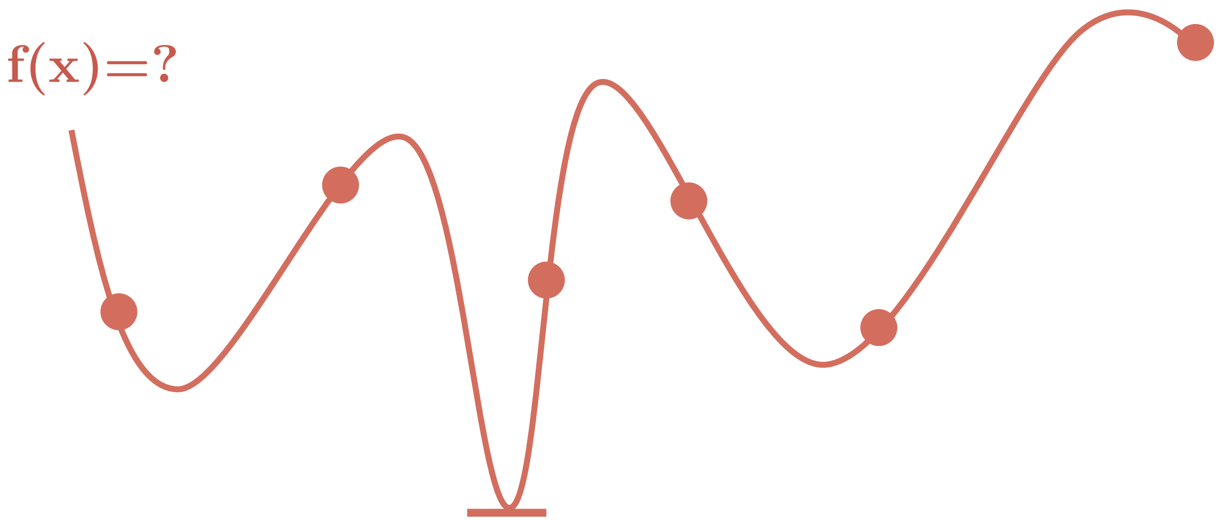

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Derivative-Free Optimization and Simulation Optimization:

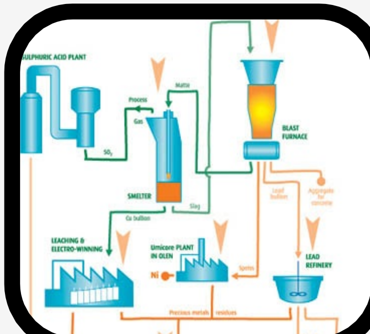
Algorithms and Comparisons

DOW Carnegie Mellon Chemical Engineering CAPD CENTER

Motivation

Query

Fix input variables



Expensive and Noisy!

Measure

Analyze response variables

Derivative-Free Optimization (DFO)

