Optimal Uncertainty Quantification for Hypervelocity Impact

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Uncertainty Quantification Short Course

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THE UNIVERSITY OF WARWICK

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Credits

Joint work with everyone (!) at the Caltech PSAAP Center, but in particular the core UQ team of Paul-Hervé Kamga, Michael McKerns, Lan Huong Nguyen, Michael Ortiz, Houman Owhadi and Clint Scovel.

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CALTECH PSAAP

National Nuclear Security Administration

Prototypical UQ Problem: Reliability Certification

- $g^\dagger \colon \mathbb{X} \to \mathbb{Y}$ is a system of interest, with random inputs X distributed according to a probability measure $\mu^\dagger$ on $\mathbb{X}$.
- For some subset $\mathcal{F} \subseteq \mathbb{Y}$, the event $[g^\dagger(X) \in \mathcal{F}]$ constitutes failure; we want to know the probability of failure

$$\mathbb{P}_{\mu^\dagger}\left[g^\dagger(X) \in \mathcal{F}\right] \equiv \underbrace{\mathbb{E}_{\mu^\dagger}\left[\mathbb{1}\left[g^\dagger(X) \in \mathcal{F}\right]\right]}_{\substack{\text{“just” an integral} \\ \text{to be evaluated} \\ \text{— directly?} \\ \text{— by MC?} \\ \text{— by quadrature?}}},$$

  or at least to know that it is acceptably small (or unacceptably large!).
- **Problem:** In practical applications, one does not know the Universe's $g^\dagger$ and $\mu^\dagger$ exactly!

Other Quantities of Interest

- For some quantity of interest (measurable function) $q \colon \mathbb{X} \times \mathbb{Y} \to \mathbb{R}$, we want to know

$$\underbrace{\mathbb{E}_{\mu^\dagger}\left[q(X, g^\dagger(X))\right]}_{\substack{\text{“just” an integral} \\ \text{to be evaluated} \\ \text{— directly?} \\ \text{— by MC?} \\ \text{— by quadrature?}}},$$

  or at least to know that it is acceptably small (or unacceptably large!).
- For example:
  - failure probability: $q(x, y) = \mathbb{1}[y \in \mathcal{F}]$,
  - mean performance: $q(x, y) = y$,
  - variance about a nominal output value: $q(x, y) = |y - y_0|^2$.
- Our interest lies in understanding $\mathbb{E}_{\mu^\dagger}\left[q(X, g^\dagger(X))\right]$ when $g^\dagger$ and $\mu^\dagger$ are only imperfectly known (i.e. epistemic uncertainty), and to obtain bounds that are optimal with respect to the known information.

Optimal UQ

- The initial step in the Optimal Uncertainty Quantification approach is specifying a feasible set of admissible scenarios (g, μ) that could be $(g^\dagger, \mu^\dagger)$ according to the available information:

$$\mathcal{A} = \left\{ (g, \mu) \;\middle|\; \begin{array}{c} (g, \mu) \text{ is consistent with the current} \\ \text{information about } (g^\dagger, \mu^\dagger) \\ \text{(e.g. legacy data, models, theory, expert judgement)} \end{array} \right\}.$$

- A priori, all we know about reality is that $(g^\dagger, \mu^\dagger) \in \mathcal{A}$; we have no idea exactly which (g, μ) in $\mathcal{A}$ is actually $(g^\dagger, \mu^\dagger)$.
  - No $(g, \mu) \in \mathcal{A}$ is "more likely" or "less likely" to be $(g^\dagger, \mu^\dagger)$.
  - Particularly in high-consequence settings, it makes sense to adopt a posture of healthy conservatism and determine the best and worst outcomes consistent with the information encoded in $\mathcal{A}$.
- Dialogue between UQ practitioners and the domain experts is essential in formulating — and revising — $\mathcal{A}$.

Optimal UQ

$$\mathcal{A} = \left\{ (g, \mu) \,\middle|\, \begin{array}{c} (g, \mu) \text{ is consistent with the current} \\ \text{information about (i.e. could be) } (g^\dagger, \mu^\dagger) \end{array} \right\}$$

- Optimal bounds (w.r.t. the information encoded in $\mathcal{A}$) on the quantity of interest $\mathbb{E}_{\mu^\dagger}[q(X, g^\dagger(X))]$ are found by minimizing/maximizing $\mathbb{E}_\mu[q(X, g(X))]$ over all admissible scenarios $(g, \mu) \in \mathcal{A}$:

$$\underline{Q}(\mathcal{A}) \leq \mathbb{E}_{\mu^\dagger}[q(X, g^\dagger(X))] \leq \overline{Q}(\mathcal{A}),$$

where $\underline{Q}(\mathcal{A})$ and $\overline{Q}(\mathcal{A})$ are defined by the optimization problems

$$\underline{Q}(\mathcal{A}) := \inf_{(g,\mu)\in\mathcal{A}} \mathbb{E}_\mu[q(X, g(X))],$$

$$\overline{Q}(\mathcal{A}) := \sup_{(g,\mu)\in\mathcal{A}} \mathbb{E}_\mu[q(X, g(X))].$$

- Cf. generalized Chebyshev inequalities in decision analysis (**Smith** (1995)), imprecise probability (**Boole** (1854)), distributionally robust optimization, robust Bayesian inference (surv. **Berger** (1984)).

