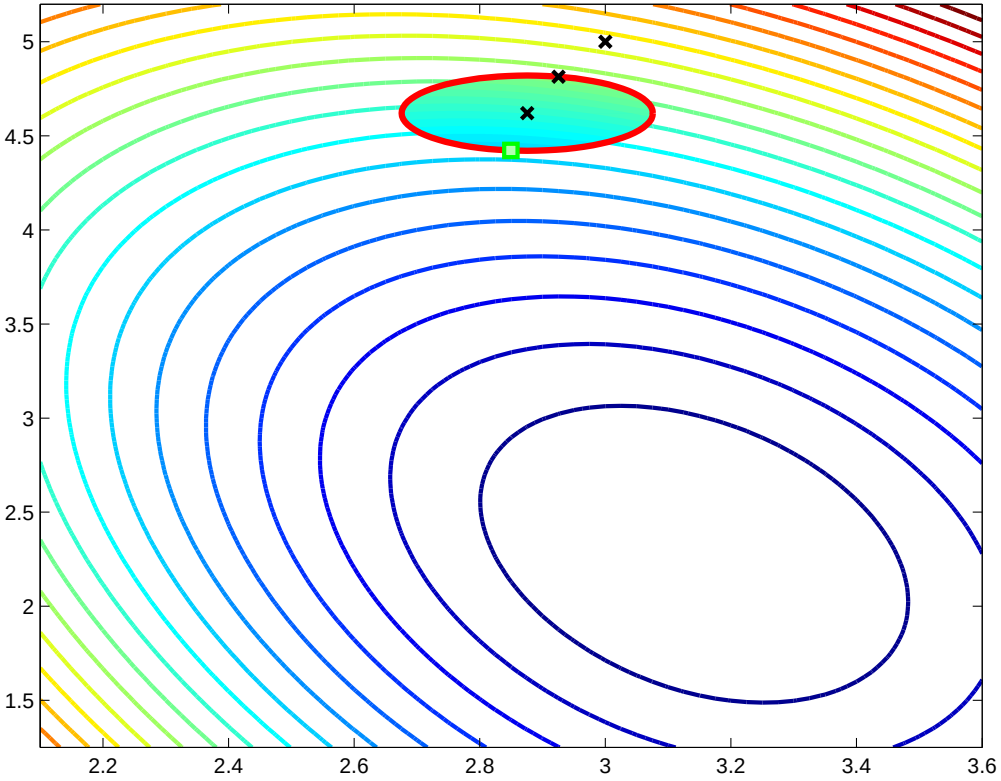

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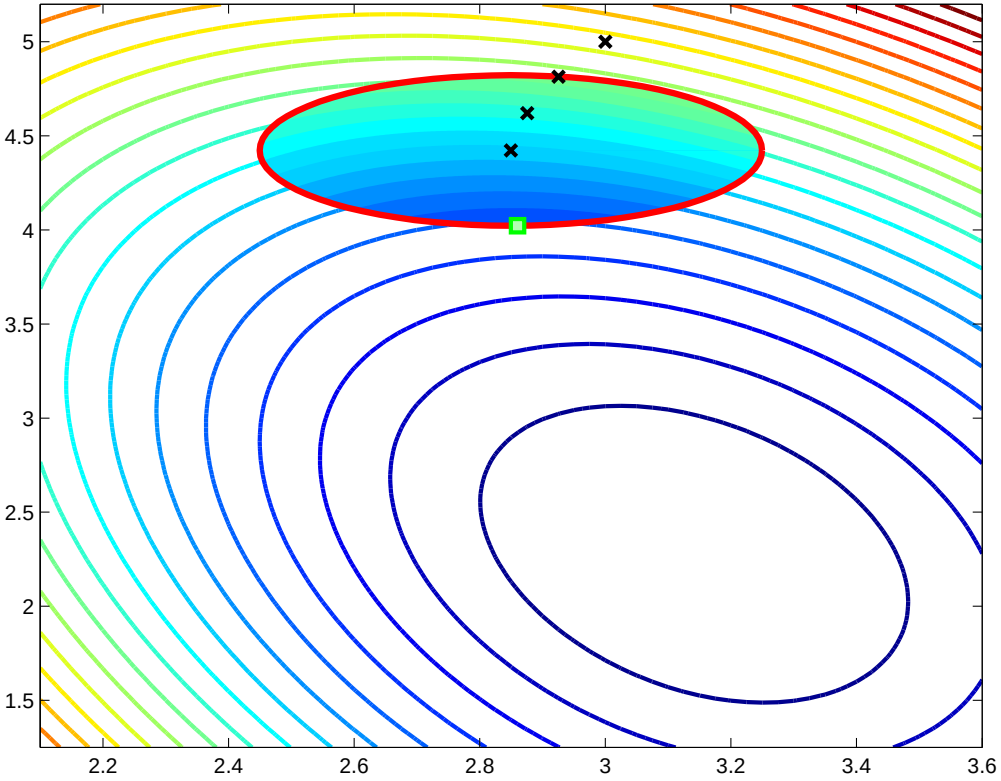

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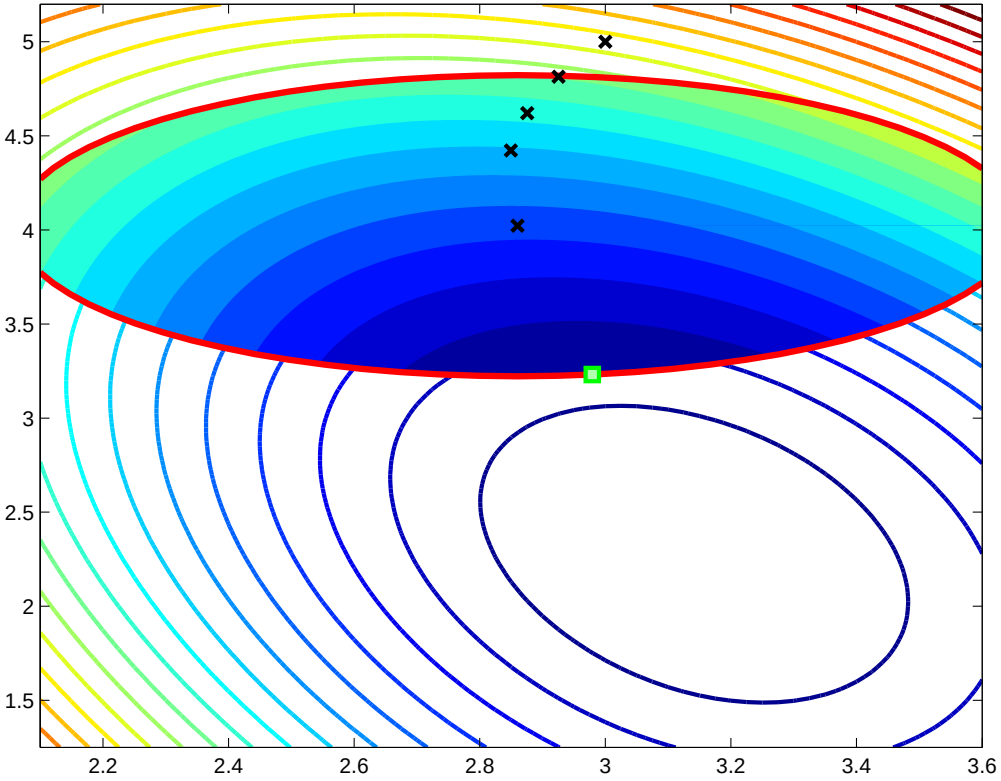

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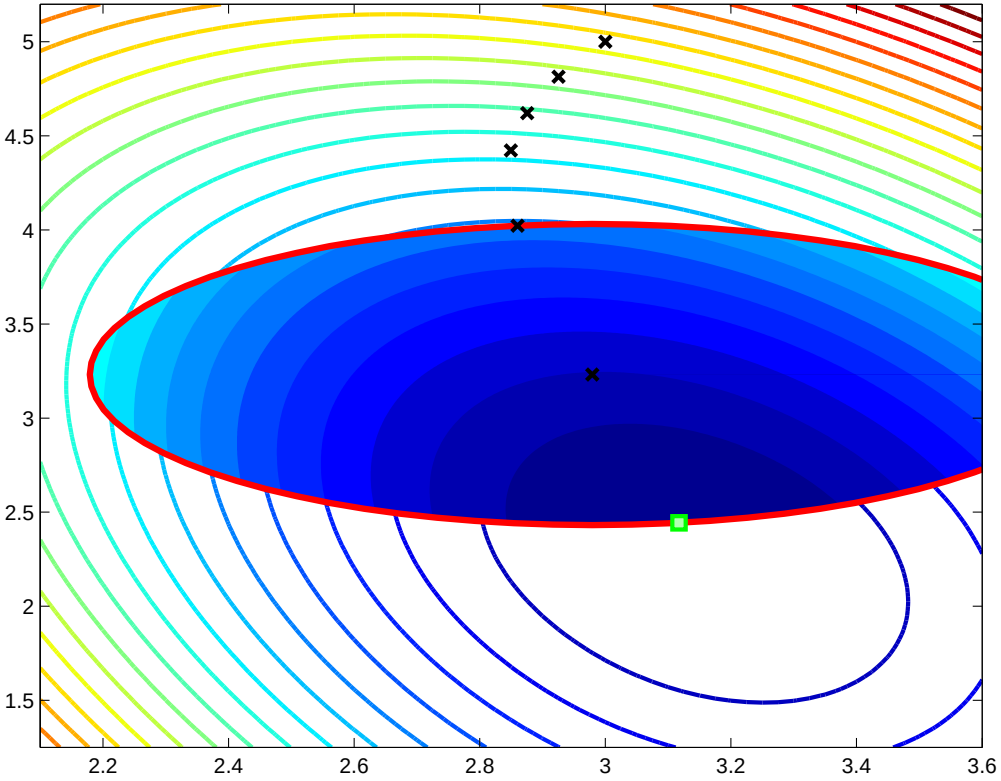