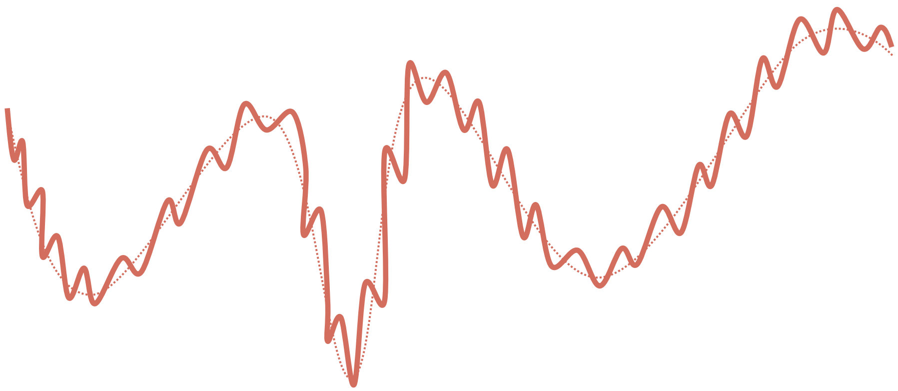
Problem definition

$$\min_{x \in \mathbb{R}^n} \quad \mathbb{E}_\omega [f(x, \omega)]$$

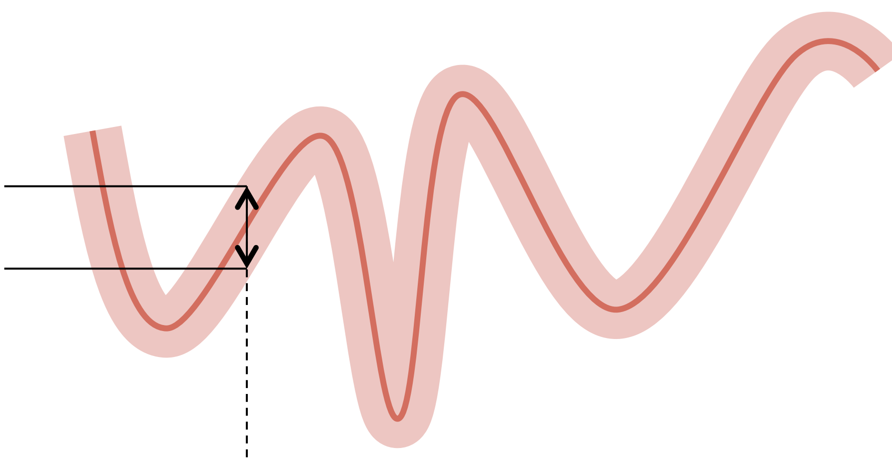
Features

- Continuous, specifiable inputs
- Bound-constrained
- Stochastic output; homogeneous uncertainty
- Expensive to evaluate
- Mono-objective
- Real-valued

Noise



- Low-amplitude, high-frequency noise
- Derivative-free optimization literature



- Inherent stochasticity in output
- Simulation optimization literature

The Challenge

- **Do the best we can when there is no model**
  - How do you exploit structure?
- **No access to derivative information**
  - Search directions? Convergence? Optimality?
- **Need to handle noise inexpensively**
  - Estimation of noise? Homogeneity?
- **Comparisons?**
- **Shift of focus**
  - Function evaluation is expensive
  - maximum decrease in few function evaluations