Reduction of OUQ Problems — LP Analogy

Dimensional Reduction

- A priori, OUQ problems are infinite-dimensional, non-convex*, highly-constrained, global optimization problems.
- However, they can be reduced to equivalent finite-dimensional problems in which the optimization is over the extremal scenarios of $\mathcal{A}$.
- The dimension of the reduced problem is proportional to the number of probabilistic inequalities that describe $\mathcal{A}$.

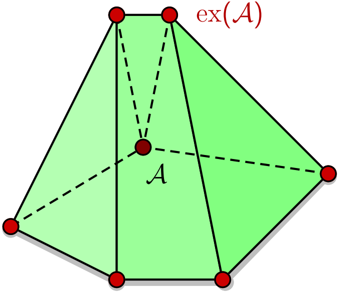

Figure : A linear functional on a convex domain in $\mathbb{R}^n$ finds its extreme value at the extremal points of the domain; similarly, OUQ problems reduce to searches over finite-dimensional families of extremal scenarios.

*But see e.g. **Bertsimas & Popescu** (2005) and **Smith** (1995) for convex special cases.

Reduction of OUQ Problems — Heuristic

Heuristic

If you have N_k pieces of information relevant to the random variable X_k, then just pretend that X_k takes at most $N_k + 1$ values in $\mathbb{X}_k$.

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- To make this heuristic rigorous, we restrict attention to Radon spaces, "nice" spaces on which every Borel probability measure is inner regular.
- Our theorem builds on now-classical results by **von Weizsäcker & Winkler** (1980) and **Winkler** (1988) characterizing the extremal measures in moment classes, and "nice" linear/affine functionals on such classes.
- Important point: the extremal measures of a moment class

$$\left\{ \mu \in \mathcal{P}(\mathbb{X}) \,\middle|\, \mathbb{E}_\mu[\varphi_1] \leq 0, \dots, \mathbb{E}_\mu[\varphi_n] \leq n \right\}$$

  are the discrete measures that have support on at most $n + 1$ distinct points of $\mathbb{X}$, which we denote by $\Delta_n(\mathbb{X})$.

Reduction of OUQ Problems — Theorem

Heuristic

If you have N_k pieces of information relevant to the random variable X_k, then just pretend that X_k takes at most $N_k + 1$ values in $\mathbb{X}_k$.

Theorem (Generalized moment and indep. constraints)

Suppose that $\mathbb{X} := \mathbb{X}_1 \times \dots \times \mathbb{X}_K$ is a product of Radon spaces. Let

$$\mathcal{A} := \left\{ (g, \mu) \,\middle|\, \begin{array}{c} g \colon \mathbb{X} \to \mathbb{R} \text{ is measurable, } \mu = \mu_1 \otimes \dots \otimes \mu_K \in \bigotimes_{k=1}^{K} \mathcal{P}(\mathbb{X}_k); \\ \langle \text{conditions on } g \text{ alone} \rangle \text{; and, for each } g, \\ \text{for some measurable functions } \varphi_i \colon \mathbb{X} \to \mathbb{R} \text{ and } \varphi_i^{(k)} \colon \mathbb{X}_k \to \mathbb{R}, \\ \mathbb{E}_{\mu}\big[\varphi_i\big] \leq 0 \text{ for } i = 1, \dots, n_0, \\ \mathbb{E}_{\mu_k}\big[\varphi_i^{(k)}\big] \leq 0 \text{ for } i = 1, \dots, n_k \text{ and } k = 1, \dots, K \end{array} \right\}$$

$$\mathcal{A}_\Delta := \left\{ (g, \mu) \in \mathcal{A} \,\middle|\, \begin{array}{c} \mu_k \in \Delta_{N_k}(\mathbb{X}_k) \\ \text{where } N_k := n_0 + n_k \end{array} \right\} \subseteq \mathcal{A}.$$

Then $\underline{Q}(\mathcal{A}) = \underline{Q}(\mathcal{A}_\Delta)$ *and* $\overline{Q}(\mathcal{A}) = \overline{Q}(\mathcal{A}_\Delta)$.

Reduction of OUQ Problems — Consequence

Heuristic

If you have N_k pieces of information relevant to the random variable X_k, then just pretend that X_k takes at most $N_k + 1$ values in $\mathbb{X}_k$.

- Computation of the OUQ bounds $\underline{Q}(\mathcal{A})$ and $\overline{Q}(\mathcal{A})$ is equivalent to finite-dimensional problems in which the optimization variables are
  - the positions of the support points $x_i \in \mathbb{X}$ of the discrete measure μ;
  - the weights $w_i \in [0, 1]$ of the points x_i; and
  - the response values $y_i \in \mathbb{Y}$ corresponding to $g(x_i)$.

  with objective function

$$\sum_{i=(0,\dots,0)}^{(N_1,\dots,N_K)} w_i \, q(x_i, y_i)$$

  and similar finite sums for the constraints.
- $\implies$ Implementation in the general-purpose open-source Mystic optimization framework, written in Python.