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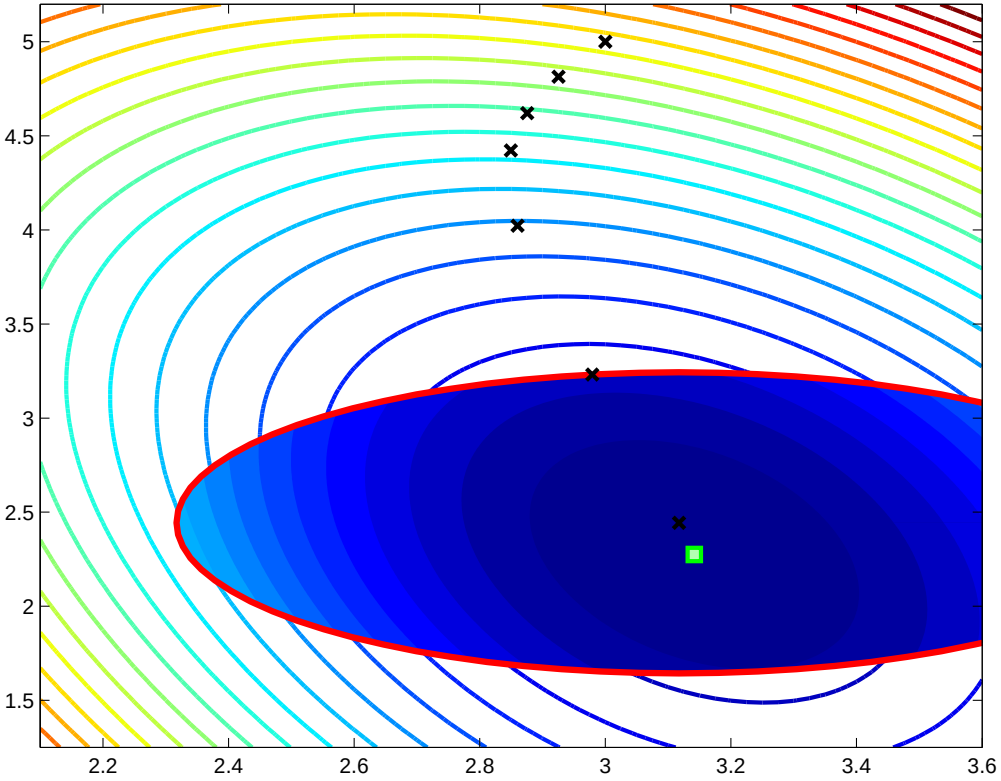

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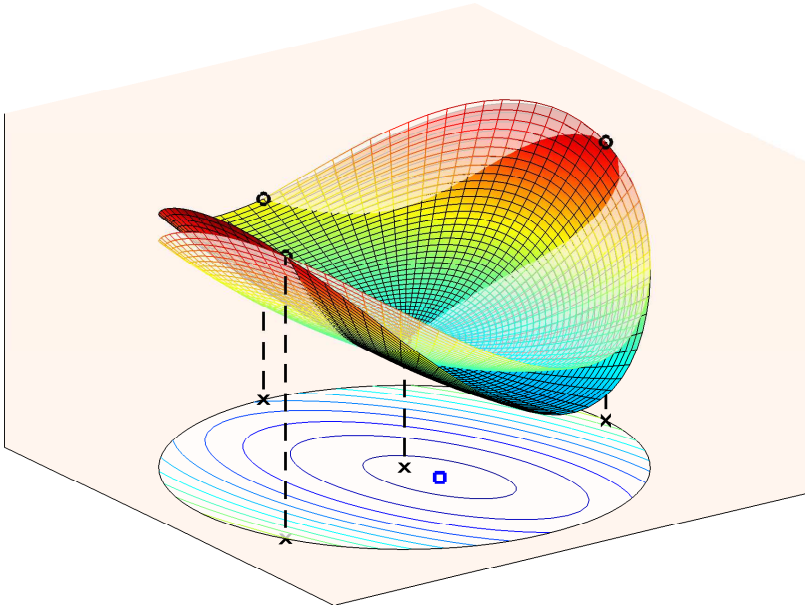
Building Models Without Derivatives

$$m_k(x) = f(x_k) + g_k^\top (x - x_k) + \frac{1}{2}(x - x_k)^\top H_k (x - x_k)$$



$n = 2$, $|\mathcal{Y}_k| = 4$

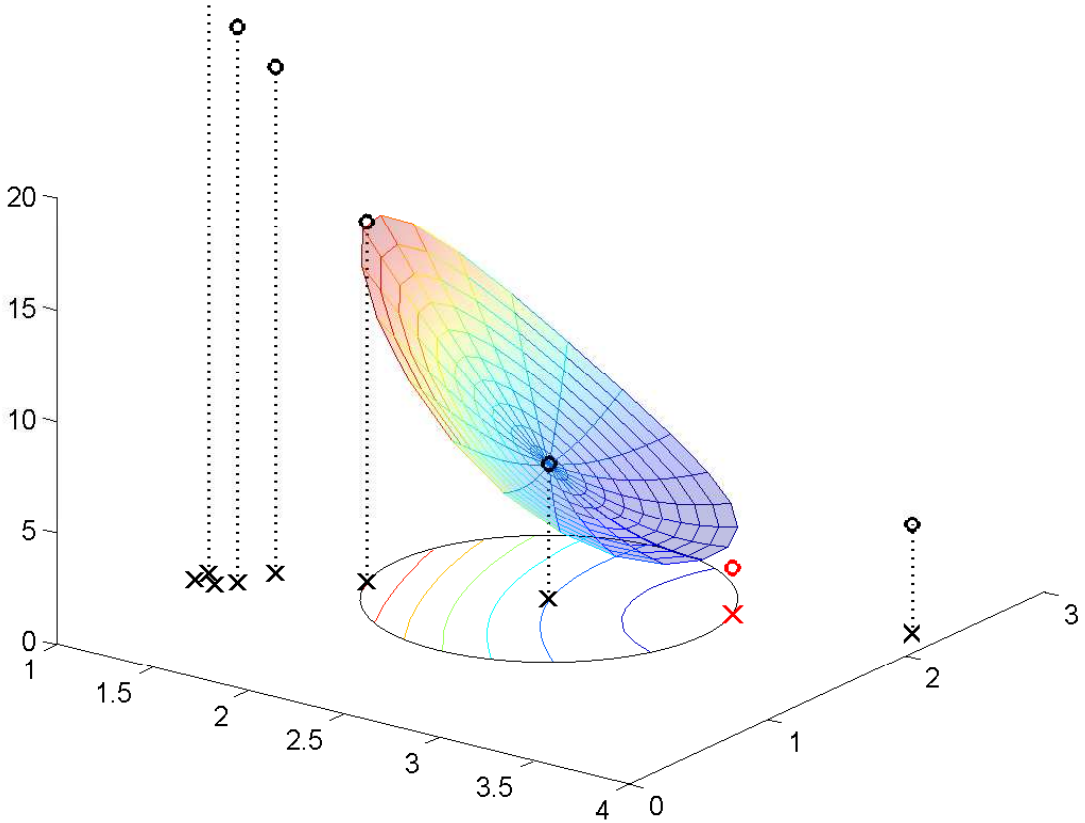
Determine (g_k, H_k) from function values

- Only need local approximation
- Numerical differentiation too expensive ($\frac{(n+1)(n+2)}{2}$ evaluations per iteration for full quadratics)
- $m_k(y_i) = f(y_i), \quad \forall y_i \in \mathcal{Y}_k$

