We Only Got Started With Dakota

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What Did We Cover?

- Using Dakota
  - Dakota command line usage
  - Interfacing your simulation program
    - Text based input and output files
- Sensitivity Analysis
  - Centered Parameter Study
  - Sampling Study
    - Latin hypercue sampling (LHS)
  - Variance Based Decomposition
    - Direct approach
    - Surrogate model
  - Surrogate Models
    - Polynomial Chaos Expansion

What Did We Cover? (continued)

- Uncertainty Quantification
  - Describing uncertainty using probability distribution functions
- Uncertainty Propagation
  - Sampling
  - Variance Based Decomposition

Many Methods in One Tool

Sensitivity Analysis	Uncertainty Quantification
• Designs: MC/LHS, DACE, sparse grid, one-at-a-time • Analysis: correlations, scatter, Morris effects, Sobol indices	• MC/LHS/Adaptive Sampling • Reliability • Stochastic expansions • Epistemic methods
Optimization	**Calibration**
• Gradient-based local • Derivative-free local • Global/heuristics • Surrogate-based	• Tailored gradient-based • Use any optimizer • Bayesian inference

Interface Dakota to your simulation once, then apply various algorithms depending on your goal…

How related tools compare to Dakota

Software	Methods	Simulation Interface	Hybrid Analyses	R&D	Parallel Computing
NASA UQTools	UQ	???	no	no	???
OpenTURNS	UQ	???	no	no	no
LLNL PSUADE	SA	yes	no	no	???
MIT MUQ	UQ, Opt	custom	no	yes	no
SNL UQTk	UQ, Cal	yes	no	yes	no
OpenMDAO	Opt	yes	no	yes	yes
COIN-OR	Opt	no	no	yes	some
NLOpt	Opt	yes	no	no	no
Nessus	UQ	yes	no	???	no
GoldSim	UQ	???	no	???	no
PEST	Cal	yes	no	???	yes

Other SA Approaches Typically Only Require Changing the Method Block

- Dakota Reference Manual guides in specifying keywords

```
method,
sampling
     sample_type lhs
     seed = 52983
     samples = 100
```

LHS Sampling

```
method,
     dace oas
     main_effects
     seed = 52983
     samples = 500
```

Main Effects Analysis using Orthogonal Arrays

```
method,
sampling
     sample_type lhs
     seed = 52983
     samples = 500
     variance_based_decomp
```

Variance-based Decomposition using LHS Sampling

```
method,
     psuade_moat
     partitions = 3
     seed = 52983
     samples = 100
```

Morris One-at-a-Time

Dakota SA Methods Summary

Category	Dakota method names	univariate trends	correlations	modified mean, s.d.	main effects Sobol inds.	importance factors / local sensis
Parameter studies	centered, vector, list	P				
	grid		D		P	
Sampling	sampling, dace lhs, dace random, fsu_quasi_mc, fsu_cvt with variance_based_decomp...	P	D		D	
DACE (DOE-like)	dace {oas, oa_lhs, box_behnken, central_composite}		D		D	
MOAT	psuade_moat			D		
PCE, SC	polynomial_chaos, stoch_collocation				D	D
Mean value	local_reliability					D

also multi-purpose!

D: Dakota-generated
P: Post-processing required
(3rd party tools)