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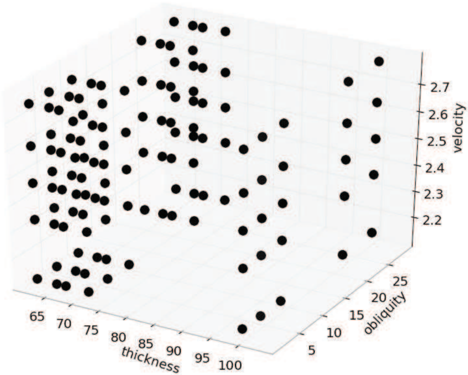

Optimal Concentration Inequalities

Classical inequalities of probability theory can be seen as OUQ statements:

Example: Markov's Inequality in OUQ Form

$$\mathcal{A}_{\mathrm{M}} := \{\mu \in \mathcal{P}([0,\infty)) \,|\, \mathbb{E}_\mu[X] \leq m\}$$

Suppose 'failure' is $X \geq t$, for $t \geq m$. Then

$$\begin{aligned}\overline{P}(\mathcal{A}_{\mathrm{M}}) &= \sup_{\mu \in \mathcal{A}_{\mathrm{M}}} \mathbb{P}_\mu[X \geq t] \\ &= \sup \left\{ \sum_{i=0}^{1} w_i \mathbb{1}[x_i \geq t] \,\middle|\, w_i, x_i \geq 0, \sum_{i=0}^{1} w_i = 1, \sum_{i=0}^{1} w_i x_i \leq m \right\} \\ &= 1 - \frac{m}{t}.\end{aligned}$$

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$$\overline{P}(\mathcal{A}_{\mathrm{M}}) = \sup_{\mu \in \mathcal{A}_{\mathrm{M}}} \mathbb{P}_\mu[X \geq t] = 1 - \frac{m}{t}.$$

How about other deviation/concentration-of-measure inequalities?

- McDiarmid's inequality: deviations from the mean of bounded-differences functions of independent random variables.
- Hoeffding's inequality: deviations from the mean of sums of independent random variables.

McDiarmid's (a.k.a. Bounded Differences) Inequality

$$\mathcal{A}_{\mathrm{McD}} := \left\{ (g,\mu) \;\middle|\; \begin{array}{c} g \colon \mathbb{X} := \mathbb{X}_1 \times \dots \times \mathbb{X}_K \to \mathbb{R}, \\ \mu = \bigotimes_{k=1}^{K} \mu_k, \text{ (i.e. } X_1, \dots, X_K \text{ independent)} \\ \mathbb{E}_\mu[g(X)] \geq m \geq 0, \\ \operatorname{osc}_k(g) \leq D_k \text{ for each } k \in \{1, \dots, K\} \end{array} \right\},$$

with componentwise oscillations/global sensitivities defined by

$$\operatorname{osc}_k(g) := \sup \left\{ |g(x) - g(x')| \;\middle|\; \begin{array}{c} x, x' \in \mathbb{X}_1 \times \dots \times \mathbb{X}_K, \\ x_i = x'_i \text{ for } i \neq k \end{array} \right\}.$$

Theorem (McDiarmid's Inequality, 1988)

$$\overline{P}(\mathcal{A}_{McD}) := \sup_{(g,\mu) \in \mathcal{A}_{McD}} \mathbb{P}_\mu[g(X) \leq 0] \overset{!!!}{\leq} \exp\left(- \frac{2m^2}{\sum_{k=1}^{K} D_k^2} \right)$$

Optimal McDiarmid and Screening Effects

Theorem (Optimal McDiarmid for $K = 1, 2$)

For $K = 1$,

$$\overline{P}(\mathcal{A}_{McD}) = \begin{cases} 0, & \text{if } D_1 \leq m, \\ 1 - \dfrac{m}{D_1}, & \text{if } 0 \leq m \leq D_1. \end{cases}$$

For $K = 2$,

$$\overline{P}(\mathcal{A}_{McD}) = \begin{cases} 0, & \text{if } D_1 + D_2 \leq m, \\ \dfrac{(D_1 + D_2 - m)^2}{4 D_1 D_2}, & \text{if } |D_1 - D_2| \leq m \leq D_1 + D_2, \\ 1 - \dfrac{m}{\max\{D_1, D_2\}}, & \text{if } 0 \leq m \leq |D_1 - D_2|. \end{cases}$$

In the highlighted case, $\min\{D_1, D_2\}$ carries no information — not in the sense of 0 bits, but the sense of being a non-binding constraint.

Optimal Hoeffding and the Effects of Nonlinearity

- Similarly, one can consider $\mathcal{A}_{\mathrm{Hfd}}$ "$\subseteq$" $\mathcal{A}_{\mathrm{McD}}$ corresponding to the assumptions of Hoeffding's inequality, which bounds deviation probabilities of sums of independent bounded random variables:

$$\mathcal{A}_{\mathrm{Hfd}} := \left\{ (g, \mu) \,\middle|\, \begin{array}{c} g \colon \mathbb{R}^K \to \mathbb{R} \text{ given by} \\ g(x_1, \dots, x_K) := x_1 + \dots + x_K, \\ \mu = \mu_1 \otimes \dots \otimes \mu_K \text{ supported on a cuboid of} \\ \text{side lengths } D_1, \dots, D_K, \text{ and } \mathbb{E}_\mu[g(X)] \geq m \geq 0 \end{array} \right\}.$$