Practical concerns

- Interpolation of scattered data (ideally, from the history of the algorithm)
- Models typically underdetermined, $|\mathcal{Y}_k| < \frac{(n+1)(n+2)}{2}$

Interpolation-based Trust-region Methods



Iteration k:

- Build a model m_k interpolating f on $\mathcal{Y}$
- Trust m_k within region $\mathcal{B}_k$
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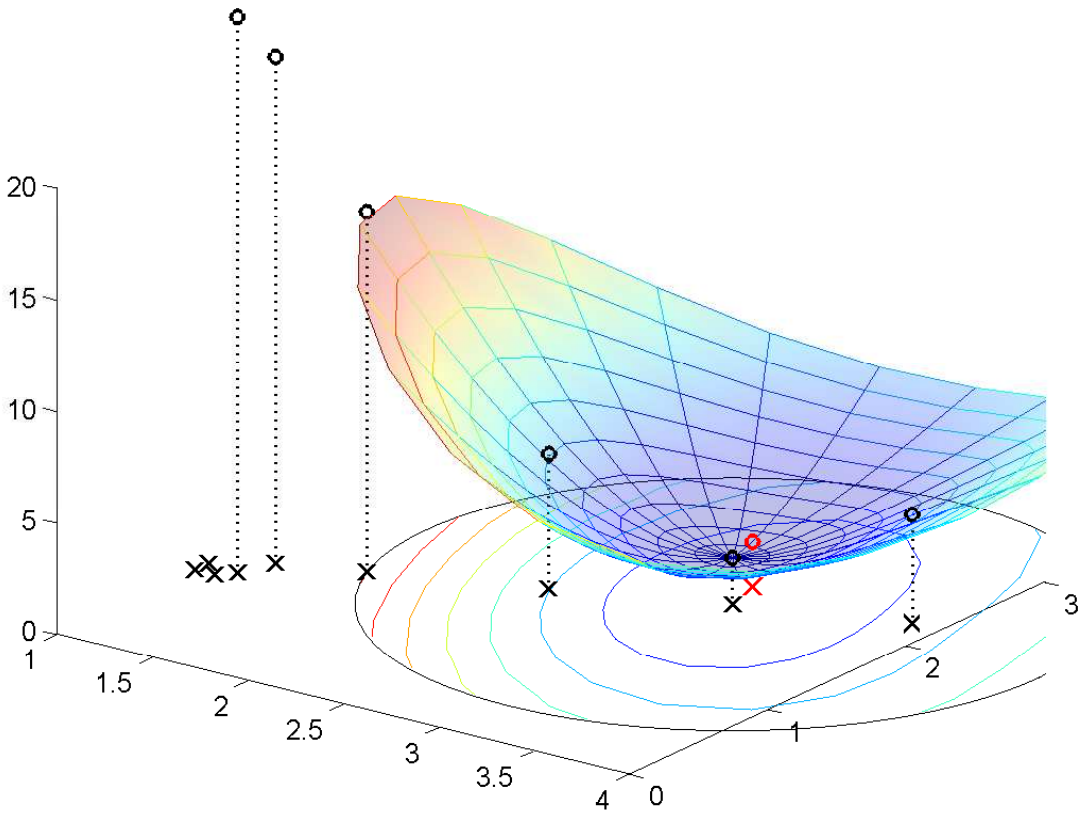

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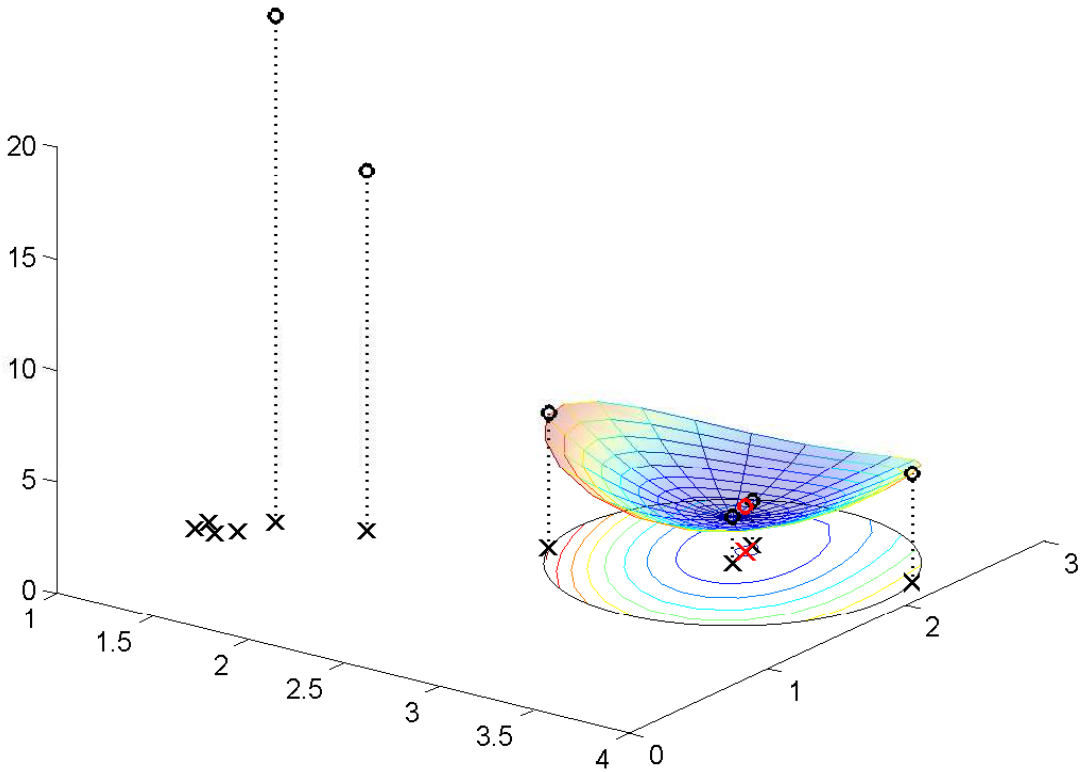

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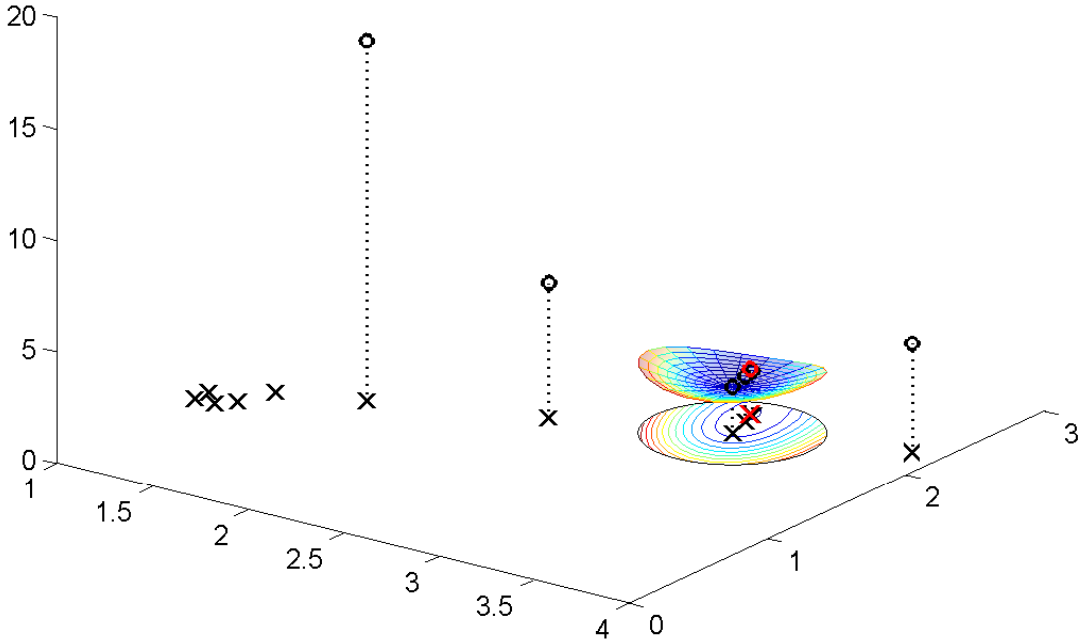

