# Measures of Residual Risk with Connections to Regression, Risk Tracking, Surrogate Models, and Ambiguity

**Johannes O. Royset**
Naval Postgraduate School, Monterey, CA
with R.T. Rockafellar, Univ. of Washington, Seattle, WA

Limoges, May 2015

This material is based upon work supported in part by the U.S. Air Force Office of Scientific Research under grants FA9550-11-1-0206 and F1ATAO1194GOO1 and by DARPA under grant HR0011412251.

# Surrogate models: learning from low-fidelity simulations

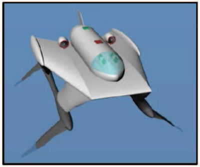
Output of costly simulation: random variable $Y$
Output of inexpensive simulation: random variable $X$

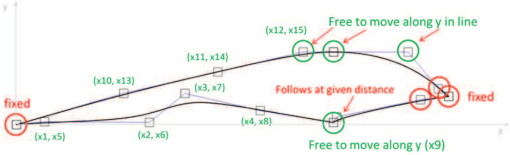
Find $f$ such that $Y \approx f(X)$, or $Y$ "safely" $\leq f(X)$

# Surrogate models: learning from low-fidelity simulations

Output of costly simulation: random variable $Y$
Output of inexpensive simulation: random variable $X$

Find $f$ such that $Y \approx f(X)$, or $Y$ "safely" $\leq f(X)$





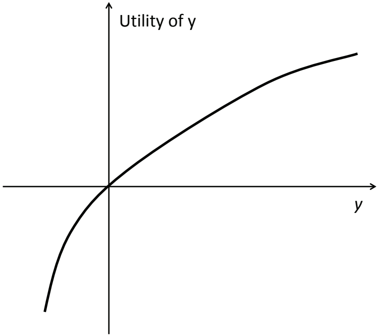

Case study: Drag-lift ratio estimation*:

Costly: Navier-Stokes solve (4 hours on 8 cores)
Inexpensive: potential flow solve (5 sec on 1 core)

*with S. Brizzolara, Mech. Engineering, MIT

# Decision problem: how to invest

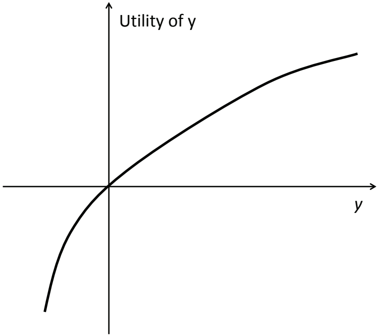
Future loss $Y$
Preferences regarding losses (utility-like functions)



# Decision problem: how to invest

Future loss $Y$

Preferences regarding losses (utility-like functions)




Opportunities:

Invest in fixed-income asset now

Invest in shares with uncertain value at the future point in time

Balance upfront cost against future (reduced) loss

# Outline

- Background: regret, risk, error, deviation
- Measures of residual risk: definition and properties
- Application to surrogate models

# Background: regret, risk, error, deviation

# Regret

Probability space $(\Omega, \mathcal{F}, P)$;
$\mathcal{L}^2 = \{Y : \Omega \to \boldsymbol{R} \mid Y \text{ measurable}, \ E[Y^2] < \infty\}$

# Regret

Probability space $(\Omega, \mathcal{F}, P)$;
$\mathcal{L}^2 = \{Y : \Omega \to \boldsymbol{R} \mid Y \text{ measurable, } E[Y^2] < \infty\}$

Measure of regret $\mathcal{V} : \mathcal{L}^2 \to (-\infty, \infty]$

# Regret

Probability space $(\Omega, \mathcal{F}, P)$;
$\mathcal{L}^2 = \{Y : \Omega \to \boldsymbol{R} \mid Y \text{ measurable, } E[Y^2] < \infty\}$

Measure of regret $\mathcal{V} : \mathcal{L}^2 \to (-\infty, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$\mathcal{V}(Y) =$ quantification of displeasure with outcomes of $Y$

For example, compensation required for being exposed to $Y$

# Regret

Probability space $(\Omega, \mathcal{F}, P)$;
$\mathcal{L}^2 = \{Y : \Omega \to \boldsymbol{R} \mid Y \text{ measurable}, E[Y^2] < \infty\}$