- Hoeffding's inequality is the bound

$$\overline{P}(\mathcal{A}_{\mathrm{Hfd}}) := \sup_{(g,\mu) \in \mathcal{A}_{\mathrm{Hfd}}} \mathbb{P}_\mu[g(X) \leq 0] \leq \exp\left(- \frac{2m^2}{\sum_{k=1}^K D_k^2} \right).$$

- Interestingly, $\overline{P}(\mathcal{A}_{\mathrm{Hfd}}) = \overline{P}(\mathcal{A}_{\mathrm{McD}})$ for $K = 1$ and $K = 2$, but $\overline{P}(\mathcal{A}_{\mathrm{Hfd}}) \leq \overline{P}(\mathcal{A}_{\mathrm{McD}})$ for $K = 3$, and the inequality can be strict. Thus, sometimes linearity is binding information, sometimes not.

OUQ with Legacy Data

- An interesting class of admissible function-measure pairs arises in the case of partially observed smooth enough functions, e.g.

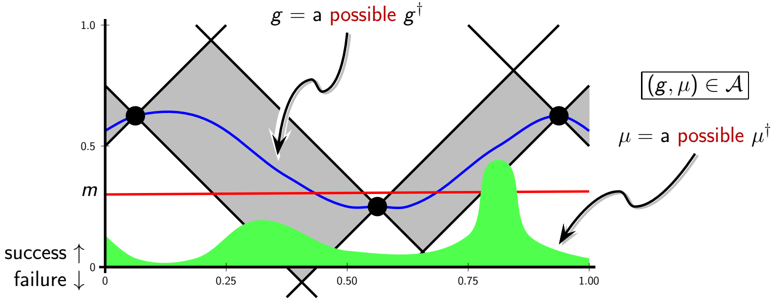
$$\mathcal{A} = \left\{ (g, \mu) \,\middle|\, \begin{array}{c} g \colon \mathbb{X} \to \mathbb{Y} \text{ has prescribed smoothness,} \\ g = g^{\dagger} \text{ on } \mathcal{O} \subseteq \mathbb{X} \text{ (i.e. some legacy data),} \\ \mu \in \mathcal{P}(\mathbb{X}),\ \mathbb{E}_{\mu}[\varphi_i] \leq 0 \text{ for } i = 1, \dots, n \end{array} \right\}$$

- Note that $\mathcal{O}$ need not be statistically representative.
- Simple examples of "smooth enough": Lipschitz constants or Hölder conditions.
- Mathematically interesting interactions between the measure-theoretic constraints and the metric geometry of the space $\mathbb{X}$, e.g. the fact that any parially-defined Lipschitz function can be extended to the whole space without changing the Lipschitz constant (**McShane** (1934)).

Example Reduction: 1 Random Variable, 1 Constraint

The original problem entails optimizing over an infinite-dimensional collection of (g, μ) that could be $(g^\dagger, \mu^\dagger)$. In the reduced problem, we only have to move around and re-weight two Dirac measures (point masses) and the values of g over those two points.

infinite-dimensional problem $\rightsquigarrow$ equivalent 5-dimensional problem!



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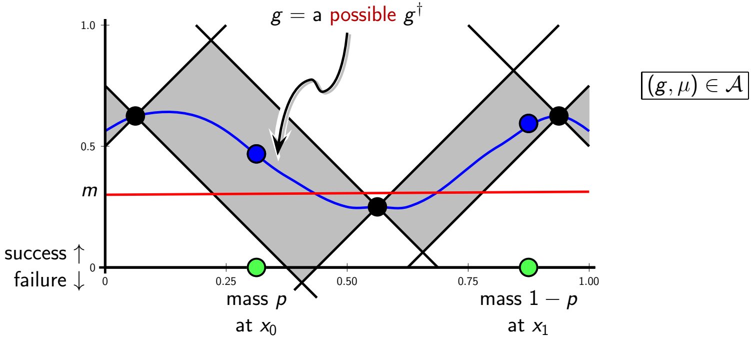

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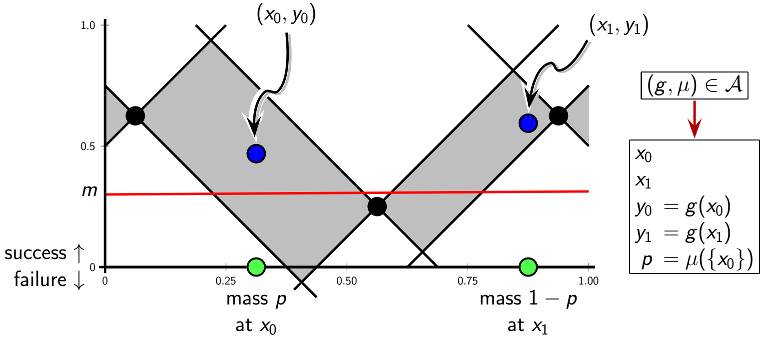

