Good and Bad Uncertainty: Consequences in UQ and Design

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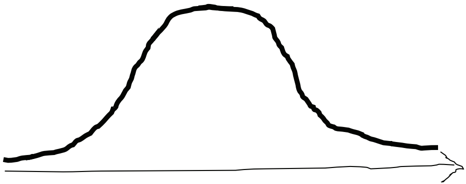
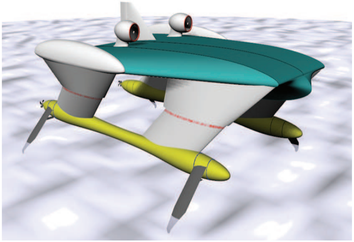
Symmetric pdfs



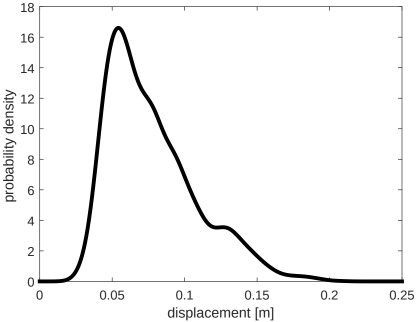
pdf for random variable

Carl Friedrich Gauss

Applications: concern about one tail



120kn marine vessel
(Patent: S. Brizzolara)

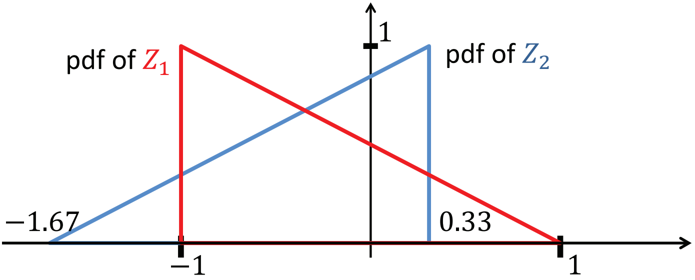


Uncertain tip displacement of hydrofoil under random cavitation index and material properties

Consequences in decision making

Design 1: uncertain response Z_1

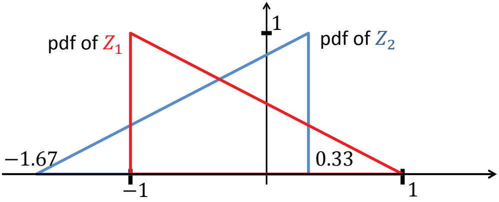
Design 2: uncertain response Z_2



Which design is less uncertain, safer?

Concern about upper tail (displacement, stress, cost)

Using mean and standard deviation?



same mean (−0.33)

same std. dev. (0.87)

Harry M. Markowitz

(www.nobelprize.org)

Designs are equally "good" from this perspective

But it gets worse..

Design 1: uncertain response W_1

Design 2: uncertain response W_2

Two possible outcomes:

With probability 0.5: $W_1 = 0$ and $W_2 = 0$

With probability 0.5: $W_1 = -2$ and $W_2 = -1$

But it gets worse..

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Obviously, Design 1 better

But, if ranking based on mean + 2 std. dev., Design 2 wins!

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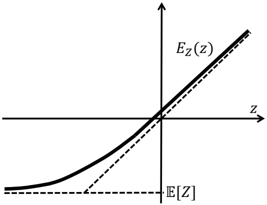
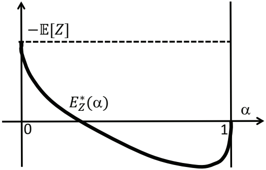
Mean plus std. deviation not suitable for decision making

Today's talk

Describe alternative way of quantifying uncertainty that

- focuses on safety, computability; avoids paradoxes
- relies on convex analysis





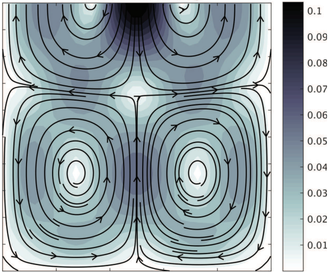
R.T. Rockafellar

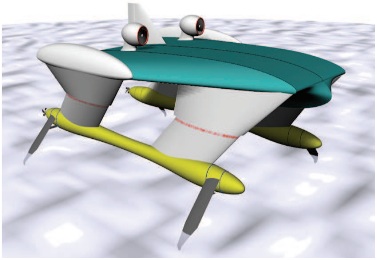
Today's talk (cont.)