Measure of regret $\mathcal{V} : \mathcal{L}^2 \to (-\infty, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$\mathcal{V}(Y) =$ quantification of displeasure with outcomes of $Y$

For example, compensation required for being exposed to $Y$

Orientation towards minimization:
For example $\mathcal{V}(Y) = -E[u(-Y)]$ for utility function $u$

# Regularity

$\mathcal{V}$ is regular if: convex

closed

$\mathcal{V}(0) = 0$

$\mathcal{V}(Y) > E[Y]$ when $Y$ not identical to 0

# Risk

Measure of risk $\mathcal{R} : \mathcal{L}^2 \to (-\infty, \infty]$

# Risk

Measure of risk $\mathcal{R} : \mathcal{L}^2 \to (-\infty, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$$\mathcal{R}(Y) = \text{quantification of the ``risk'' in } Y$$

$$Y \text{ safely } \leq Y' \iff Y \leq_{\mathcal{R}} Y' \iff \mathcal{R}(Y) \leq \mathcal{R}(Y')$$

# Risk

Measure of risk $\mathcal{R} : \mathcal{L}^2 \to (-\infty, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$$\mathcal{R}(Y) = \text{quantification of the ``risk'' in } Y$$

$$Y \text{ safely } \leq Y' \iff Y \leq_{\mathcal{R}} Y' \iff \mathcal{R}(Y) \leq \mathcal{R}(Y')$$

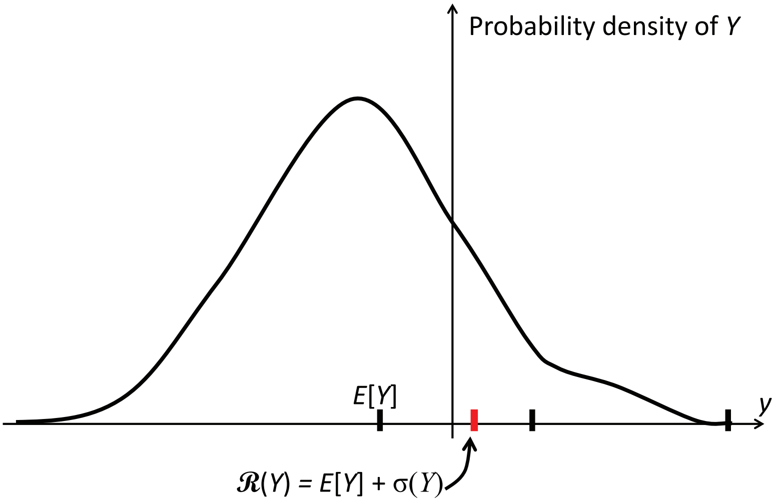
$\mathcal{R}$ is regular if: convex

closed

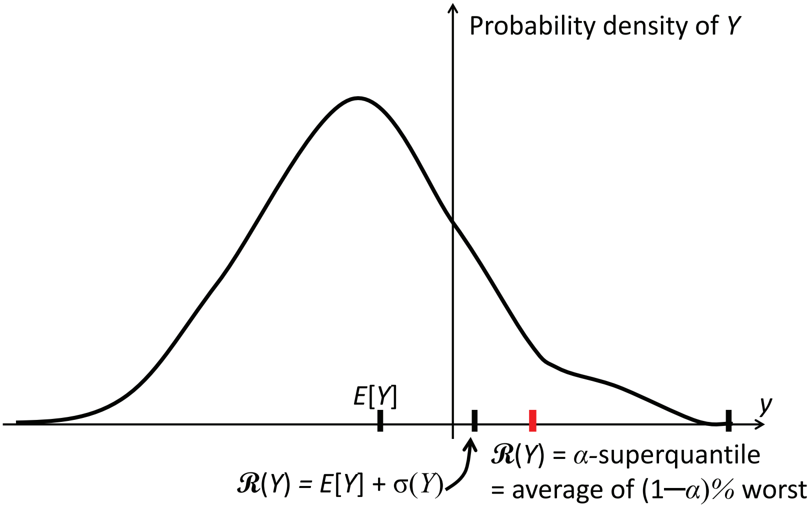
$\mathcal{R}(Y) = c$ when $Y$ is identical to constant $c$