Explicit Solution: 1 Random Variable, 1 Data Point

- The case of a single observation in 1d can be solved explicitly.
- Suppose that you have one observation $(z, g^\dagger(z)) \in [0, \frac{1}{2}] \times \mathbb{R}$ of a function $g^\dagger \colon [0, 1] \to \mathbb{R}$ with Lipschitz constant $L \geq 0$.
- Explicit piecewise and discontinuous least upper bound on $\mathbb{P}_{\mu^\dagger}[g^\dagger(X) \leq 0]$ given L, $(z, g^\dagger(z))$, and that $\mathbb{E}_{\mu^\dagger}[g^\dagger(X)] \geq m$:

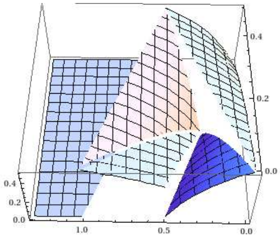

Figure : Surface plot of the least upper bound $\overline{P}$ on $\mathbb{P}_{\mu^\dagger}[g^\dagger(X) \leq 0]$, as a function of the observed data point $(z, g^\dagger(z))$.

Caltech's Hypervelocity Impact Setup

Figure : Caltech's Small Particle Hypervelocity Impact Range (SPHIR): a two-stage light gas gun that launches 1–50 mg projectiles at speeds of 2–10 $\text{km} \cdot \text{s}^{-1}$.

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3-Variable Hypervelocity Impact Example

- Legacy data = 32 data points (steel-on-aluminium shots A48–A81, less two mis-fires) from summer 2010 at Caltech's SPHIR facility:

$$X = (h, \alpha, v) \in \mathbb{X} := [0.062, 0.125]\,\text{in} \times [0, 30]\,\text{deg} \times [2300, 3200]\,\text{m/s}.$$

  Output $g^\dagger(h, \alpha, v)$ = the induced perforation area in mm^2; the data set contains results between $6.31\,\text{mm}^2$ and $15.36\,\text{mm}^2$.
- Failure event is $[g^\dagger(h, \alpha, v) \leq \theta]$, for various values of θ.
- Constrain the mean perf. area: $\mathbb{E}_{\mu^\dagger}[g^\dagger(h, \alpha, v)] \geq m := 11.0\,\text{mm}^2$.
- Modified Lipschitz constraint (multi-valued data):

$$L = \left(\frac{175.0}{\text{in}}, \frac{0.075}{\text{deg}}, \frac{0.1}{\text{m/s}} \right) \text{mm}^2$$

$$|y - y'| \leq \sum_{k=1}^{3} L_k |x_k - x'_k| + 1.0\,\text{mm}^2.$$

3-Parameter Hypervelocity Impact Example: Results

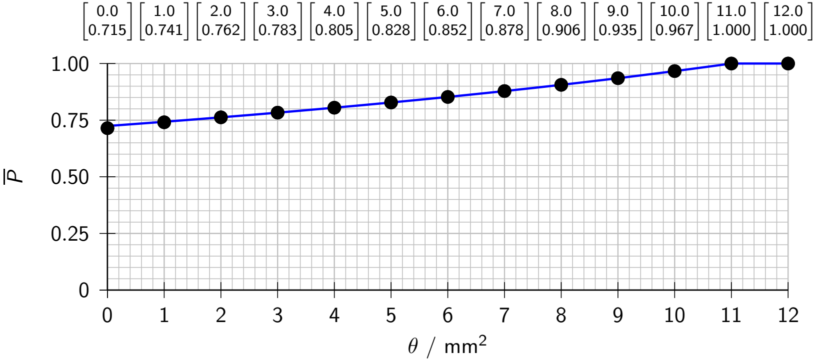

Figure : Maximum probability that perforation area is $\leq \theta$, for various θ, with the data and assumptions of the previous slide, including mean perforation area $\mathbb{E}[g^\dagger(h, \alpha, v)] \geq 11.0\,\mathrm{mm}^2$. For $\theta \geq 2\,\mathrm{mm}^2$, the results are within 10^{-6} of Markov's bound, which indicates that 2 binding data points are those that constrain the maximum of the response function; the other 30 are non-binding.

Models and Neighbourhoods

- One can consider feasible sets in which the constraints on g are of the form $d(g, F) \leq C$ for some model function F.
- There are good and bad choices for the distance function d:

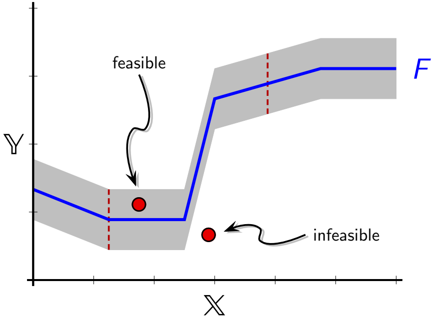

Figure : Assuming that reality $g^\dagger$ is uniformly close to the model F means assuming that the model has approximately the right cliffs in exactly the right places; Hausdorff (graphical) closeness is a much looser assumption.