Show how to carry out

- design optimization under uncertainty
- surrogate building using multi-fidelity analysis

with this alternative way of quantifying uncertainty



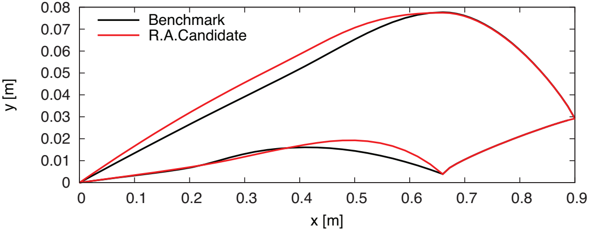


Impact in multi-disciplinary 3D hydrofoil design

17 design variables; 5 uncertain parameters

Quantities of interest: hydrodynamical and structural

Multi-fidelity 3D URANSE for turbulent cavitating flow, 3D FEM



	displ. [m]	drag/lift	lift [t]	stress margin [MPa]
Prediction	0.109	0.139	36.8	−142
Actual	0.060	0.130	37.7	−410
Benchmark	0.097	0.132	35.3	−294

Bonfiglio, Royset, Karniadakis, '18

Alternative way: superquantile risk

For $\alpha \in [0,1]$, the α-superquantile of random variable Z:

$R_\alpha(Z)$ = average of $(1-\alpha)100\%$ worst outcomes of Z

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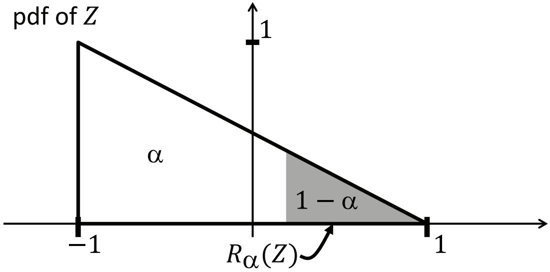

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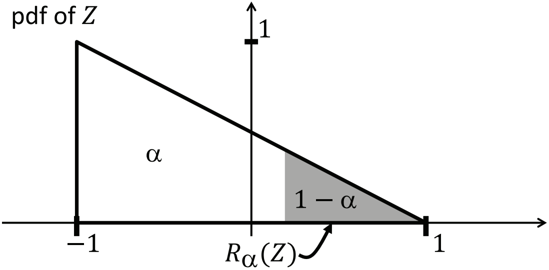

$\alpha = 0$: $R_\alpha(Z) = \mathbb{E}[Z]$ = expected value (mean) of Z

$\alpha = 1$: $R_\alpha(Z)$ = worst outcome of Z that can occur

Z_1 safely below Z_2 when $R_\alpha(Z_1) \leq R_\alpha(Z_2)$

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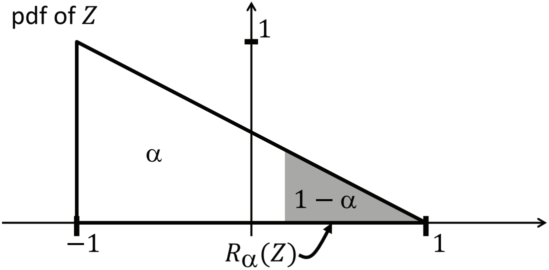

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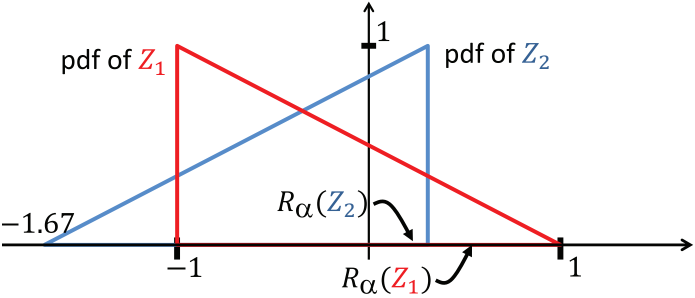
Rockafeller & Uryasev '00, '02 (CVaR); Acerbi & Tasche '02 (exp. shortfall)

Also called AVaR (Föllmer & Schied '04) in finance and OR

Return to triangular example

Design 1: uncertain response Z_1

Design 2: uncertain response Z_2



Averages of worst 10% outcomes:

$R_{0.9}(Z_1) = 0.58$ and $R_{0.9}(Z_2) = 0.28$ (better)

Response of Design 2 **safely below** that of Design 1

Advantages of superquantile risk (s-risk)

Modeling considerations:

adapts to any level of “safety” (can vary α)

focuses on the “bad” tail (promotes resilience)

promotes diversification

connects with dual utility theory

probes deeper than expected utility theory

relates to risk-neutral decisions under stochastic ambiguity

Computational considerations:

preserves convexity (continuity)

easier to find globally optimal designs and decisions

when using s-risk,
optimization under uncertainty “no harder” than deterministic

Design optimization under uncertainty

Design variables: deterministic vector x

Uncertain parameters: random vector V

System response (quantity of interest): $g(x, V)$

Cost of design: $\varphi(x)$

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Find design x that

$$\begin{aligned} \min\ & \varphi(x) \\ \text{subject to}\ & R_\alpha\big(g(x, V)\big) \le t \\ & \text{and other (deterministic) constraints} \end{aligned}$$

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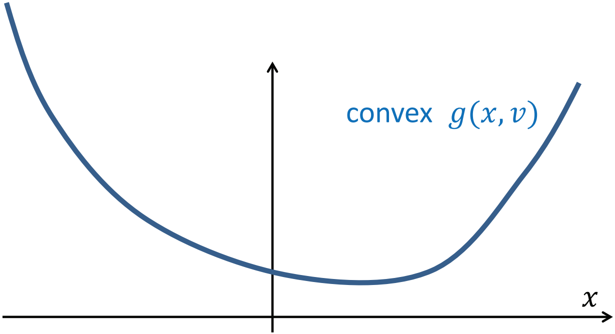
Resulting design $x^\star$: on average in the $(1-\alpha)100\%$ worst outcomes of $g(x^\star, V)$, response will not exceed t