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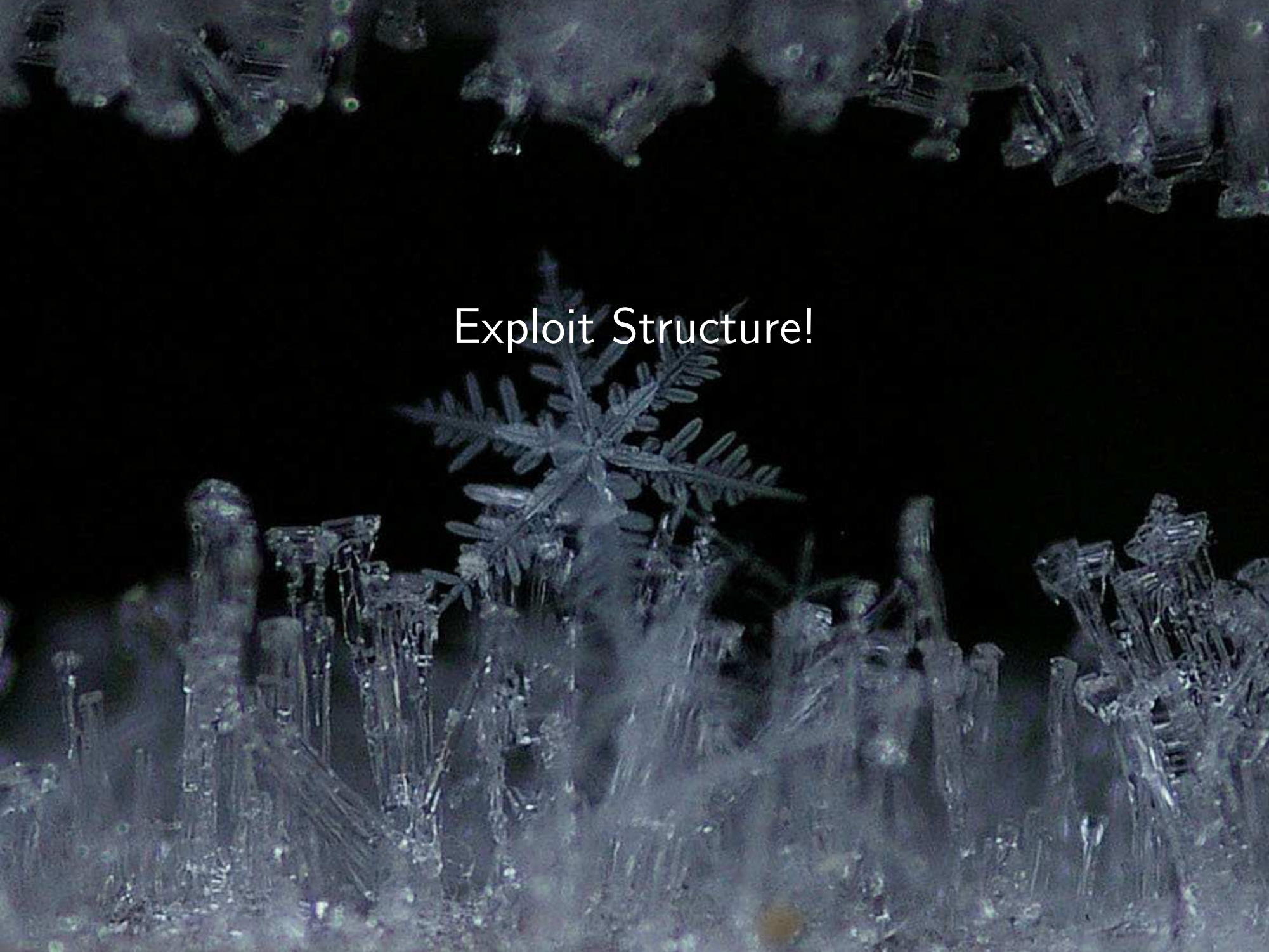
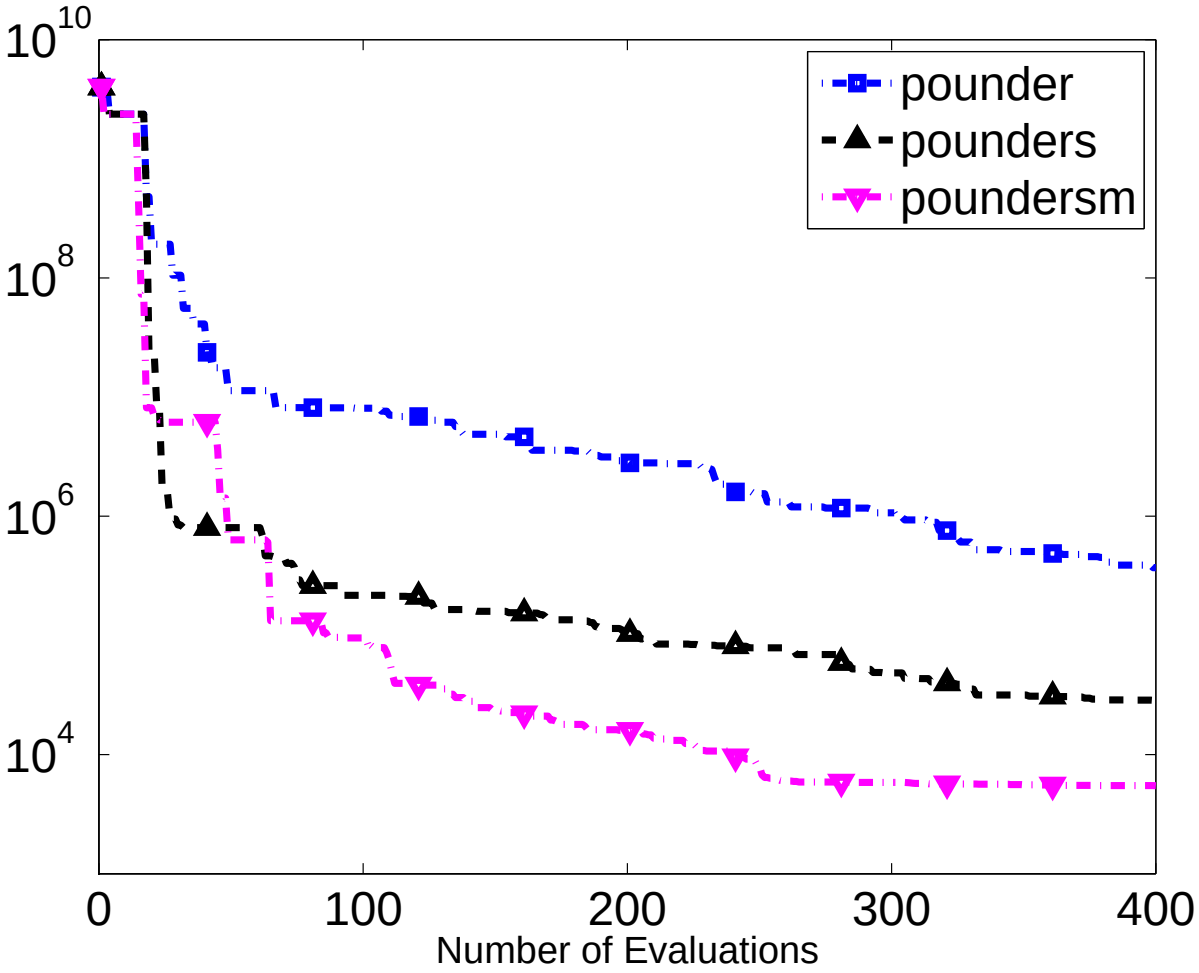

Exploit Structure!

Performance of Model-Based Methods



Optimizing EDF in [Bertolli et al., PRC 2012]

Calibration is not a Blackbox Problem

Generic:

$$\min_{\mathbf{x}} \{ f(\mathbf{x}) : \mathbf{x} \in \Omega \subseteq \mathbb{R}^{n_x} \}$$

- $\mathbf{x}$ n_x decision variables
- f $: \mathbb{R}^{n_x} \to \mathbb{R}$ objective function
- Ω feasible region, $\{\mathbf{x} : c_E(\mathbf{x}) = 0, c_I(\mathbf{x}) \leq 0\}$
  - c_E (vector of) equality constraints
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- Ω feasible region, $\{\mathbf{x} : c_E(\mathbf{x}) = 0, c_I(\mathbf{x}) \leq 0\}$
  - c_E (vector of) equality constraints
  - c_I (vector of) inequality constraints

Typical calibration problem:

$$f(\mathbf{x}) = \|\mathbf{F}(\mathbf{x})\|_2^2 = \sum_{i=1}^{n_d} F_i(\mathbf{x})^2$$

- $\mathbf{x}$ n_x coupling constants
- F_i $: \mathbb{R}^{n_x} \to \mathbb{R}$ residual function
  - Ex.- $\frac{1}{w_i}\left(S(\mathbf{x}; \boldsymbol{\nu}_i) - d_i\right)$
    - $S(\mathbf{x}; \boldsymbol{\nu}_i)$: numerical simulation
  - Ex.- Obtain $\chi^2(\mathbf{x})$ by $\frac{1}{n_d - n_x} f(\mathbf{x})$
- Ω $= \{\mathbf{x} : \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}\}$
  - Finite bounds (for some x_i)
  - Often dictated by dom($\mathbf{S}$)

[Ekström et al, PRL 2013] [Kortelainen et al, PRC 2014]

