Optimization Using Surrogates for Engineering Design

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Background: Introduction

Target problems
The strawman surrogate algorithm
Closed and Open Constraints

The surrogate management framework

Selected numerical results

Software and Conclusions

Our aim is to provide usable algorithms for expensive simulation-driven design. We use surrogates, but we solve the simulation-driven problem

(*NLP*) minimize
$$f(x)$$
 subject to $x \in \Omega$,

The strawman surrogate algorithm Closed and Open Constraints

Target Class of Problems

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where $f: \Re^n \to \Re \cup \{\infty\}$ may be discontinuous and:

the functions are expensive black boxes - secs, mins, days, weeks

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- accurate approximation of derivatives is problematic



Relation of target problems to design

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- Optimization or design or control variables x

The strawman surrogate algorithm Closed and Open Constraints

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▶ p is fixed in the simulation, but it is subject to uncertainty because of incomplete knowledge (e.g. material properties) or because the product is used differently (e.g., the altimeter is off by 5%)

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- $ightharpoonup C_p(x) \le 0$ only has to hold at the solution

The strawman surrogate algorithm Closed and Open Constraints

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- ➤ Some variables are categorical, i.e., the simulations only run with certain discrete choices, e.g., choice and sequencing of manufacturing processes. We rigorously treat categorical optimization variables in our algorithms

The strawman surrogate algorithm Closed and Open Constraints

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Robustify against such "variability" by giving up some optimality at a given point in return for optimality over nearby designs

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We would be willing to give up some performance at the exact conditions p in return for optimal performance over all likely nearby conditions q - or we can constrain probability of failure for the nominal p

Seems to be "chance constrained" stochastic programming - nothing new



The strawman surrogate algorithm Closed and Open Constraints

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Still belongs to target class, Bring 'em on for now, but seek tighter coupling

A confidence builder

Meckesheimer, Booker, and Torng report very good performance of our approach on some structural engineering problems in dealing with probability of failure by constraints or as the objective

Appeared in OTPE special issue: "Reliability based design optimization using Design Explorer" (Design Explorer is Boeing's implementation of the surrogate management framework - SMF)

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From this point on, assume the formulation incorporates uncertainty

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 - 1.1 simplified physical models; or
 - 1.2 surfaces obtained from f, C values at selected sites

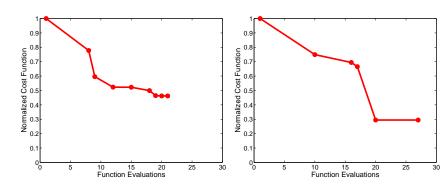
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- 3. Compute $f(x_s)$, $C(x_s)$ to determine if improvement has been made over the best x found to date Stalls when surrogate stagnates

Trailing edge design for unsteady flow

Optimize shape for total acoustic noise reduction. Work of Stanford fluids grad student Alison Marsden, strawman left and SMF right



Closed constraints - a barrier approach

To enforce X constraints, replace f by a barrier objective

$$f_X(x) := \begin{cases} f(x) & \text{if } x \in X, \\ +\infty & \text{otherwise.} \end{cases}$$

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Our theory is powerful for this approach, which saves LES runs in Alison Marsden's application to trailing edge design in fully turbulent flow.

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Note that $h_X(x) = 0$ iff x is feasible for both open and closed constraints

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We use the filter. (originally idea from Fletcher & Leyffer)

We admit that our filter theory is currently weaker than for other approaches.

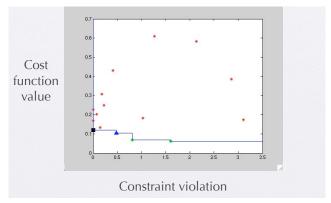
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Final filter for RANS trailing edge design

A trial point x is *unfiltered* if $h_X(x) < h_{max}$ and no earlier point is at least as optimal and as feasible Successful iterations find unfiltered points UNSUCCESSFUL iterations don't



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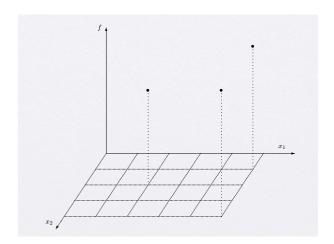
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1. (Strawman)Search on s_f, s_C to find an unfiltered $x_{k+1} \in M_k$. If found, then set $M_{k+1} = M_k$ and update the surrogates;

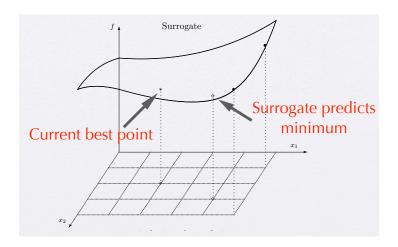
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- 2. Else if p_k is the only unfiltered point in P_k ; Then set $x_{k+1}=x_k$ and $M_{k+1}=M_k/4$ and update the surrogates; Else return to 1