(Easily extended to multiple quantities of interests, uncertain cost)

Role of convexity

If $g(x, v)$ is convex in x for all outcomes v of V:



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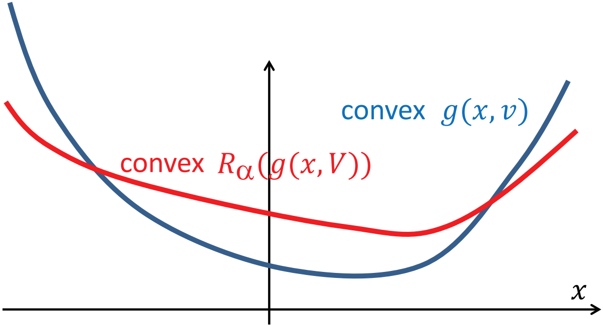


What about failure probability?

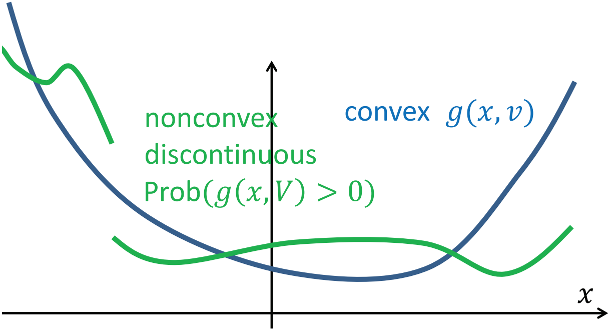
Find design x that

$$\begin{aligned} &\min \varphi(x) \\ \text{subject to } &\text{Prob}\big(g(x, V) > 0\big) \leq 1 - \alpha \\ &\text{and other (deterministic) constraints} \end{aligned}$$

Common formulation in reliability-based design optimization

Lack of convexity for failure probability

If $g(x, v)$ is convex in x for all outcomes v of V:

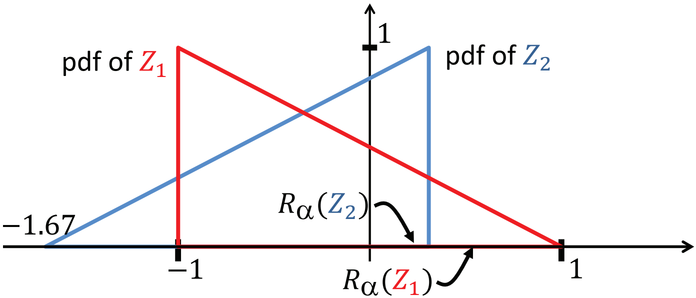


Using failure probability makes optimization harder

Again return to triangular example

Design 1: uncertain response Z_1

Design 2: uncertain response Z_2



Recall: $R_{0.9}(Z_1) = 0.58$ and $R_{0.9}(Z_2) = 0.28$ (better)

Prob$(Z_1 > 0) = 0.25$ (better) and Prob$(Z_2 > 0) = 0.31$

Failure probability doesn't account for **magnitude** of exceedance

..but sometimes failure probability is needed..

Failure probability common in regulatory requirements

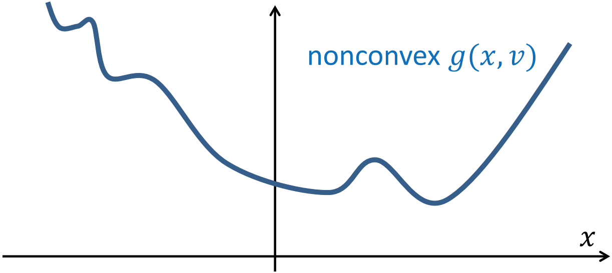
Superquantiles lead to a (best) conservative approximation of failure probability through **buffered failure probability** (Rockafellar & Royset '10, Norton et al. '17, Mafusalov et al. '18):

$$
\begin{aligned}
& R_\alpha\big(g(x,V)\big) \leq 0 \\
\iff & \text{buffered failure probability of } g(x,V) \leq 1-\alpha \\
\implies & \text{Prob}\big(g(x,V) > 0\big) \leq 1-\alpha
\end{aligned}
$$

Constraints on s-risk can be reinterpreted in probabilistic terms

Role of convexity

But, $g(x, v)$ may not be convex in x:



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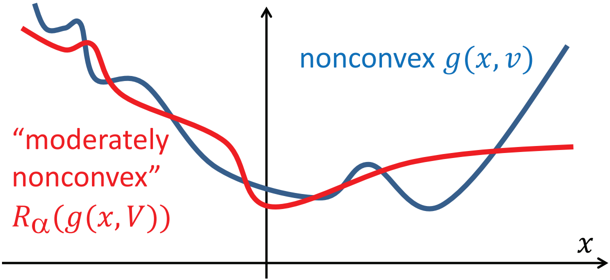