Guide to Optimization Methods

See Usage Guidelines in User's Manual

Sandia National Laboratories

Category	Dakota method names	Continuous Variables	Categorical/ Discrete Variables	Bound Constraints	General Constraints
Gradient-Based Local (smooth)	`optpp_cg`	x			
	`dot_bfgs, dot_frcg, conmin_frcg`	x		x	
	`npsol_sqp, nlpql_sqp, dot_mmfd, dot_slp, dot_sqp, conmin_mfd, optpp_newton, optpp_q_newton, optpp_fd_newton`	x		x	x
Gradient-Based Global (smooth)	`hybrid, multi_start`	x		x	x
Derivative-Free Local (nonsmooth)	`optpp_pds`	x		x	
	`coliny_cobyla, coliny_pattern_search, coliny_solis_wets, surrogate_based_local`	x		x	x
	`asynch_pattern_search, mesh_adaptive_search`	x	x	x	x
Derivative-Free Global (nonsmooth)	`ncsu_direct, genie_direct, genie_opt_darts`	x		x	
	`coliny_direct, efficient_global, surrogate_based_global`	x		x	x
	`coliny_ea, soga, moga (multiobjective)`	x	x	x	x

For multi-objective problems: use weighted sum with any method, pareto_set, or moga.

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Category	Dakota method names	Continuous Variables	Categorical/ Discrete Variables	Bound Constraints	General Constraints
Gradient-Based Local (smooth)	`optpp_cg`	x			
	`dot_bfgs, dot_frcg, conmin_frcg`	x		x	
	`npsol_sqp, nlpql_sqp, dot_mmfd, dot_slp, dot_sqp, conmin_mfd, optpp_newton, optpp_q_newton, optpp_fd_newton`	x		x	x
Gradient-Based Global (smooth)	`hybrid, multi_start`	x		x	x
Derivative-Free Local (nonsmooth)	`optpp_pds`	x		x	
	`coliny_cobyla, coliny_pattern_search, coliny_solis_wets, surrogate_based_local`	x		x	x
	`asynch_pattern_search, mesh_adaptive_search`	x	x	x	x
Derivative-Free Global (nonsmooth)	`ncsu_direct, genie_direct, genie_opt_darts`	x		x	
	`coliny_direct, efficient_global, surrogate_based_global`	x		x	x
	`coliny_ea, soga, moga (multiobjective)`	x	x	x	x

For multi-objective problems: use weighted sum with any method, pareto_set, or moga.

Guide to Calibration Methods

See Usage Guidelines in User's Manual

Category	Specialized Calibration Methods	General Optimization Methods	Continuous Variables	Categorical/ Discrete Variables	Bound Constraints	General Constraints
Gradient-Based Local (smooth)		optpp_cg	x			
	nl2sol	dot_bfgs, dot_frcg, conmin_frcg	x		x	
	nlssol_sqp, optpp_g_newton	npsol_sqp, nlpql_sqp, dot_mmfd, dot_slp, dot_sqp, conmin_mfd, optpp_newton, optpp_q_newton, optpp_fd_newton	x		x	x
Gradient-Based Global (smooth)	hybrid*, multi_start*	hybrid, multi_start	x		x	x
Derivative-Free Local (nonsmooth)		optpp_pds	x		x	
	surrogate_based_local*	coliny_cobyla, coliny_pattern_search, coliny_solis_wets	x		x	x
		asynch_pattern_search, mesh_adaptive_search	x	x	x	x
Derivative-Free Global (nonsmooth)		ncsu_direct, genie_direct, genie_opt_darts	x		x	
		coliny_direct, efficient_global, surrogate_based_global	x		x	x
		coliny_ea, soga	x	x	x	x

**: in conjunction with a specialized gradient-based method (nl2sol, nlssol, optpp_g_newton)*

Dakota UQ Methods Summary

character	method class	problem character	variants
aleatory	probabilistic sampling	nonsmooth, multimodal, modest cost, # variables	Monte Carlo, LHS, importance
	local reliability	smooth, unimodal, more variables, failure modes	mean value and MPP, FORM/SORM,
	global reliability	nonsmooth, multimodal, low dimensional	EGRA
	stochastic expansions	nonsmooth, multimodal, low dimension	polynomial chaos, stochastic collocation
epistemic	interval estimation	simple intervals	global/local optim, sampling
	evidence theory	belief structures	global/local evidence
both	nested UQ	mixed aleatory / epistemic	nested

Also see Usage Guidelines in User's Manual