$\mathcal{R}(Y) > E[Y]$ when $Y$ is not constant

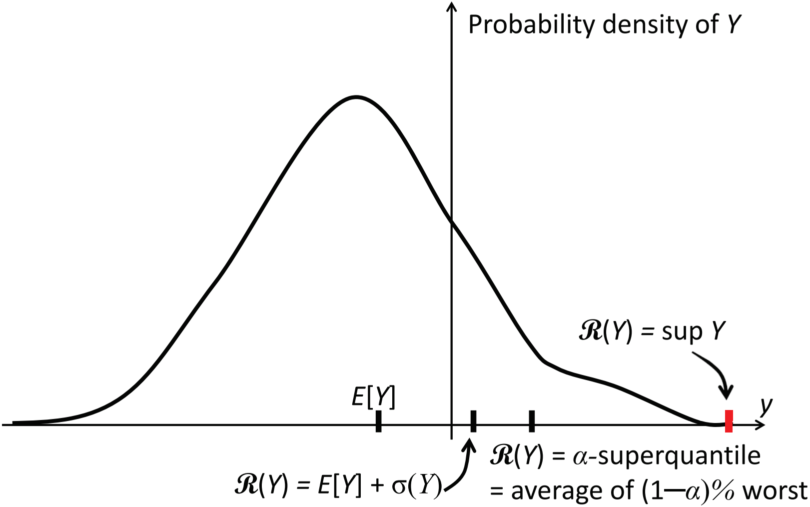
# Examples of risk measures



# Examples of risk measures



# Examples of risk measures



# Risk-regret connection

Theorem:

Any regular measure of regret $\mathcal{V}$ constructs a regular measure of risk

$$\mathcal{R}(Y) = \min_{c_0 \in \boldsymbol{R}} \left\{ c_0 + \mathcal{V}(Y - c_0) \right\}.$$

# Error

Measure of error $\mathcal{E} : \mathcal{L}^2 \to [0, \infty]$

# Error

Measure of error $\mathcal{E} : \mathcal{L}^2 \to [0, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$\mathcal{E}(Y) =$ quantification of nonzeroness of $Y$

For example: $\mathcal{E}(Y) = E[Y^2]$

$$\mathcal{E}(Y) = E[\alpha \max\{0, Y\}/(1-\alpha) + \max\{0, -Y\}]$$

# Error

Measure of error $\mathcal{E} : \mathcal{L}^2 \to [0, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$\mathcal{E}(Y) =$ quantification of nonzeroness of $Y$

For example: $\mathcal{E}(Y) = E[Y^2]$

$\mathcal{E}(Y) = E[\alpha \max\{0, Y\}/(1-\alpha) + \max\{0, -Y\}]$

$\mathcal{E}$ is regular if: convex

closed

$\mathcal{E}(0) = 0$

$\mathcal{E}(Y) > 0$ when $Y$ is not identical 0

# Deviation

Measure of deviation $\mathcal{D} : \mathcal{L}^2 \rightarrow [0, \infty]$

# Deviation

Measure of deviation $\mathcal{D} : \mathcal{L}^2 \to [0, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$$\begin{aligned}\mathcal{D}(Y) &= \text{quantification nonconstancy of } Y \\ &\quad \text{For example standard deviation}\end{aligned}$$

# Deviation

Measure of deviation $\mathcal{D} : \mathcal{L}^2 \to [0, \infty]$

For random variable $Y \in \mathcal{L}^2$,

$$\begin{aligned} \mathcal{D}(Y) = &\text{ quantification nonconstancy of } Y \\ &\text{ For example standard deviation} \end{aligned}$$

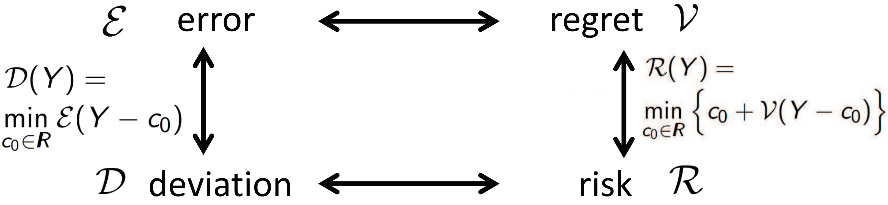
$$\begin{aligned} \mathcal{D} \text{ is regular if: } &\text{convex} \\ &\text{closed} \\ &\mathcal{D}(Y) = 0 \text{ when } Y \text{ is a constant} \\ &\mathcal{D}(Y) > 0 \text{ when } Y \text{ is nonconstant} \end{aligned}$$