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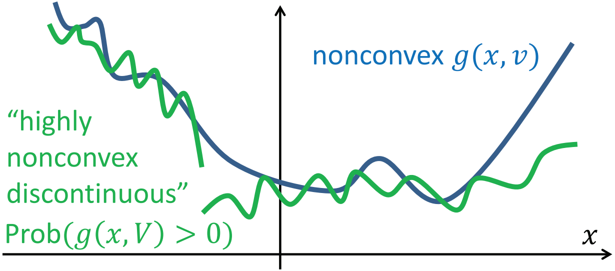

Further simplifications

Defining formula for superquantiles (Rockafeller & Uryasev '00, '02):

$$R_\alpha\big(g(x,V)\big) = \min_{y_0 \in \mathbb{R}} \left\{ y_0 + \frac{1}{1-\alpha} \mathbb{E}\big[\max\{0, g(x,V) - y_0\}\big] \right\}$$

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If V has outcomes $v^1, v^2, \ldots, v^m$ with probabilities $p_1, p_2, \ldots, p_m$,

$$\begin{aligned} &\min\ \varphi(x) \\ &\text{subject to } R_\alpha\big(g(x,V)\big) \le t \end{aligned}$$

can **equivalently be replaced** by finding $x, y_0 \in \mathbb{R}, y \in \mathbb{R}^m$ that

$$\begin{aligned} &\min\ \varphi(x) \\ \text{subject to } y_0 + \frac{1}{1-\alpha}\sum_{i=1}^m p_i y_i &\le t \\ g(x, v^i) - y_0 \le y_i &\text{ for all } i = 1, \ldots, m \\ 0 \le y_i &\text{ for all } i = 1, \ldots, m \end{aligned}$$

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Optimization under uncertainty "no harder" than deterministic

Risk-adaptive learning and surrogate building

Response $g(x, V)$ **costly to compute** (high-fidelity simulation)

Leverage approximating responses $h(x, V)$ (low-fidelity simulations)

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Risk-adaptive surrogate building:

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i.e., $R_\alpha\big(g(x, V)\big) \leq R_\alpha\big(f(h(x, V))\big)$

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Flexibility: $h(x, v)$ vector-valued, possibly $h_j(x, v) = x_j$, etc.

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Example: $\hat{h}(x, v)$ = lower-level surrogate and $f\big(h(x, v)\big) =$

$$a_0 + a^\top x + c^\top v + b_0 \hat{h}(x, v) + \bar{a}^\top x \hat{h}(x, v) + \bar{c}^\top v \hat{h}(x, v) + b[\hat{h}(x, v)]^2$$

Finding f amounts to finding coefficients $a_0, a, \bar{a}, b_0, b, c, \bar{c}$

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Notation: $Y = g(x, V)$, $X = h(x, V)$; view x as "random" over design space (set-based design)

Risk-adaptive learning and surrogates (cont.)

Response quantity: random variable Y (high-fidelity simulation)
Approximations: random vector X (low-fidelity simulations)

Find f such that $R_\alpha(Y) \leq R_\alpha\big(f(X)\big)$

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How can this be achieved without being overly conservative?

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Reasonable: minimize the error of $Y - f(X)$

But using what measure of error? **Least-squares will not do**

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Superquantile regression possible (but not discussed here)

(Rockafellar, Royset, Miranda '14)

Risk-adaptive learning algorithm

For simplicity, $f(X) = c_0 + c^\top X$, with $c \in \mathbb{R}^k$

Two-step algorithm:

1. Solve $\min_{c \in \mathbb{R}^k} \left\{ c^\top \mathbb{E}[X] + R_\alpha(Y - c^\top X) \right\} + \lambda \|c\|_1$
2. Set $c_0 = R_\alpha(Y - c^\top X)$

Step 1 (Residual risk minimization)

convex problem; scalable

problem size is data independent

resembling problem in SVM

Step 2 (s-risk computation)

either 1D convex problem or sorting (quick)

Rockafellar & Royset '15a; Royset, Bonfiglio, Vernengo, Brizzolara '17

Theoretical results

Conservative surrogate on training data:

For $\alpha \in (0,1)$ and (c_0, c) computed by risk-adaptive learning,

$$R_\alpha(\tilde{Y}) \leq R_\alpha(c_0 + c^\top \tilde{X})$$

with $(\tilde{X}, \tilde{Y})$ distributed according to training data

Rockafellar & Royset '15a

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Consistency:

For $\alpha \in (0,1)$ and (c_0, c) computed by risk-adaptive learning,

$$\mathcal{R}_\alpha(Y) \leq \mathcal{R}_\alpha(c_0 + c^\top X) \text{ in the limit as training size } \to \infty$$

with (X, Y) having the actual (true) distribution

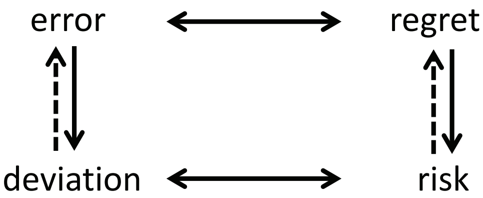
Rockafellar & Royset '15a

Broader landscape: risk-regression connections

Residual risk problem equivalent to quantile regression

Extensions to (regular) measures of risk beyond s-risk

Risk (design) connected with error (regression, prediction)