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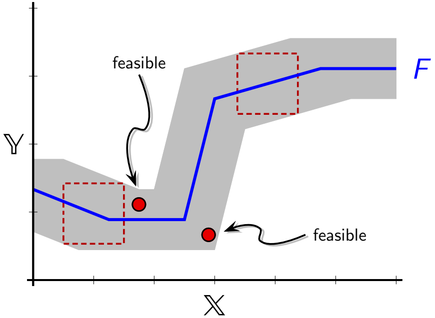

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Hypervelocity Impact Application

- System is characterized by three input parameters: target plate thickness h, obliquity α, and impact velocity v, with assumed ranges $h \in \mathbb{X}_h := \{0.5, 1.5, 3.0\}\,\mathrm{mm}$, $\alpha \in \mathbb{X}_\alpha := [0, 60]^\circ$, and $v \in \mathbb{X}_v := [4.5, 7.0]\,\mathrm{km} \cdot \mathrm{s}^{-1}$. Input space is $\mathbb{X} := \mathbb{X}_h \times \mathbb{X}_\alpha \times \mathbb{X}_v$.
- Perforation area is the main performance measure of the system, which is expected to lie in the output space $\mathbb{Y} := [0, 39.73]\,\mathrm{mm}^2$. We want to bound $\mathbb{P}[g^\dagger(h, \alpha, v) \leq \theta]$ for threshold area values θ.
- The model function F is the Optimal Transportation Meshfree method. (A **lot** swept under the carpet here!)
- Model-reality mismatch quantified as $d(g^\dagger, F) \leq \delta$. In practice, we fix a confidence level $0 < \eta < 1$, and use legacy data points to find $\delta(\eta)$ such that $d(g^\dagger, F) \leq \delta(\eta)$ with probability $\geq \eta$.

Mean Constraints on Outputs

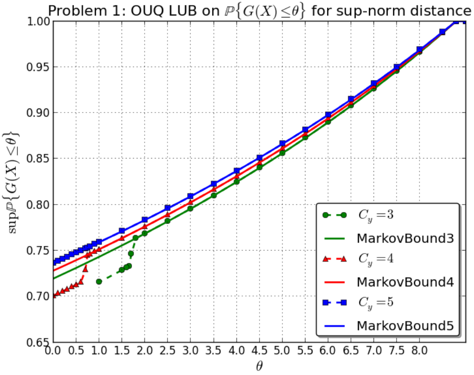

Figure : OUQ least upper bounds on perforation area probabilities given $d(g^\dagger, F) \leq \delta$ and bounds on $\mathbb{E}_\mu[g^\dagger]$. Note the relative insensitivity (for $\theta \geq 2\,\mathrm{mm}^2$) to both δ and the choice of d as the uniform or Hausdorff distance. Note also that the closeness to the Markov bounds (solid curves), indicating that the binding information is the implied maximum perforation area.

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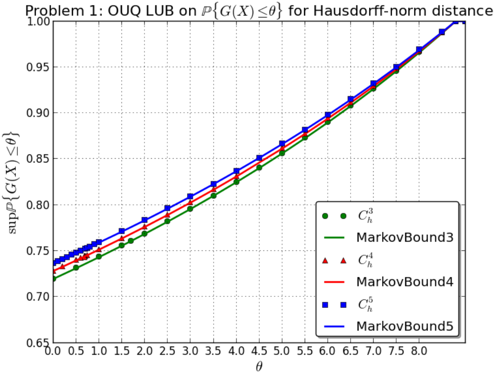

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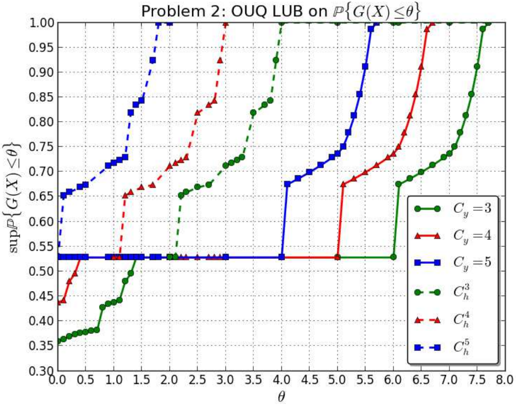


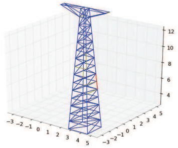
Figure : OUQ least upper bounds on perforation area probabilities given $d(g^\dagger, F) \leq \delta$ and bounds on $\mathbb{E}_\mu[h]$, $\mathbb{E}_\mu[\alpha]$, $\mathbb{E}_\mu[v]$. Note the strong sensitivity to both δ and the choice of d as the uniform (solid curves) or Hausdorff (dashed curves) distance.

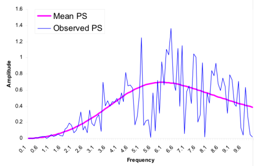
Seismic Safety Certification

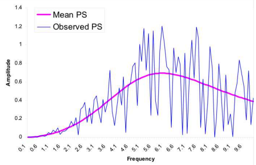
- Consider the survivability of a truss structure under an random earthquake of known intensity drawn from an incompletely specified probability distribution.
- Consider a random ground motion u, with the constraint that the mean power spectrum is the Matsuda–Asano shape function s_{MA}:

$$\mathbb{E}_{u\sim\mu}\left[|\hat{u}(\omega)|^2\right] = s_{\mathrm{MA}}(\omega) \propto \frac{\omega_{\mathrm{g}}^2\omega^2 e^{M_{\mathrm{L}}}}{(\omega_{\mathrm{g}}^2 - \omega^2)^2 + 4\xi_{\mathrm{g}}^2\omega_{\mathrm{g}}^2\omega^2}.$$

- Such shape functions are a common tool in the seismological community, but usually u is generated by filtering white noise through s.
- We used 200 3d Fourier modes, leading to a 1200-dimensional OUQ problem.