# Deviation-error connection

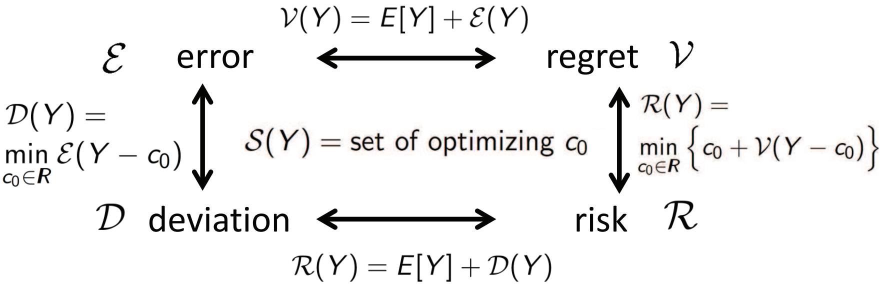
Theorem:
Any regular measure of error $\mathcal{E}$ constructs a regular measure of deviation

$$\mathcal{D}(Y) = \min_{c_0 \in \boldsymbol{R}} \mathcal{E}(Y - c_0)$$

# Connections



# Connections




Corresponding measures and statistics

# Measures of residual risk: definition and properties

# Motivation: How to invest

- future loss $Y$, given in present money

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now
- invest $c$ shares in a stock with random value $X$, in present terms, at the future point in time

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now
- invest $c$ shares in a stock with random value $X$, in present terms, at the future point in time
- price of each share $E[X]$

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now
- invest $c$ shares in a stock with random value $X$, in present terms, at the future point in time
- price of each share $E[X]$
- future regret, as perceived now: $\mathcal{V}(Y - [c_0 + cX])$

# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now
- invest $c$ shares in a stock with random value $X$, in present terms, at the future point in time
- price of each share $E[X]$
- future regret, as perceived now: $\mathcal{V}(Y - [c_0 + cX])$
- balance current cost with future regret:

$$\text{residual risk} = \min_{c_0, c} \left\{ c_0 + cE[X] + \mathcal{V}(Y - [c_0 + cX]) \right\}$$

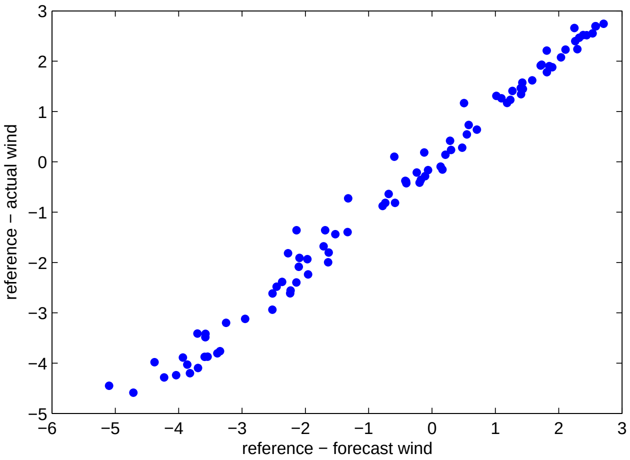
# Motivation: How to invest

- future loss $Y$, given in present money
- preference captured by measure of regret $\mathcal{V}$
- invest $c_0$ in a risk-free asset now
- invest $c$ shares in a stock with random value $X$, in present terms, at the future point in time
- price of each share $E[X]$
- future regret, as perceived now: $\mathcal{V}(Y - [c_0 + cX])$
- balance current cost with future regret:

$$\text{residual risk} = \min_{c_0, c} \left\{ c_0 + cE[X] + \mathcal{V}(Y - [c_0 + cX]) \right\}$$

With optimal $c_0$ and $c$:
$(c_0 + cE[X]) + (Y - [c_0 + cX]) \leq_{\mathcal{R}}$ residual risk

# Motivation: wind prediction on day $D$




$Y = 3 - (\text{actual wind power}) \;\; = \text{shortfall}$

$X = 3 - (\text{forecast wind power}) \;\; = \text{legacy forecast}$

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$
- form of point prediction $c_0 + cE[X]$