Rockafellar & Uryasev '13; Rockafellar & Royset '15a

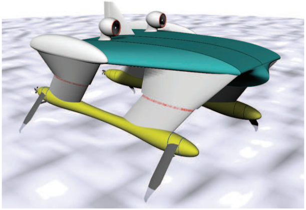
Detail: multi-disciplinary 3D hydrofoil design

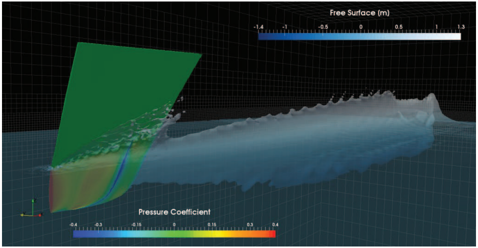
Surface-piercing super-cavitating hydrofoil

17 design variables; 5 uncertain parameters

Quantities of interest: hydrodynamical and structural

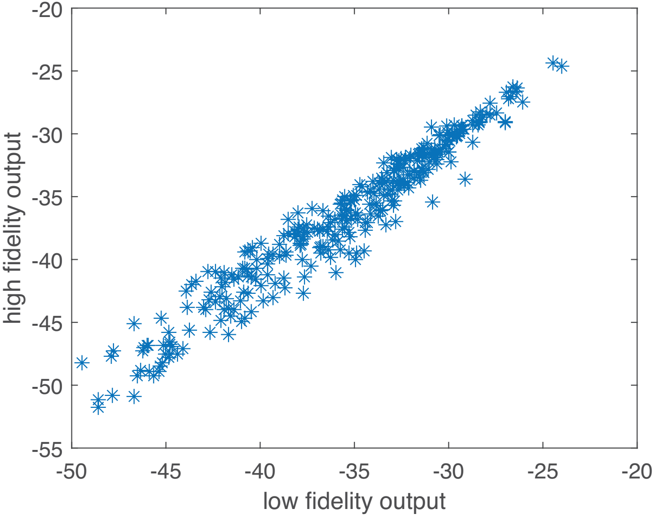
308 high-fidelity 3D URANSE solves
3063 high-fidelity 3D FEM solves
19830 low-fidelity 3D URANSE solves and 3D FEM solves





Bonfiglio, Royset, and Karniadakis '18

Risk-adaptive learning of lift force

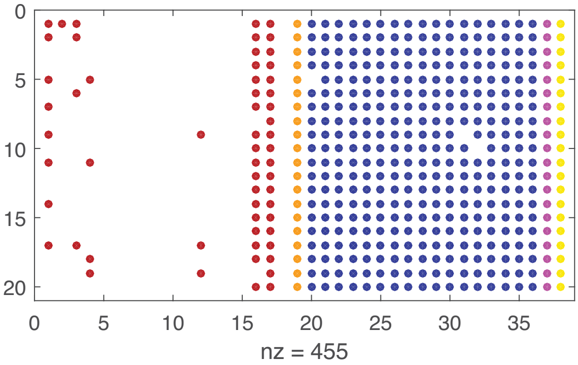


Accurate predictions possible

Risk-adaptive learning of lift force (cont.)

Surrogate has 1+38 coefficients to be learned

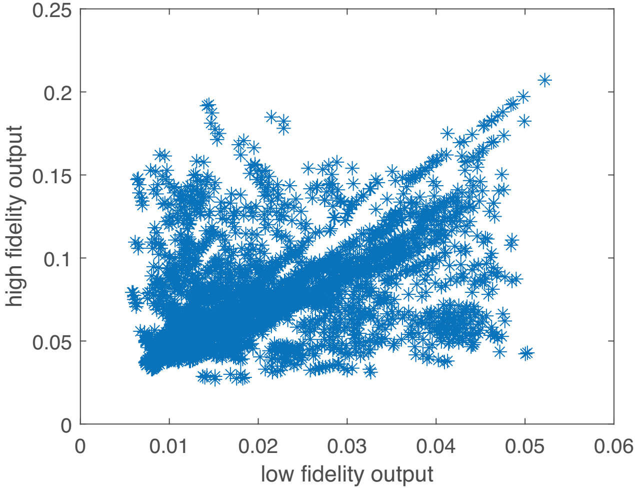
Sparsity (model selection) across 20 surrogates:



Red, gray, orange, blue, pink, and yellow colors correspond to a, c, b_0, $\bar{a}$, $\bar{c}$, and b, respectively

$$a_0 + a^\top x + c^\top v + b_0 \hat{h}(x,v) + \bar{a}^\top x \hat{h}(x,v) + \bar{c}^\top v \hat{h}(x,v) + b[\hat{h}(x,v)]^2$$