Trust-region based algorithm

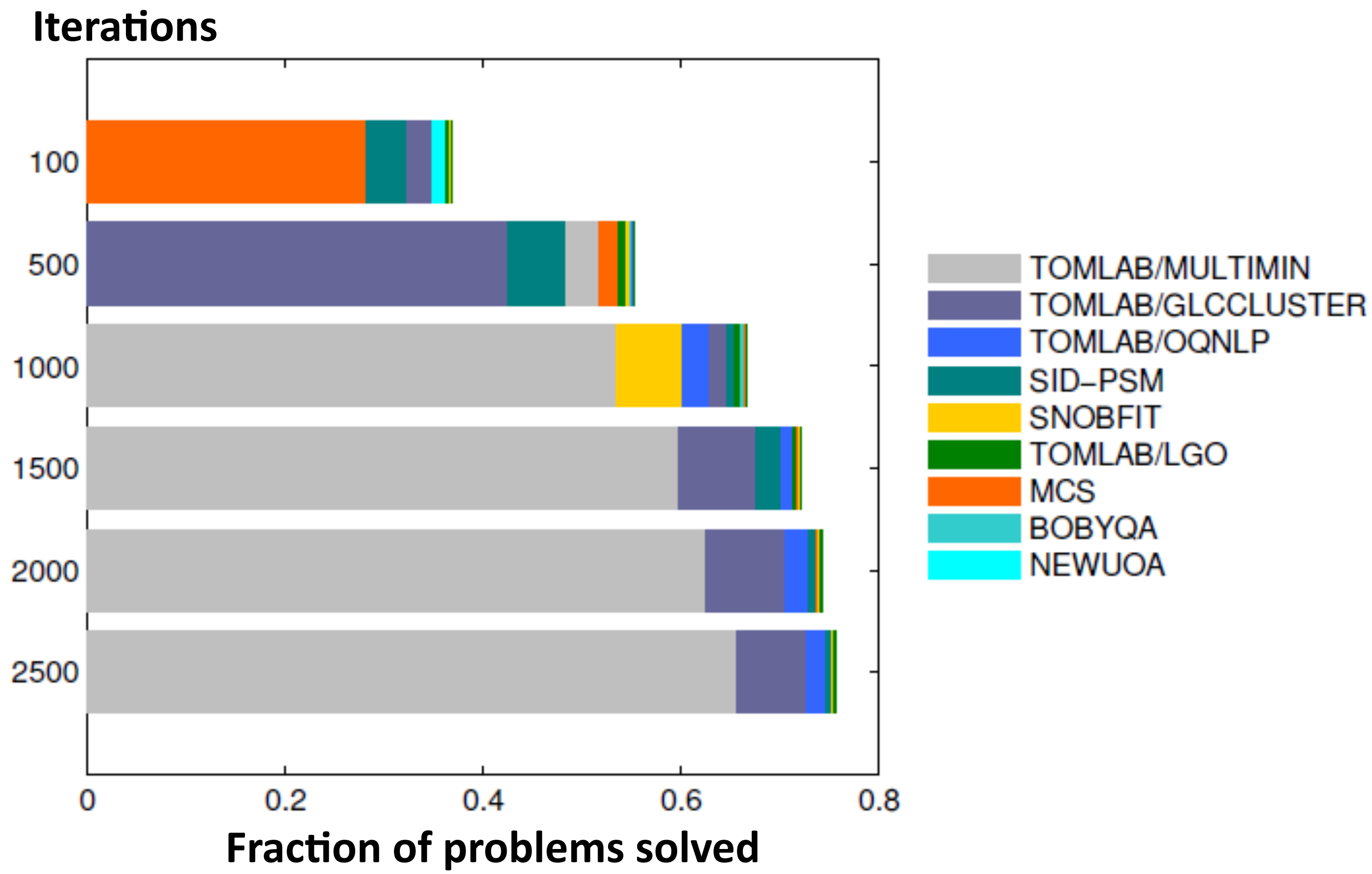
- **Algorithm based on interpolation of sample points using Radial Basis Functions**
- **Routine embedded in a trust-region framework**
- **Adapted to perform global optimization of surrogate, simple bounds on variables**

Comparisons

- **Limitations in comparing algorithms for truly stochastic problems**
  - Many implementations don't have a well-defined stopping criterion; many don't tell you what point they think is the best
  - Even if solver gives 'solution', the only way to compare is to fully characterize the point it is confident in
  - Requires human intervention; not fully automated
  - Noise may not be homogeneous or Gaussian; most solvers assume Gaussian distributions/homogeneity. Heteroscedasticity may need a different objective
  - Lack of standard libraries

DFO results

- **What we've learnt from comparing DFO solvers:**



Rios and Sahinidis (2012)

List of algorithms tested

Algorithm	Type	Author (year)
SPSA – basic	Stochastic approximation	Spall (2003)
SPSA – 2^{nd} order	Stochastic approximation	Spall (2003)
STRONG	Local quadratic response + trust region	Chang, Hong, Wan (2011)
SKO	Global kriging response surface	Huang, Allen, Notz, Zeng (2006)
SNOBFIT	Multi-start local quadratic response	Huyer, Neumaier (2008)
SNM	Nelder-Mead	Chang (2012)