Calibration is not a Blackbox Problem

Generic:

$$\min_{\mathbf{x}} \{ f(\mathbf{x}) : \mathbf{x} \in \Omega \subseteq \mathbb{R}^{n_x} \}$$

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- Taking advantage of structure should further reduce # of expensive evaluations

Exploiting Nonlinear Least Squares Structure

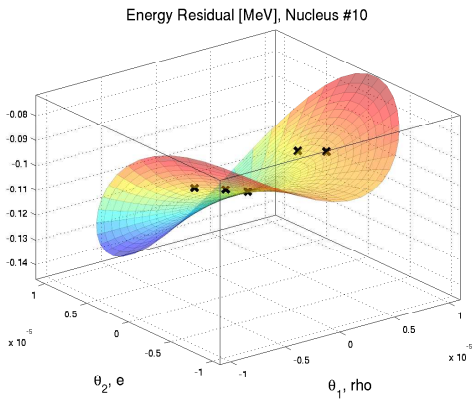
Obtain a vector of output $F_1(x), \ldots, F_p(x)$

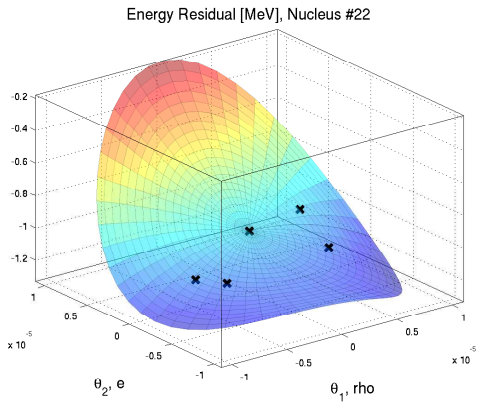
- Model each F_i

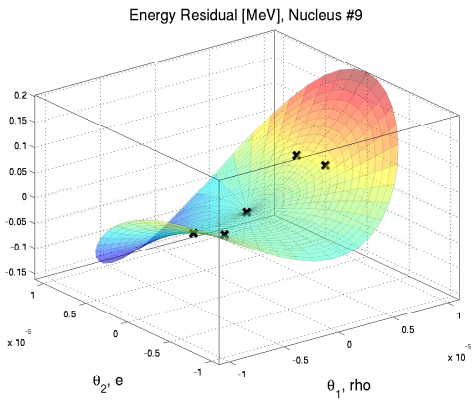
$$F_i(x) \approx q_k^{(i)}(x) = F_i(x_k) + (x - x_k)^\top g_k^{(i)} + \frac{1}{2}(x - x_k)^\top H_k^{(i)}(x - x_k)$$

- Employ models in the approximation

$$\begin{aligned} \nabla f(x) &= \textstyle\sum_i \nabla \mathbf{F_i}(\mathbf{x}) F_i(x) && \rightarrow \textstyle\sum_i \mathbf{g_k^{(i)}}(\mathbf{x}) F_i(x) \\ \nabla^2 f(x) &= \textstyle\sum_i \nabla \mathbf{F_i}(\mathbf{x}) \nabla \mathbf{F_i}(\mathbf{x})^T + F_i(x) \nabla^2 \mathbf{F_i}(\mathbf{x}) && \rightarrow \textstyle\sum_i \mathbf{g_k^{(i)}}(\mathbf{x}) \mathbf{g_k^{(i)}}(\mathbf{x})^T + F_i(x) \mathbf{H_k^{(i)}}(\mathbf{x}) \end{aligned}$$







The POUNDERS Method & Open-Source Software

Practical Optimization Using No DERivatives for sums of Squares

- a local, model-based, full Newton-like, trust-region algorithm
- for unconstrained and bound-constrained
- nonlinear-least squares problems
- in the absence of some derivatives (derivative-free)

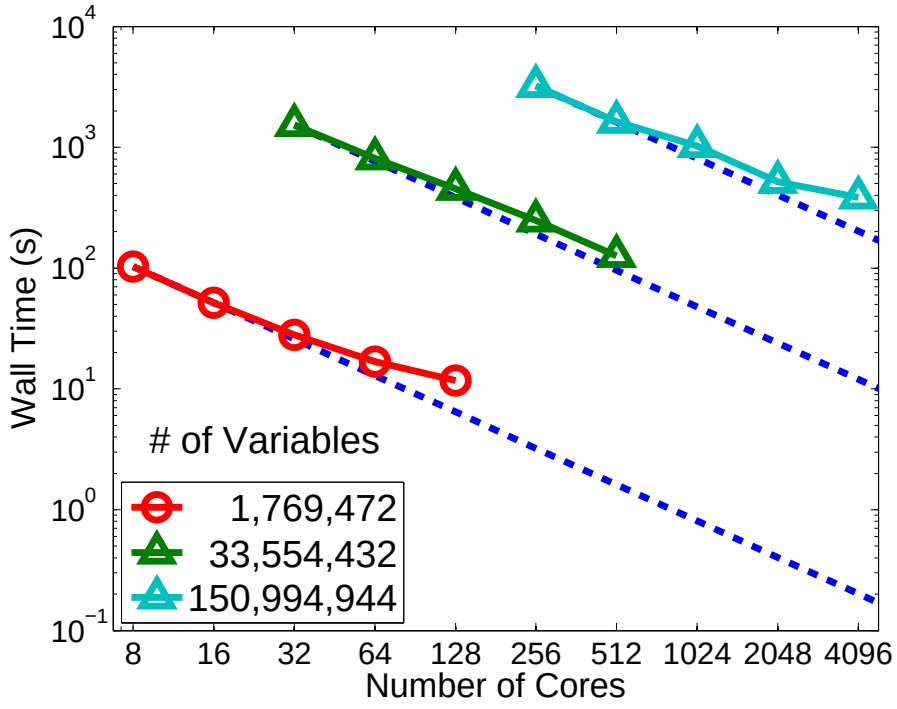
that

- is a misnomer (uses some derivatives)
- is robust to noise/poor local minima
- has a simple interface (provide routine for $\mathbf{S}$)
- allows for parallel evaluation of $\mathbf{S}$
- has asymptotic convergence guarantees
- performs well in practice
- is available in TAO [http://mcs.anl.gov/tao]

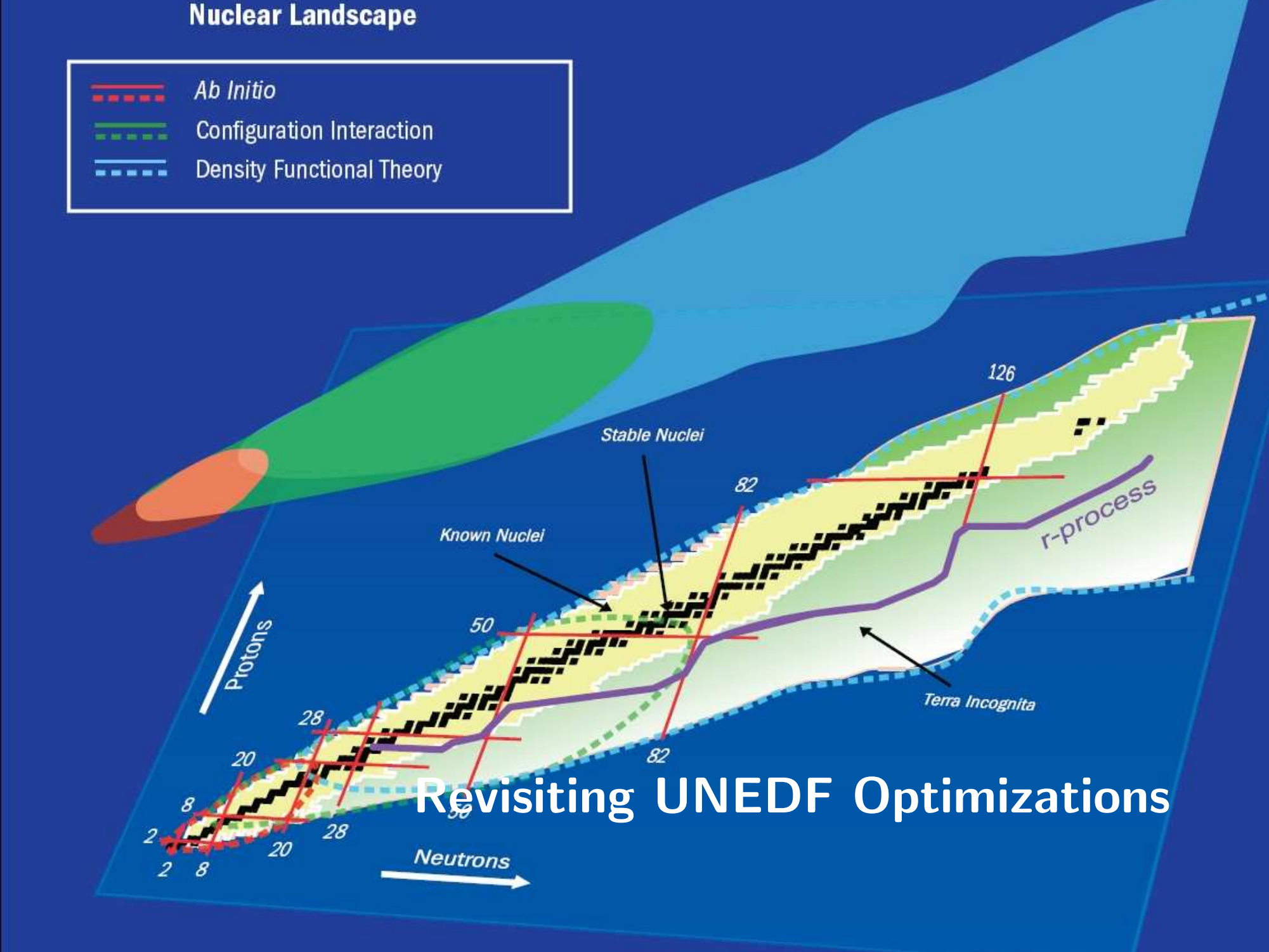
What is TAO?