Risk-adaptive learning of displacement

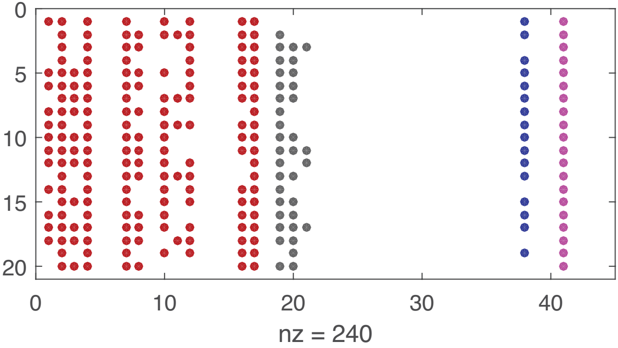


Poor correlation between low- and high-fidelity simulations

Risk-adaptive learning of displacement (cont.)

Surrogate has 1+44 coefficients to be learned

Sparsity (model selection) across 20 surrogates:

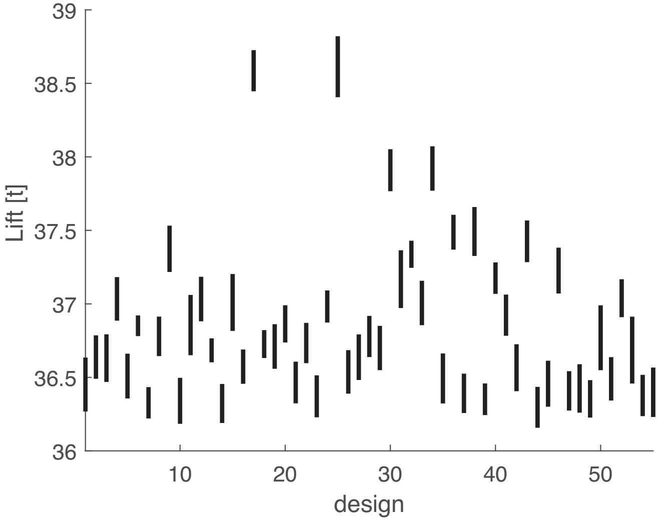


Red, gray, orange, blue, pink, and yellow colors correspond to a, c, b_0, $\bar{a}$, $\bar{c}$, and b, respectively

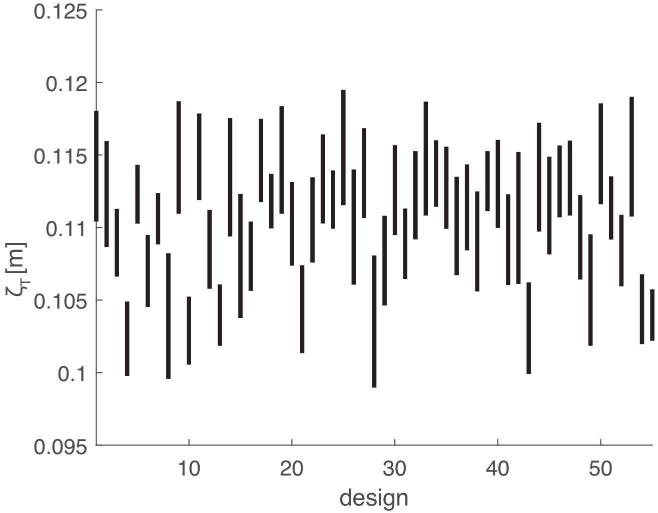
$$a_0 + a^\top x + c^\top v + b_0 \hat{h}(x,v) + \bar{a}^\top x \hat{h}(x,v) + \bar{c}^\top v \hat{h}(x,v) + b[\hat{h}(x,v)]^2$$

Uncertainty in surrogates: lift

Not standard deviation, but superquantile deviation!



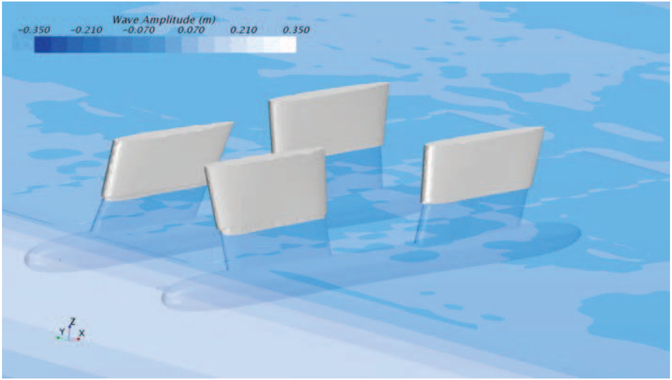
Uncertainty in surrogates: displacement



Poor low-fidelity: uncertain surrogates, **but still conservative**

Design of torpedo hull: seakeeping

Motion of vessel in regular and irregular waves



Torpedo hull fully submerged at medium speed (60kn)

Ongoing w/ L. Bonfiglio, MIT, and G. Karniadakis, Brown Univ.

Design of torpedo hull: seakeeping (cont.)