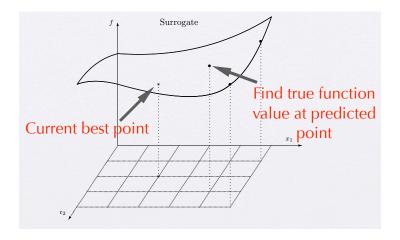
Gather surrogate training set



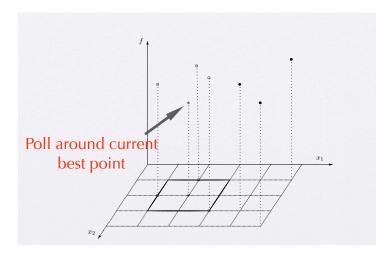
Use surrogate to predict better design



Check for improvement



If surrogate fails, then POLL



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There are NO assumptions on the surrogate, but better surrogates provide better predictions and hence fewer expensive function calls.

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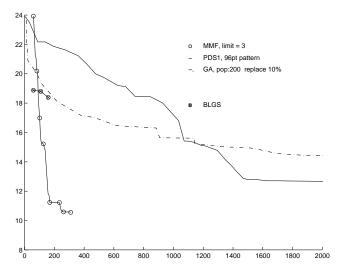
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Is the SMF that good?

Presently it is the only realistic possibility for really expensive problems

Here are some results:

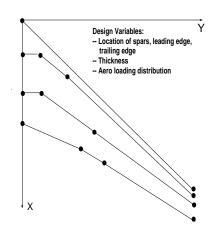
Comparisons on 31d helicopter example



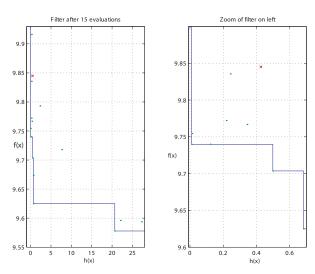
Boeing wing planform design - infeasible baseline

Infeasible baseline design

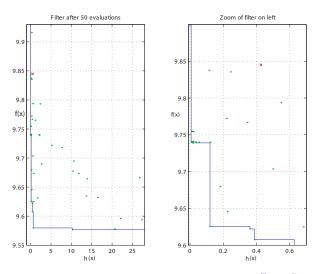
		# of	# of
	n	ctrs	fevals
Α	15	11	304
В	15	11	292



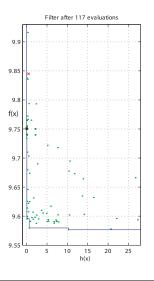
Boeing SonicCruiser planform initial filter

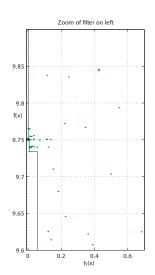


A planform filter after 50 evaluations

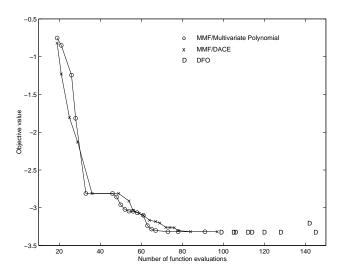


Feasibility after 117 evaluations

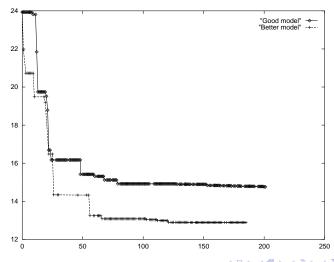




Polynomial vs DACE surrogates



Recovering from a bad surrogate



Implementations

- *=freely available. Red=under active development.
 - NOMAD C++*: MADS with barrier and filter
 - ▶ in use in company-wide tool at ExxonMobil
 - NOMADm*: Our MatLab version with everything
 - ▶ in use at Siemens
 - Design Explorer: Boeing's implementation available to nonBoeing users from Phoenix Integration
 - includes DACE surrogates, used on the Boeing 777 and in use on the 7e7
 - Alison Marsden's Matlab code Used for trailing edge design
 - she has completed one iteration with her SMF implementation on LES turbulent flow trailing edge design with a 54% reduction in noise - 3 weeks per simulation

Conclusions and Claims

- ► The SMF is a completely rigorous tool for engineering design governed by expensive simulations. It solves the expensive problem - not the surrogate problem
- ▶ The SMF is based on our derivative-free MADS algorithms
- ► The quality of the surrogate as an approximation is not an assumption, but a good surrogate saves expensive simulations
- ► The ANOVA implementation in Boeing's Design Explorer suggests which are the important design variables
- ► The work to find an approximation based on a large training set is not justified for its use in surrogate optimization, but it may be justified if the approximation has other purposes -Phillips Research NL does this