Toolkit for Advanced Optimization

- Open-source library for large-scale optimization problems
- Emphasize portability, performance, scalable parallelism, and architecture-independent interface
- Bi-directional connection to lower level linear algebra
- Works with PETSc (3.3)
- Current version 2.1
- `www.mcs.anl.gov/tao`



Strong scaling of TAO's PDE-constrained optimization solver on an elliptic problem



Revisiting UNEDF Optimizations

Validation of the UNEDF DFT Optimizations

Changes to evaluation engine $\mathbf{S}(\mathbf{x})$

- ◇ HFBTHO Ver 201 [Stoitsov, Schunck, et al., CPC 2013]

2010 MPI-only
single core per nucleus, 72 nuclei evaluated concurrently

2014 Hybrid MPI+OpenMP
98 nuclei evaluated concurrently using 784 cores

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Look back over previous results

- Local optimization
- Computational noise – changes in the code
- Sensitivity analysis – error bars, σ_i

UNEDF0, revisited

	Starting from SLy4		Starting from UNEDF0		Scaled Diff.
	$\hat{\mathbf{x}}^{1,\text{initial}}$	$\hat{\mathbf{x}}^{1,\text{final}}$	$\hat{\mathbf{x}}^{2,\text{initial}}$	$\hat{\mathbf{x}}^{2,\text{final}}$	
ρ_c	0.159539	**0.160**486	0.160526	**0.160**482	0.005
E^{NM}/A	-15.9721	-**16.06**85	-16.0559	-**16.05**81	-0.189
K^{NM}	229.901	**<u>230</u>**	<u>230</u>	**<u>230</u>**	-
a_{sym}^{NM}	32.0043	**31**.3393	30.5429	**30**.6643	0.221
L_{sym}^{NM}	45.9618	54.2493	45.0804	**4**6.2421	0.200
$1/M_s^*$	1.43955	**<u>0.9</u>**	<u>0.9</u>	**<u>0.9</u>**	-
$C_0^{\rho\Delta\rho}$	-76.9962	-**55**.2344	-55.2607	-**55.3**410	0.063
$C_1^{\rho\Delta\rho}$	15.6571	-64.1619	-55.6226	-**55**.4700	-0.153
V_0^n	-258.2	-**170**.796	-170.374	-**170**.575	-0.105
V_0^p	-258.2	-**19**7.782	-199.202	-**198**.759	0.292
$C_0^{\rho\nabla J}$	-92.25	-**7**7.9436	-79.5308	-**79**.4576	0.442
$C_1^{\rho\nabla J}$	-30.75	27.4519	45.6302	**45**.3042	-0.606
$f(\hat{\mathbf{x}})$	1188.75	**67**.9034	67.9854 67.310	**67**.8692	

- Scaled differences: $\frac{\hat{x}_i^{1,\text{final}} - \hat{x}_i^{2,\text{final}}}{\sigma_{\mathbf{i}}}$
- XXX: Reported in UNEDF0 [Kortelainen et al., PRC 2010]
- **XXX**: Agreement with UNEDF0
- <u>XXX</u>: Active bound constraints

Many-Start Results for UNEDF Optimizations

UNEDF0, UNEDF1 [Kortelainen et al., PRC 2012], UNEDF2 [Kortelainen et al., PRC 2014]:

POUNDERS obtains consistent solutions (relative to the original reported uncertainties)

Explanations (other than "very lucky!") include

- POUNDERS is robust: avoids poor local minimizers
- starting points conducive to staying in same basin of attraction
- the data $\mathbf{d}$ and simulation S result in an objective function that is not very multimodal in this part of the parameter space

→ Likely some combination of the above

Contributes further confidence in process

- optimization
- Jacobian-based error bars/SA

Jacobian

Jacobian matrix $J(\mathbf{x}) \in \mathbb{R}^{n_d \times n_x}$

- $[J(\mathbf{x})]_{i,j} = \frac{\partial F_i(\mathbf{x})}{\partial x_j} = \frac{1}{w_i} \frac{\partial S(\mathbf{x};\boldsymbol{\nu}_i)}{\partial x_j}$
- Obtain through algorithmic differentiation (AD) [autodiff.org]
- Approximate by numerical differentiation

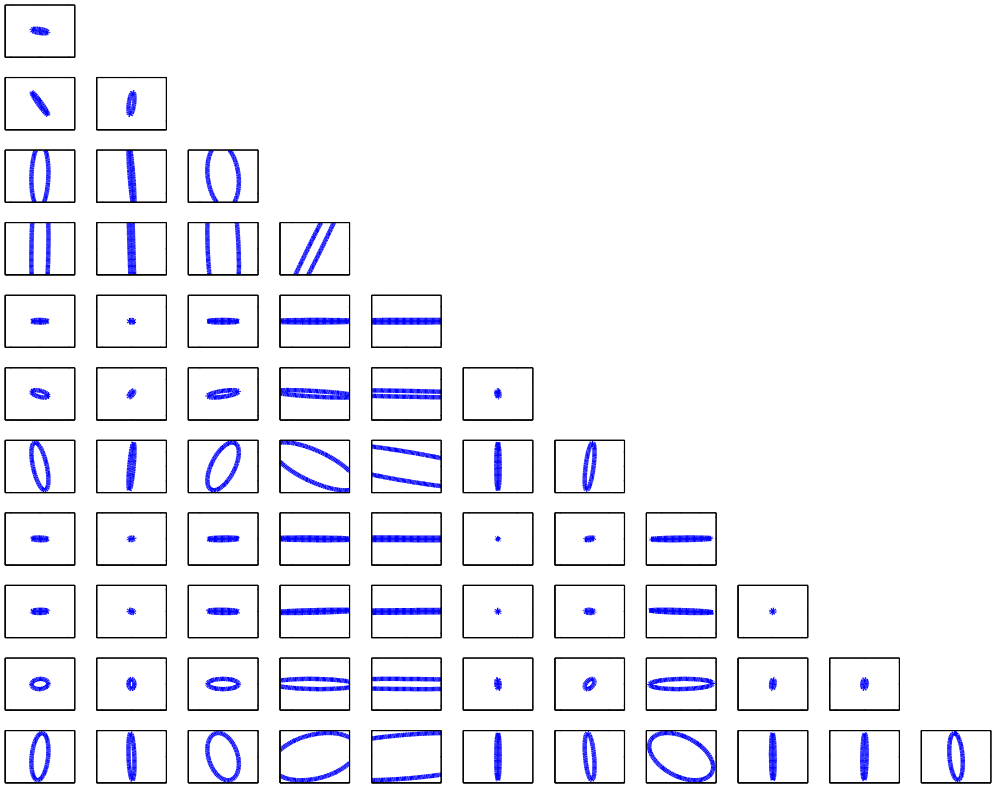
$$\frac{1}{2 w_i h^*_{i,j}} \left(S(\mathbf{x} + h^*_{i,j}\mathbf{e}_j; \boldsymbol{\nu}_i) - S(\mathbf{x} - h^*_{i,j}\mathbf{e}_j; \boldsymbol{\nu}_i) \right)$$

  $h^*_{i,j}$: optimal step size [Moré & W., TOMS 2011] based on the noise in $S(\mathbf{x};\boldsymbol{\nu}_i)$ along the direction $\mathbf{e}_j$
- Requires $2 n_d n_x$ (=2*130*14 for UNEDF2) concurrent evaluations