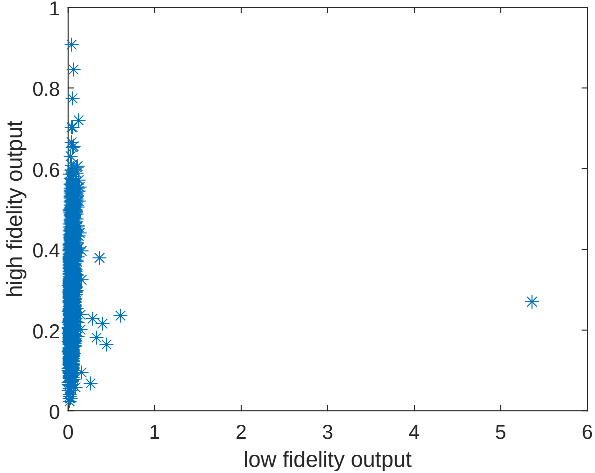
Acceleration (pitch) of vessel

1000 high- and low-fidelity simulations (2D strip theory)

Design of torpedo hull: seakeeping (cont.)

Acceleration (pitch) of vessel

1000 high- and low-fidelity simulations (2D strip theory)

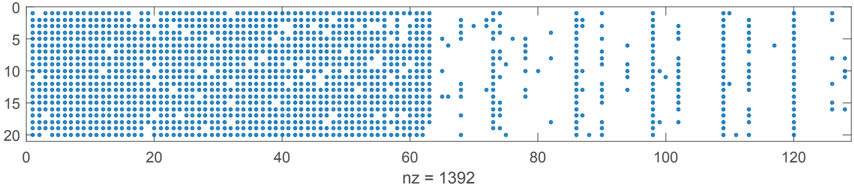


Design of torpedo hull: seakeeping (cont.)

60 design variables; 3 uncertain parameters

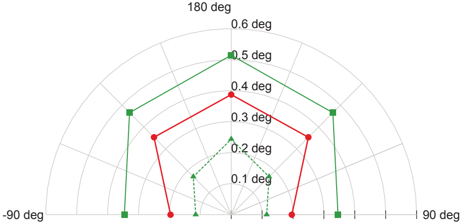
Surrogate has 1+128 coefficients to be learned

Sparsity (model selection) across 20 surrogates:

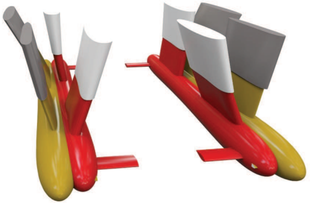


Similar surrogate form as before: $f\left(h(x,V)\right) =$
$a_0 + a^\top x + c^\top v + b_0 \hat{h}(x,v) + \bar{a}^\top x \hat{h}(x,v) + \bar{c}^\top v \hat{h}(x,v) + b[\hat{h}(x,v)]^2$

Accuracy of surrogates and design improvement

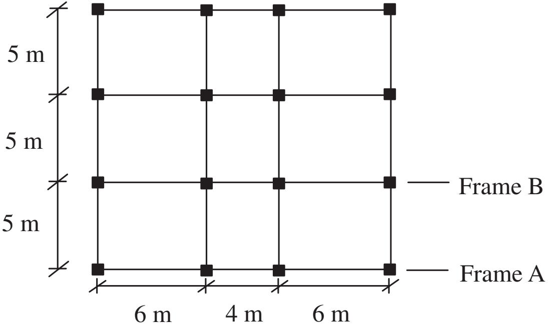


Actual (red) response between conservative and nominal (green) predictions regardless of wave direction



Optimized (green) compared with benchmark (red) torpedo hull

Application in earthquake engineering



12-story reinforced concrete symmetrical frame

High-fidelity: nonlinear time-history analysis

Low-fidelity: linear-time history, pushover, response spectrum

Input uncertainty: ground motion (79 ground motions)

Response quantity: inter-story drift ratio

Ongoing w/ S. Gunay and K. Mosalam, Berkeley

Accuracy of surrogates

Pushover surrogate: $c_0 + cX$ (PO only)

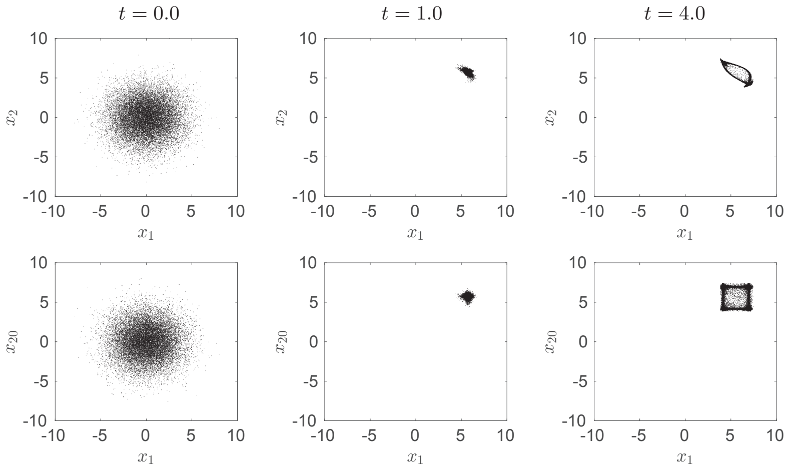
Full surrogate: $c_0 + c_1X_1 + c_2X_2 + c_3X_3$ (LTH, PO, RS)