Reduction of the Random Power Spectrum

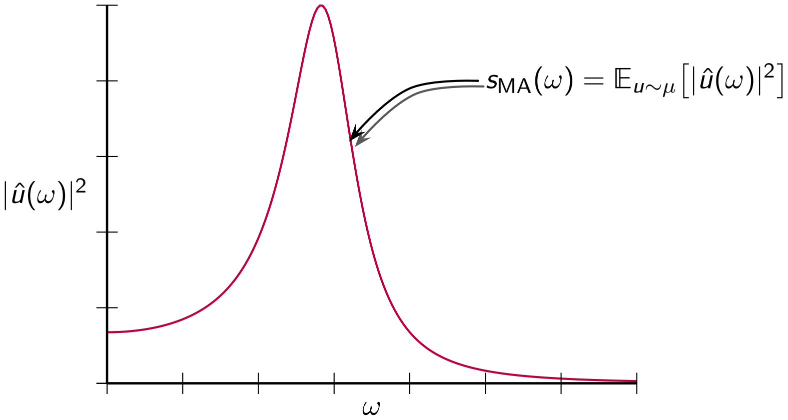
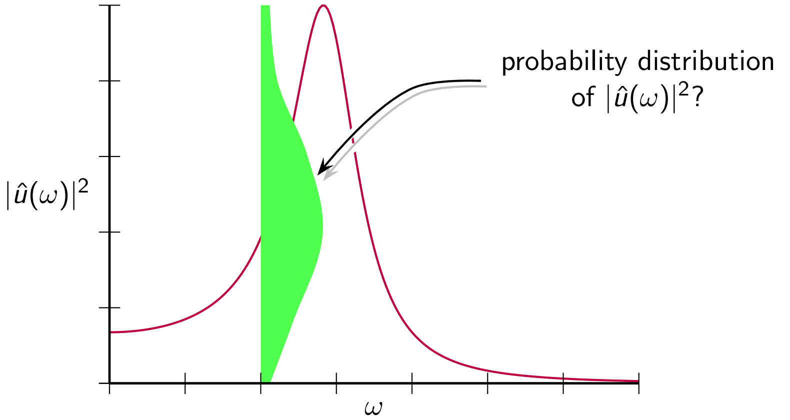


Figure : One mean constraint on each independent random Fourier mode $\hat{u}(\omega)$ (i.e. that $\mathbb{E}_{u\sim\mu}\left[|\hat{u}(\omega)|^2\right] = s_{\mathrm{MA}}(\omega)$) $\implies$ we get to pretend that $u(\omega)$ takes at most two distinct values which together satisfy this mean constraint.

Reduction of the Random Power Spectrum



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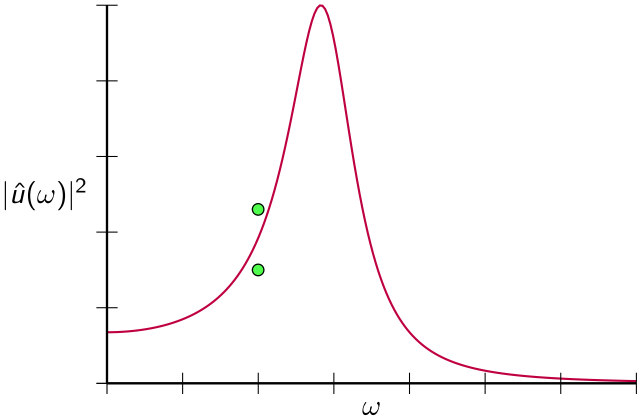

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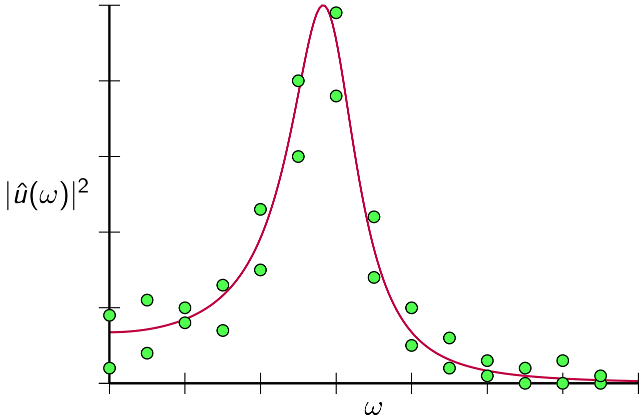

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Numerical Vulnerability Curves (CDF Envelopes)