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$
- form of point prediction $c_0 + cE[X]$
- regret about prediction $\mathcal{V}(Y - [c_0 + cX])$

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D - 1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$
- form of point prediction $c_0 + cE[X]$
- regret about prediction $\mathcal{V}(Y - [c_0 + cX])$
- want small shortfall and regret

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$
- form of point prediction $c_0 + cE[X]$
- regret about prediction $\mathcal{V}(Y - [c_0 + cX])$
- want small shortfall and regret
- balance the two by solving

$$\min_{c_0, c} \left\{ c_0 + cE[X] + \mathcal{V}(Y - [c_0 + cX]) \right\}$$

# Preference-based predication

- $Y$ = shortfall on day $D$; to be predicted
- $X = (D-1)$ legacy forecast; known or known distribution
- form of shortfall prediction $c_0 + cX$
- form of point prediction $c_0 + cE[X]$
- regret about prediction $\mathcal{V}(Y - [c_0 + cX])$
- want small shortfall and regret
- balance the two by solving

$$\min_{c_0, c} \left\{ c_0 + cE[X] + \mathcal{V}(Y - [c_0 + cX]) \right\}$$

- Same problem as faced by investor!

# Measures of residual risk

For given random vector $X \in \mathcal{L}_n^2$ and regular measure of regret $\mathcal{V}$, a measure of residual risk $\mathcal{R}(\cdot|X) : \mathcal{L}^2 \to [-\infty, \infty]$ is defined by

$$\mathcal{R}(Y|X) = \inf_{c_0 \in \boldsymbol{R}, c \in \boldsymbol{R}^n} \left\{ c_0 + \langle c, E[X] \rangle + \mathcal{V}(Y - [c_0 + \langle c, X \rangle]) \right\}$$

# Measures of residual risk

For given random vector $X \in \mathcal{L}^2_n$ and regular measure of regret $\mathcal{V}$, a measure of residual risk $\mathcal{R}(\cdot|X) : \mathcal{L}^2 \to [-\infty, \infty]$ is defined by

$$\mathcal{R}(Y|X) = \inf_{c_0 \in \mathbf{R}, c \in \mathbf{R}^n} \left\{ c_0 + \langle c, E[X] \rangle + \mathcal{V}(Y - [c_0 + \langle c, X \rangle]) \right\}$$

Interpretation: lowest $K \in \mathbf{R}$ such that

$$Y - [c_0 + \langle c, X \rangle] + [c_0 + \langle c, E[X] \rangle] \leq_{\mathcal{R}} K$$

# Properties

Theorem:

Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

(i) $E[Y] \leq \mathcal{R}(Y|X) \leq \mathcal{R}(Y) \leq \mathcal{V}(Y)$.

# Properties

Theorem:
Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

(i) $E[Y] \leq \mathcal{R}(Y|X) \leq \mathcal{R}(Y) \leq \mathcal{V}(Y)$.

(ii) $\mathcal{R}(\cdot|X)$ is convex.

# Properties

Theorem:
Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

(i) $E[Y] \leq \mathcal{R}(Y|X) \leq \mathcal{R}(Y) \leq \mathcal{V}(Y)$.

(ii) $\mathcal{R}(\cdot|X)$ is convex.

(iii) If $X$ is nondegenerate*, then $\mathcal{R}(\cdot|X)$ is closed and infimum attained.

*$X$ is nondegenerate if $\langle c, X \rangle$ is a constant implies $c = 0$

# Dual expression

Theorem:

For finite regular risk measure with conjugate $\mathcal{R}^*$ and risk envelope $\mathcal{Q} = \{Q \in \mathcal{L}^2 \mid \mathcal{R}^*(Q) < \infty\}$:

$$\mathcal{R}(Y|X) = \sup_{Q \in \mathcal{Q}} \left\{ E[QY] - \mathcal{R}^*(Q) \;\middle|\; E[QX] = E[X] \right\}$$

# Dual expression

Theorem:
For finite regular risk measure with conjugate $\mathcal{R}^*$ and risk envelope $\mathcal{Q} = \{Q \in \mathcal{L}^2 \mid \mathcal{R}^*(Q) < \infty\}$:

$$\mathcal{R}(Y|X) = \sup_{Q \in \mathcal{Q}} \left\{ E[QY] - \mathcal{R}^*(Q) \;\middle|\; E[QX] = E[X] \right\}$$

Applications in optimization under stochastic ambiguity

# Alternative perspective: linear regression

Find regression coefficients $c_0$ and $c$ that

$$\text{minimize } \mathcal{E}(Y - [c_0 + \langle c, X \rangle])$$

What will we obtain for "nonstandard" error measures?