Training replicated 10 times

	Story 5 drift (%)		Story 12 drift (%)	
Surrogate:	Full	Pushover	Full	Pushover
nominal	8.901	8.846	1.896	1.964
conservative	9.189	9.204	2.156	2.321
Actual $R_{0.8}(Y)$	8.344		1.614	

High-dim nonlinear stochastic dynamical system

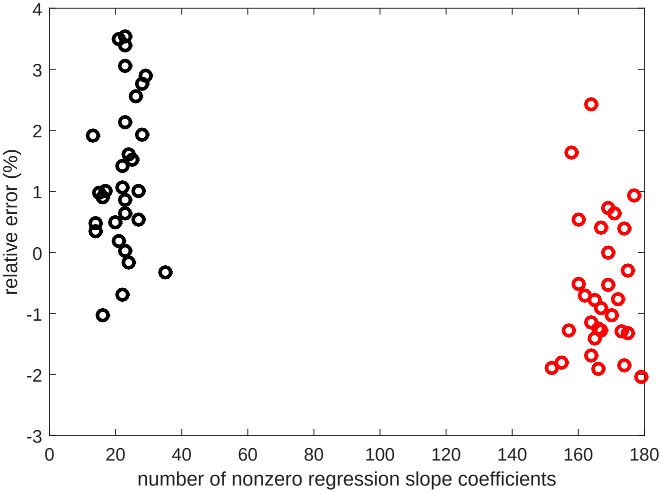
Venturi-16 system: $\dot{x}_i(t) = -x_i \sin x_{i-1} - a x_i + b,\ i = 1, ..., 1000$
Random initial condition $x(0) = W$ independent Gaussian



Find surrogate of state 1 at time 20: $x_1(20)$
Ongoing w/ D. Venturi, UC Santa Cruz

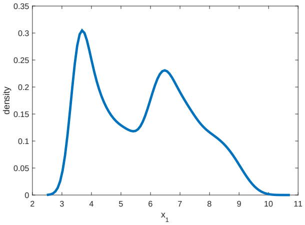
Risk-adaptive learning in 1000 dimensions

Training of $c_0 + c^\top W$ using 500 samples; 30 reps; $\alpha = 0.8$

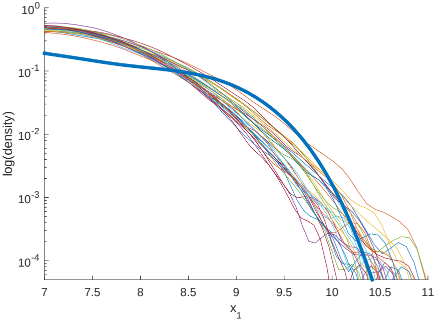


Sparsity parameter $\lambda = 0.2$ (black) and $\lambda = 0.1$ (red)

Tail-focused Gaussian approximation of pdf



Actual pdf of $x_1(20)$
$R_{0.8}\left(x_1(20)\right) = 8.16$



Upper tails of pdf for

$x_1(20)$ (thick blue line)
$c_0 + c^\top W$ (thin lines)

Summary

Prediction and design based on superquantiles

Promotes safety, resilience, and tractability

Scalable surrogate building from multi-fidelity simulations

Surrogates adapts to decision maker's preferences

Applications in naval architecture, earthquake engineering, semi-conductor manufacturing (ongoing w/ D. Kouri, Sandia)

More risk...

MT8 Optimization and Control Under Uncertainty
Drew Kouri
2:30 PM-4:30 PM
Grand Ballroom G - 1st Floor

Rockafellar & Uryasev, 2000, Optimization of conditional value-at-risk, *J. Risk* 2:493-517

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Rockafellar & Royset, 2010, On Buffered Failure Probability in Design and optimization..., *Reliability Eng. Sys. Safety* 95:499-510

Rockafellar & Uryasev, 2013, The fundamental risk quadrangle in risk management, optimization..., *Surveys in Op. Res. and Manag. Sci.* 18:33-53

Rockafellar & Royset, 2015a, Measures of Residual Risk with Connections to Regression, Risk Tracking, Surrogate..., *SIAM J. Optim.* 25(2):1179-1208

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Rockafellar, Royset, Miranda, 2014, Superquantile Regression with Applications to Buffered Reliability..., *European J. Operational Research* 234(1):140-154

Royset, Bonfiglio, Vernengo, Brizzolara, 2017, Risk-Adaptive Set-Based Design and Applications..., *ASME J. Mechanical Design* 139(10): 1014031-1014038

Bonfiglio, Royset, Karniadakis, 2018, Multi-Disciplinary Risk-Adaptive Design of Super-Cavitating Hydrofoils, *AIAA Non-Deterministic Approaches Conf.*

See http://faculty.nps.edu/joroyset for papers and code