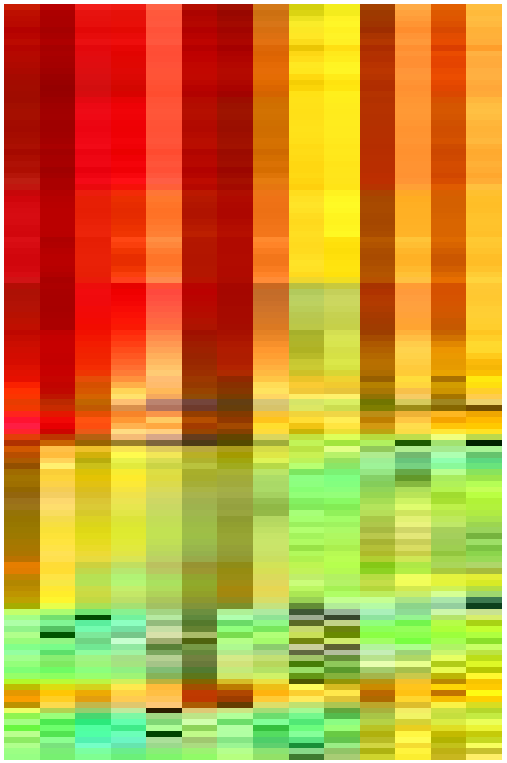
Jacobian-based Sensitivity Analysis

$$\nabla^2_{x,x} f \approx J^T J$$

$$\mathsf{Cov}(x_*) \propto \left(\nabla^2_{x,x} f(x_*)\right)^{-1}$$



Pairwise 95% confidence regions for UNEDF0



Jacobian structure for UNEDF2

Applications Using the Jacobian $\hat{J} = J(\hat{\mathbf{x}})$

Residual $\mathbf{F}(\mathbf{x}) \in \mathbb{R}^{n_d}$ undergoes a change by $\boldsymbol{\epsilon} \in \mathbb{R}^{n_d}$

- Ex.- normalized datum $\frac{d_i}{w_i}$ is changed to $\frac{d_i}{w_i} + \epsilon_i$

$$\hat{\mathbf{x}} \in \arg\min_{\hat{\mathbf{x}} \in \mathbb{R}^{n_x}} f^0(\mathbf{x}) = \|\mathbf{F}(\mathbf{x})\|_2^2 \qquad \hat{\mathbf{x}}_\epsilon \in \arg\min_{\hat{\mathbf{x}} \in \mathbb{R}^{n_x}} f(\mathbf{x}) = \|\mathbf{F}(\mathbf{x}) + \boldsymbol{\epsilon}\|_2^2$$

A second-order expansion of $f = \|\mathbf{F}(\mathbf{x}) + \boldsymbol{\epsilon}\|_2^2$ about $\hat{\mathbf{x}}$:

$$f(\hat{\mathbf{x}}) + 2\boldsymbol{\epsilon}^T \hat{J}(\mathbf{x} - \hat{\mathbf{x}}) + \frac{1}{2}(\mathbf{x} - \hat{\mathbf{x}})^T \left(\nabla^2 f^0(\hat{\mathbf{x}}) + 2\sum_{i=1}^{n_d} \epsilon_i \nabla^2 F_i(\hat{\mathbf{x}}) \right) (\mathbf{x} - \hat{\mathbf{x}}),$$

When $\boldsymbol{\epsilon}$ is small, this quadratic will be convex and hence minimized at

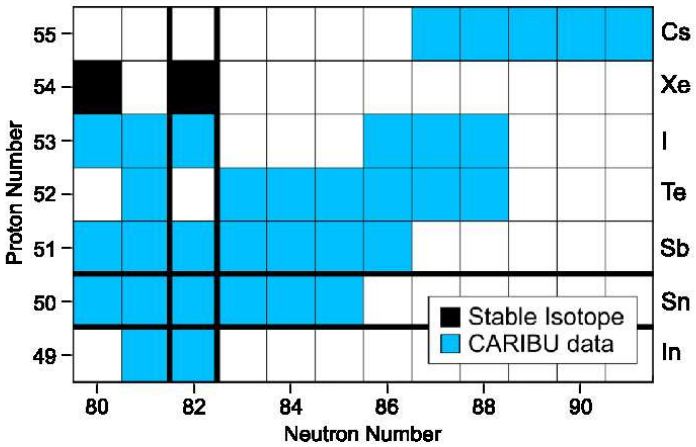
$$\mathbf{x}_\epsilon - \hat{\mathbf{x}} = 2\left(\nabla^2 f^0(\hat{\mathbf{x}})\right)^{-1} \hat{J}^T \boldsymbol{\epsilon} + \mathcal{O}(\|\boldsymbol{\epsilon}\|^2).$$

When $\mathbf{F}(\hat{\mathbf{x}})$ is small, $\nabla^2 f^0(\hat{\mathbf{x}}) \approx 2\hat{J}^T \hat{J}$ and

$$\tilde{\mathbf{x}}_\epsilon \approx \hat{\mathbf{x}} + \left(\hat{J}^T \hat{J}\right)^{-1} \hat{J}^T \boldsymbol{\epsilon}$$

Changes to the Data: Argonne Masses

New nuclear mass data from CARIBU [van Schelt et al., PRL 2014] for 17 neutron-rich, even-even nuclei



UNEDF1 [Kortelainen et al., PRC 2012]:
$n_d = 115$ data

- 75 Masses/binding energies
- 28 RMS radii
  - 8 Pairing gaps/Odd-even mass differences
  - 4 Excitation energies of fission isomers

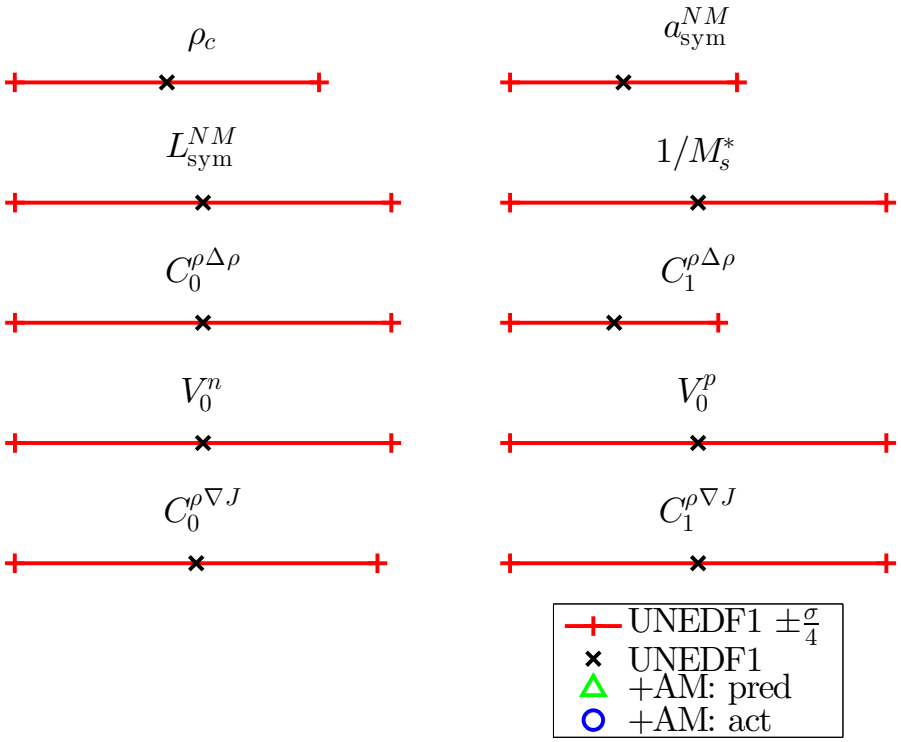
from 75 even-even nuclei

- ◇ 39 deformed (mass only)
- ◇ 28 spherical (mass and rms)
- ◇ 8 deformed (mass and pairing),

11 with $A < 66$, 64 with $A > 106$

Changes to the Data: Argonne Masses (II)

- $\hat{\mathbf{x}}$ UNEDF1 parameterization
- $\mathbf{d}$ UNEDF1 + AM predictions
- $\boldsymbol{\epsilon}$ Zeros except for new mass data
- σ Uncertainties based on $\hat{J}$