# Connection regression and residual risk

Regression Problem:

$$\min_{c_0,c} \mathcal{E}(Y - [c_0 + \langle c, X \rangle])$$

Residual Risk Problem:

$$\min_{c_0,c} \left\{ c_0 + \langle c, E[X] \rangle + \mathcal{V}(Y - [c_0 + \langle c, X \rangle]) \right\}$$

# Connection regression and residual risk

Regression Problem:

$$\min_{c_0, c} \mathcal{E}(Y - [c_0 + \langle c, X \rangle])$$

Residual Risk Problem:

$$\min_{c_0, c} \left\{ c_0 + \langle c, E[X] \rangle + \mathcal{V}(Y - [c_0 + \langle c, X \rangle]) \right\}$$

Theorem:

Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

(i) Optimal solution sets are identical.

# Connection regression and residual risk

Regression Problem:

$$\min_{c_0,c} \mathcal{E}(Y - [c_0 + \langle c, X\rangle])$$

Residual Risk Problem:

$$\min_{c_0,c} \Big\{c_0 + \langle c, E[X]\rangle + \mathcal{V}(Y - [c_0 + \langle c, X\rangle])\Big\}$$

Theorem:

Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

(i) Optimal solution sets are identical.

(ii) They are closed, convex, and if $X$ is nondegenerate, then also nonempty.

# Connection regression and residual risk

Regression Problem:

$$\min_{c_0, c} \mathcal{E}(Y - [c_0 + \langle c, X \rangle])$$

Residual Risk Problem:

$$\min_{c_0, c} \left\{ c_0 + \langle c, E[X] \rangle + \mathcal{V}(Y - [c_0 + \langle c, X \rangle]) \right\}$$

Theorem:
Given $X \in \mathcal{L}_n^2$ and corresponding regular measures:

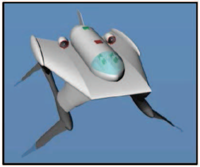
(i) Optimal solution sets are identical.

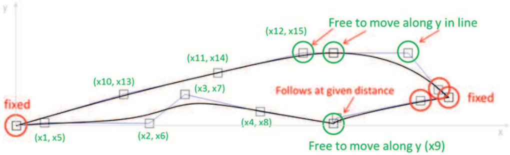
(ii) They are closed, convex, and if $X$ is nondegenerate, then also nonempty.

(iii) They are bounded if the residual risk is finite and $X$ is nondegenerate.

# Application to surrogate models

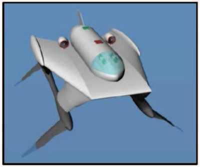
# Learn from low-fidelity simulation: drag/lift estimation

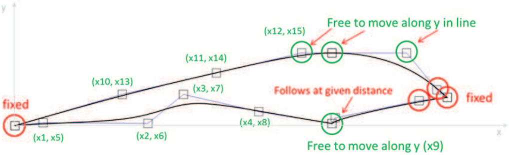





$Y$ drag-to-lift ratio; costly realization (4 hours on 8 cores)
$X$ approx. ratio; inexpensive realizations (5 sec on 1 core)

# Learn from low-fidelity simulation: drag/lift estimation

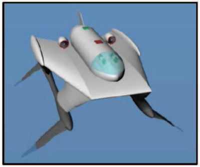


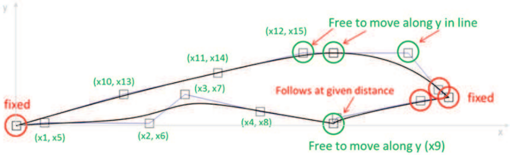



$Y$ drag-to-lift ratio; costly realization (4 hours on 8 cores)
$X$ approx. ratio; inexpensive realizations (5 sec on 1 core)