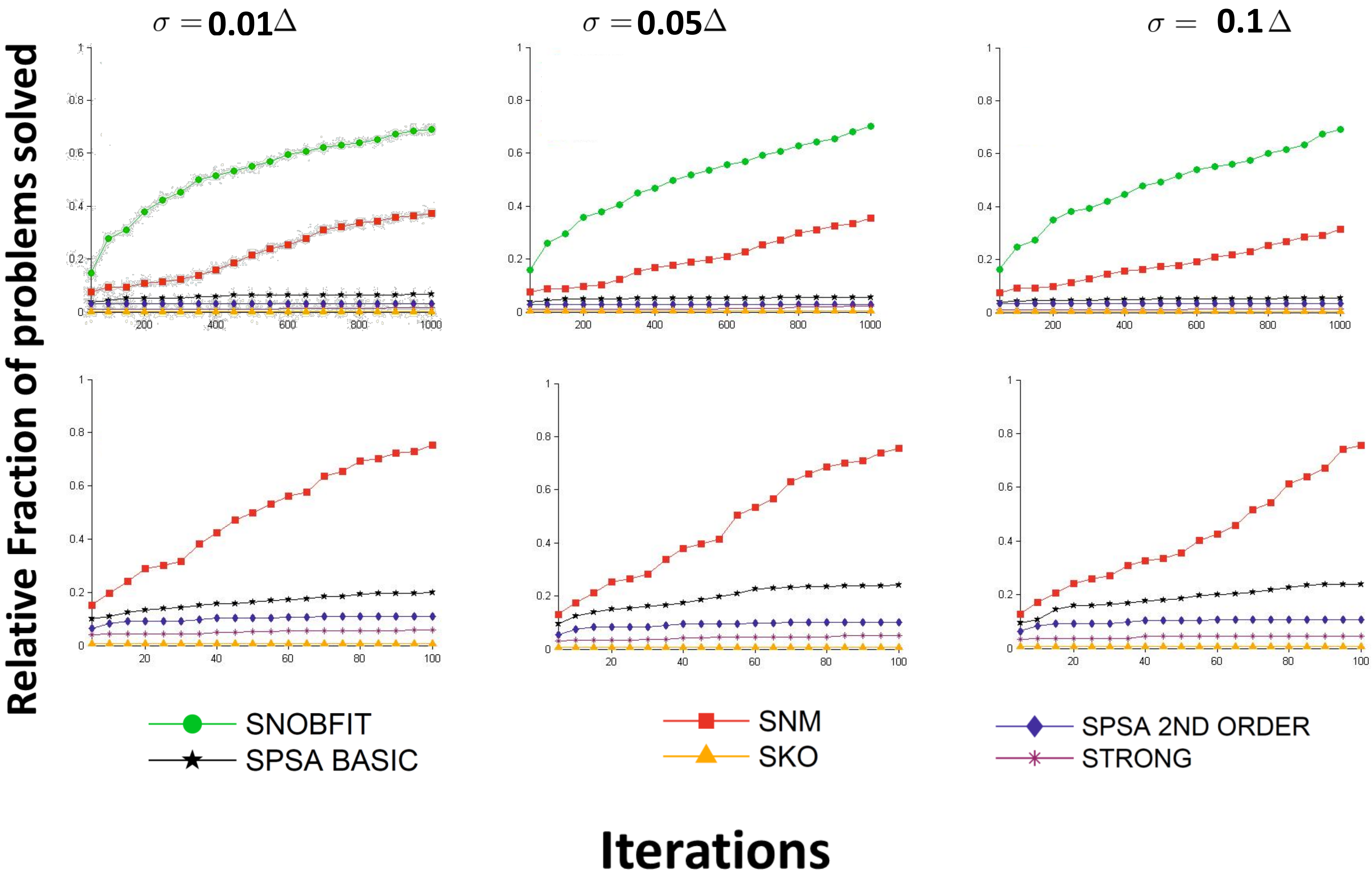
Test problems

	smooth	non-smooth	Total
Convex	**78**	**161**	**239**
Non-convex	**245**	**18**	**263**
Total	**323**	**179**	**502**

Sources:

- **Richtarik (2010), Nesterov (2007), Conn et al (1994), globallib, princetonlib, Lukšan and Vlček (2000)**

Results



$\sigma = 0.01\Delta$
$\sigma = 0.05\Delta$
$\sigma = 0.1\Delta$
Relative Fraction of problems solved
SNOBFIT
SPSA BASIC
SNM
SKO
SPSA 2ND ORDER
STRONG
Iterations

Conclusions and Future Work

- **SNOBFIT performed best**
- **Add more solvers**
  - Academic
  - Commercial
- **Real problem testbeds**
  - SimOpt
- **Give feedback to community**
  - few well-documented codes available
- **Continue to develop algorithms**
  - Deterministic
  - Stochastic
  - Hybrid