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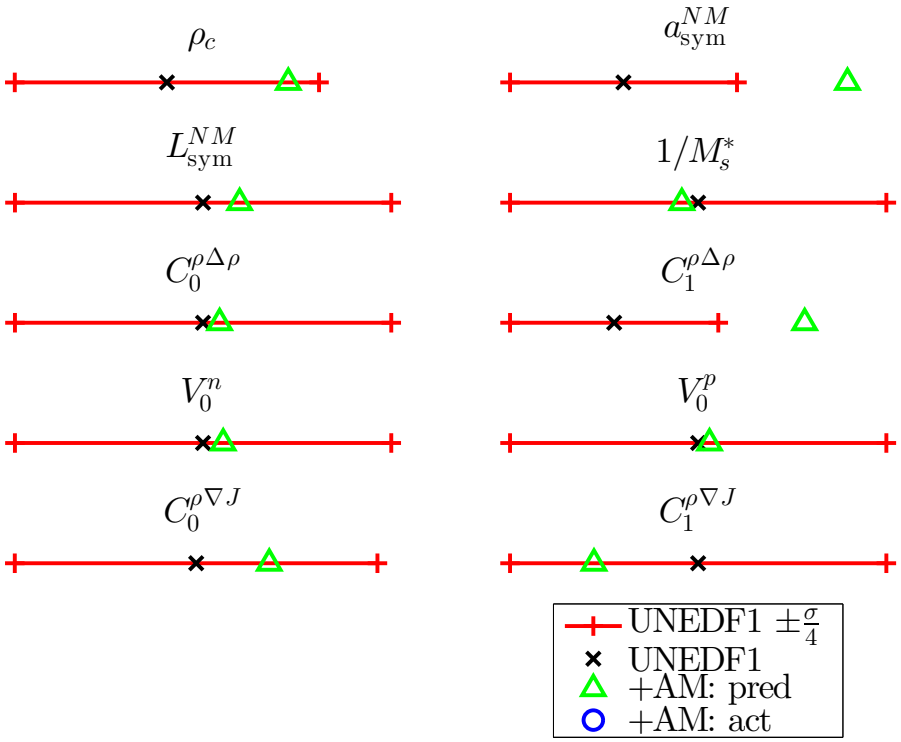

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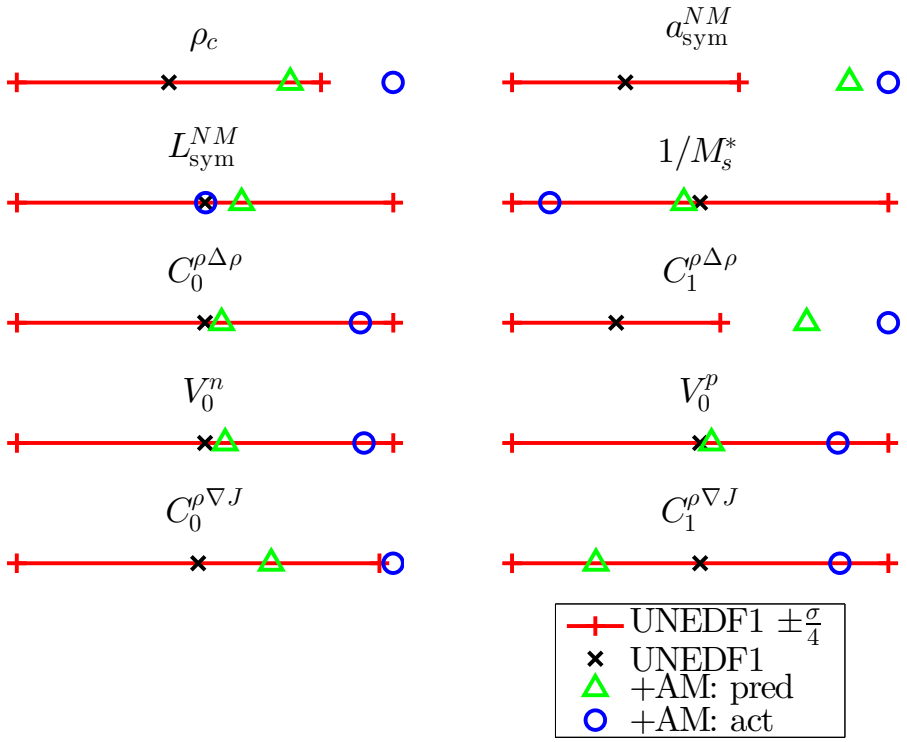
- $\mathbf{x}_*$ Actual POUNDERS solution
  - $\chi^2 = \frac{f(\hat{\mathbf{x}})}{n_d - n_x} = \frac{51.058}{103} = 0.496$
  - $\chi^2 = \frac{f(\mathbf{x}_*)}{n_d - n_x} = \frac{54.01}{120} = 0.450$



Summary

- Move beyond "blackbox" optimization
- Exploiting structure yields better solutions, in fewer simulations
- Promote optimization/modeling considerations during code development
- Bridge theoretical calculations to experiments and ab initio approaches to DFT codes through calibration for new observables
- `www.mcs.anl.gov/tao` (Optimization toolkit)
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Merci!

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Optimization Formulation Plays a Crucial Role

- Solution speed and quality
- Comparing results and extrapolation
  - *What is your χ^2 value?*

$\longrightarrow$ What is your χ^2 function?

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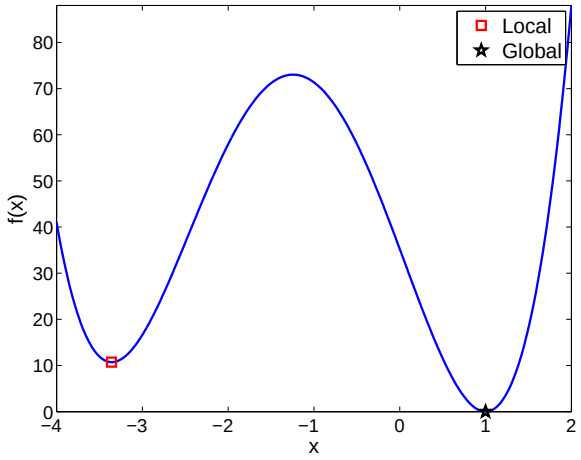
Ex.-: Different norms in fitting

- Now: $f(\mathbf{x}) = \|\mathbf{S}(\mathbf{x}) - \mathbf{d}\|_A^2$, $A =$diag(w_i^{-1})
- Correlations: $f(\mathbf{x}) = \|\mathbf{S}(\mathbf{x}) - \mathbf{d}\|_A^2 = \sum_i \sum_j A_{ij} \left(S_i(\mathbf{x}) - d_i\right)\left(S_j(\mathbf{x}) - d_j\right)$, $A \succ 0$
- $f(\mathbf{x}) = \sum_i \left(\frac{S_i(\mathbf{x}) - d_i}{w_i(\mathbf{x})}\right)^2 + \lambda \|\mathbf{x} - \mathbf{x}^{\mathrm{nom}}\|_0$
- Other regularization terms (total variation, Tikhonov, ...)

Global Optimization, $\min_{x \in \Omega} f(x)$

Careful:

- Global convergence: Convergence (to a local solution/stationary point) from anywhere in Ω
- Convergence to a global minimizer: Obtain x_* with $f(x_*) \leq f(x) \, \forall x \in \Omega$



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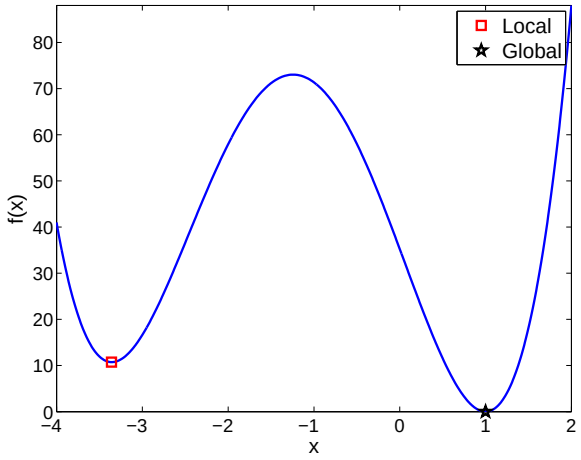

Anyone selling you global solutions when derivatives are unavailable:

either assumes more about your problem (e.g., convex f)

or expects you to wait forever

Törn and Žilinskas: An algorithm converges to the global minimum for any continuous f if and only if the sequence of points visited by the algorithm is dense in Ω.

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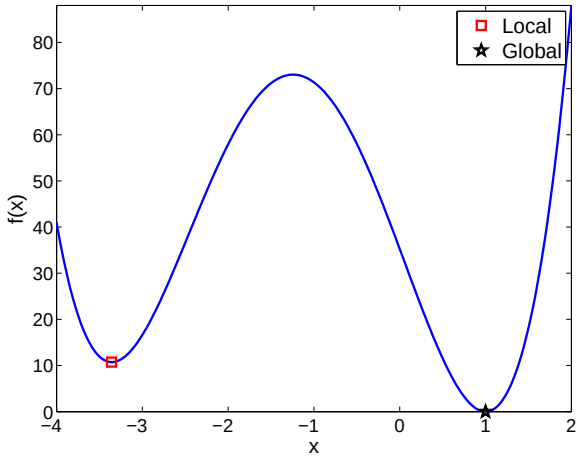

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Instead:

- Rapidly find good local solutions and/or be robust to poor solutions
- Consider multistart approaches and/or structure of multimodality

Heuristics: Experimental X-ray Beam Design