Find $c_0 + cX$ such that $Y$ safely $\leq c_0 + cX$

# Learn from low-fidelity simulation: drag/lift estimation



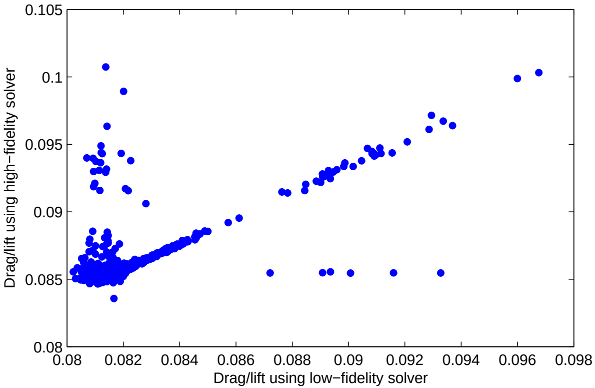



$Y$ drag-to-lift ratio; costly realization (4 hours on 8 cores)
$X$ approx. ratio; inexpensive realizations (5 sec on 1 core)

Find $c_0 + cX$ such that $Y$ safely $\leq c_0 + cX$
$\mathcal{R}(Y) \leq \mathcal{R}(c_0 + cX)$, with 0.8-superquantile risk

# Distribution of drag/lift

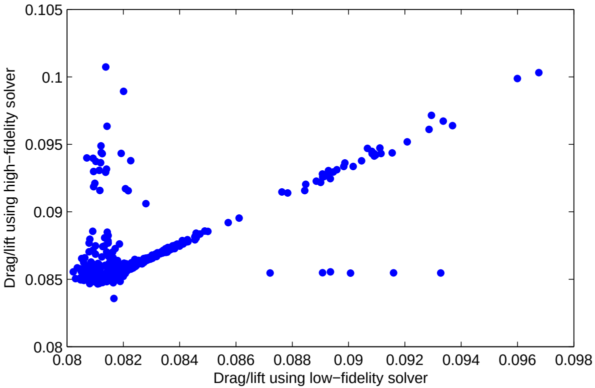
Randomness due to manufacturing tolerance (689 “scenarios”)




Mean $E[Y] = 0.0864$; 0.8-superquantile $\mathcal{R}(Y) = 0.0901$

# Distribution of drag/lift

Randomness due to manufacturing tolerance (689 “scenarios”)




Mean $E[Y] = 0.0864$; 0.8-superquantile $\mathcal{R}(Y) = 0.0901$

Want to bound $\mathcal{R}(Y)$ from above cheaply

# Risk-tuned surrogate estimation

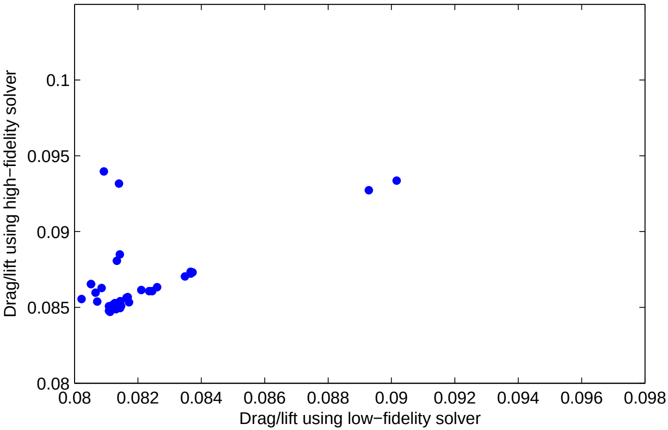
Theorem:
For positively homogeneous regular measure of risk $\mathcal{R}$,

$$\text{the model } c_0 + \langle c, X \rangle \text{ of } Y,$$

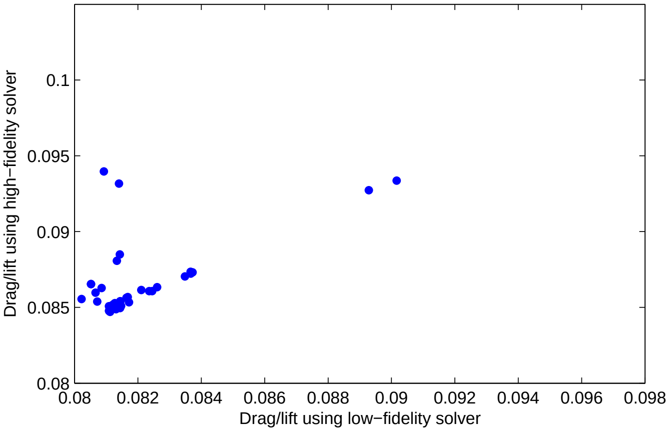
with $c$ obtained by corresponding regression and $c_0 = \mathcal{R}(Y - \langle c, X \rangle)$, satisfies