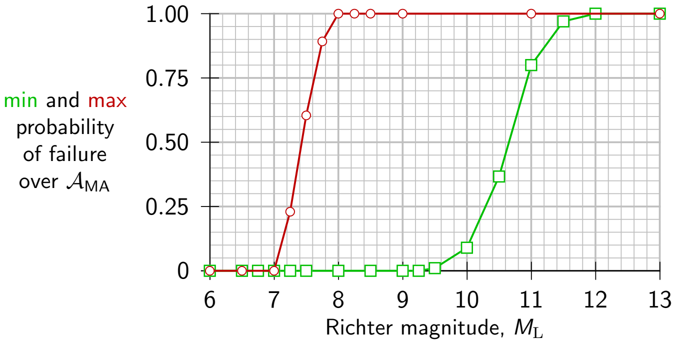

Figure : The minimum and maximum probability of failure as a function of Richter magnitude, M_{L}, where the ground motion u is constrained to have $\mathbb{E}_{\mu}[|\hat{u}|^2] =$ the Matsuda–Asano shape function s_{MA} with natural frequency ω_{g} and natural damping ξ_{g} taken from the 24 Jan. 1980 Livermore earthquake. Each data point required $\approx$ 1 day on 44+44 AMD Opterons (*shc* and *foxtrot* at Caltech). The forward model used 200 Fourier modes for a 3-dimensional ground motion u.

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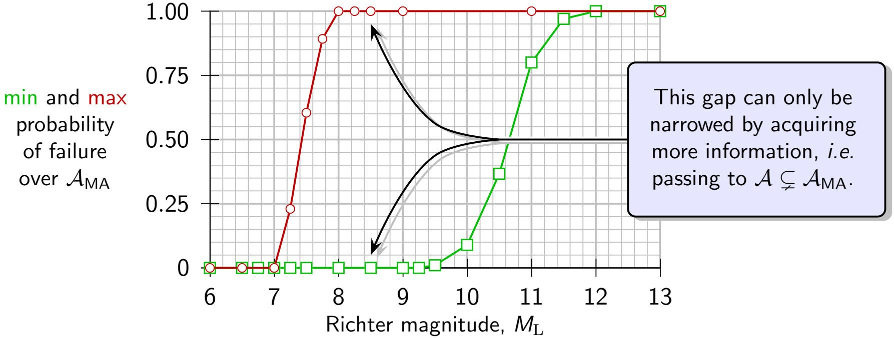

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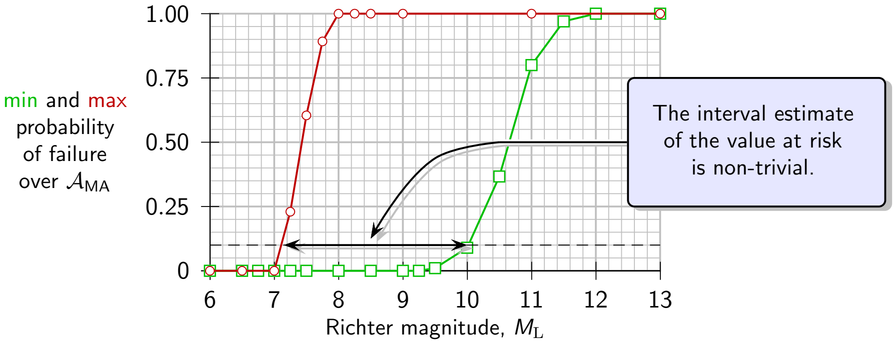

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When and How to Use OUQ

- Use OUQ if you are strongly risk-averse, have unavoidable epistemic uncertainties, and have enough time to compute your way through the problem.
- Conversely, for real-time applications with simple and well-understood uncertainties, OUQ is impractical and overkill.
- Good features to include in your optimizer:
    - keep the functional parts of your optimizer as swappable modules, and pay attention to enforcing constraints;
    - cache past function evaluations;
    - look out for convex sub-problems in the non-convex OUQ problem;
    - look out for numerical 'collapse' of the discrete measure (dimension reduction $\implies$ huge cost savings).
- Personal rules of thumb: Differential Evolution works well with pop. size ≈ 40, 200 to 400 generations convergence criterion, run problems with 10s of support points and a fast model on a laptop overnight.

Conclusions

- By posing **UQ as an optimization problem** we
  - place the available information ($\cong$ constraints) about the input uncertainties at the centre of the problem;
  - obtain optimal bounds on output uncertainties w.r.t. that information;
  - get natural notions of information content in optimization-theoretic terms about constraints: active/inactive, binding/non-binding, . . .
- We have theoretical (closed-form pen-and-paper) and real (high-dimensional engineering systems) examples in hand showing these phenomena at work.
- Growing computational resources make large OUQ-type problems increasingly tractable, cf. Bayesian methods in 20th Century.
- Many research questions, especially concerning the inclusion of random sample data, algorithmic properties of OUQ, &c.

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- Caltech (O)UQ Publications
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  - H. Owhadi & al. "Optimal Uncertainty Quantification." *SIAM Rev.* **55**(2):271–345, 2013. doi:10.1137/10080782X
  - T. J. Sullivan & al. "Optimal uncertainty quantification for legacy data observations of Lipschitz functions." *Math. Mod. Num. Anal.* **47**(6):1657–1689, 2013. doi:10.1051/m2an/2013083
  - Kidane & al. "Rigorous model-based uncertainty quantification with application to terminal ballistics. Part I" *J. Mech. Phys. Solids* **60**(5):983–1001, 2011. doi:10.1016/j.jmps.2011.12.001
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- Software
  - Mystic (optimization): http://trac.mystic.cacr.caltech.edu/project/mystic
  - Pathos (distribution): http://trac.mystic.cacr.caltech.edu/project/pathos