$$\mathcal{R}(Y) \leq \mathcal{R}(c_0 + \langle c, X \rangle)$$

# 50 training data points

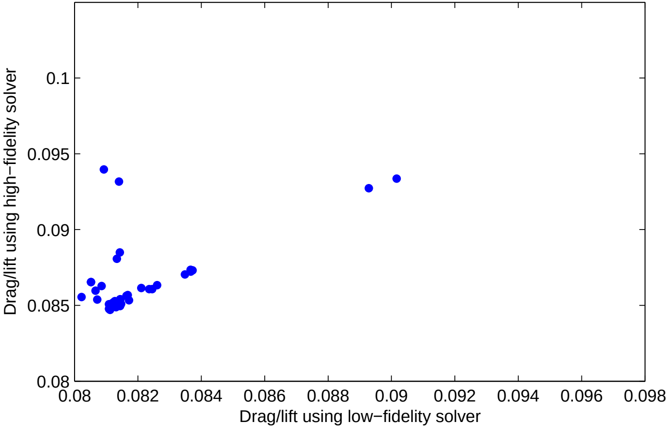


# 50 training data points




Quantile regression/residual risk problem $\longrightarrow c = 0.7859$

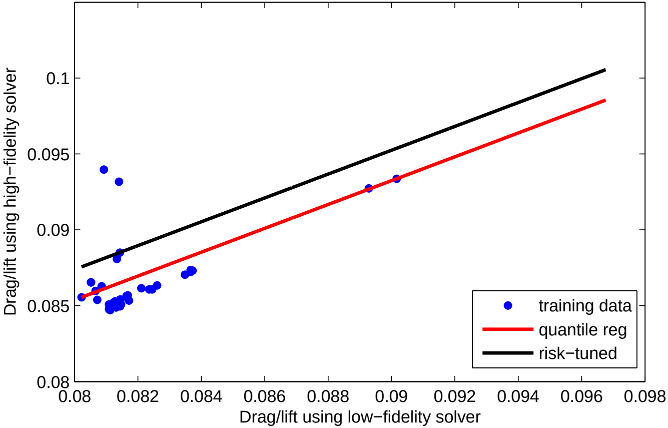
# 50 training data points



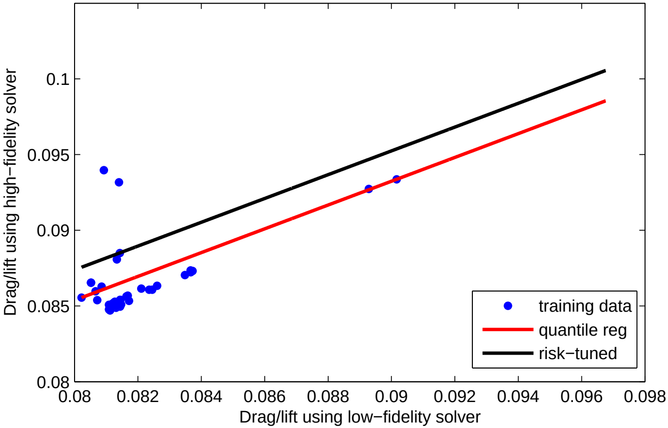

Quantile regression/residual risk problem $\longrightarrow c = 0.7859$

Following theorem $\longrightarrow c_0 = 0.0245$

# Illustration of fit



# Illustration of fit




$\mathcal{R}(c_0 + cX) = 0.0918$ (mean $0.0912$, st.dev. $0.0016$)

Recall: $\mathcal{R}(Y) = 0.0901$

# Summary

Connecting estimation and decision making (risk-tuning)

Enabling construction of risk-averse, preference-driven data tools

Applications in “risk-averse” regression and robust optimization

# Reference

R.T. Rockafellar and J.O. Royset,
"Measures of Residual Risk with Connections to Regression, Risk Tracking, Surrogate Models, and Ambiguity,"
SIAM J. Optimization, to appear

http://faculty.nps.edu/joroyset