The worst case approach to UQ

Houman Owhadi

"The gods to-day stand friendly, that we may,
Lovers of peace, lead on our days to age!
But, since the affairs of men rests still uncertain,
Let's reason with the worst that may befall."

Julius Caesar, Act 5, Scene 1
William Shakespeare (1564 –1616)

CALTECH PSAAP Predictive Science Academic Alliance Program

National Nuclear Security Administration

You want to certify that

$$\mathbb{P}[G(X) \geq a] \leq \epsilon$$

Problem

- You don't know G.

and

- You don't know $\mathbb{P}$

You want to certify that

$$\mathbb{P}[G(X) \geq a] \leq \epsilon$$

Problem

- You don't know G.

and

- You don't know $\mathbb{P}$

You only know

$$\boxed{(G, \mathbb{P}) \in \mathcal{A}}$$

$$\mathcal{A} \subset \left\{ (f, \mu) \,\middle|\, \begin{matrix} f : \mathcal{X} \to \mathbb{R}, \\ \mu \in \mathcal{P}(\mathcal{X}) \end{matrix} \right\}$$

Compute **Worst and best case**

optimal bounds $\mathbb{P}[G(X) \geq a]$
given available information.

$$\boxed{\mathcal{U}(\mathcal{A}) := \sup_{(f,\mu)\in\mathcal{A}} \mu[f(X) \geq a]}$$

$$\boxed{\mathcal{L}(\mathcal{A}) := \inf_{(f,\mu)\in\mathcal{A}} \mu[f(X) \geq a]}$$

$$\boxed{\mathcal{L}(\mathcal{A}) \leq \mathbb{P}[G(X) \geq a] \leq \mathcal{U}(\mathcal{A})}$$

$\mathcal{U}(\mathcal{A}) \leq \epsilon$: Safe even in worst case.
$\epsilon < \mathcal{L}(\mathcal{A})$: Unsafe even in best case.
$\mathcal{L}(\mathcal{A}) \leq \epsilon < \mathcal{U}(\mathcal{A})$: Cannot decide.
Unsafe due to lack of information.

Optimal Uncertainty Quantification

H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz. **Optimal Uncertainty Quantification**. *SIAM Review*, 55(2):271–345, 2013.

Robust Optimization

A. Ben-Tal, L. El Ghaoui, and A.Nemirovski. ***Robust optimization***. Princeton Series in Applied Mathematics. Princeton University Press, Princeton, NJ, 2009

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A. Ben-Tal and A. Nemirovski. **Robust convex optimization**. *Math. Oper. Res.*, 23(4):769–805, 1998

I. Elishakoff and M. Ohsaki. ***Optimization and Anti-Optimization of Structures Under Uncertainty***. World Scientific, London, 2010.

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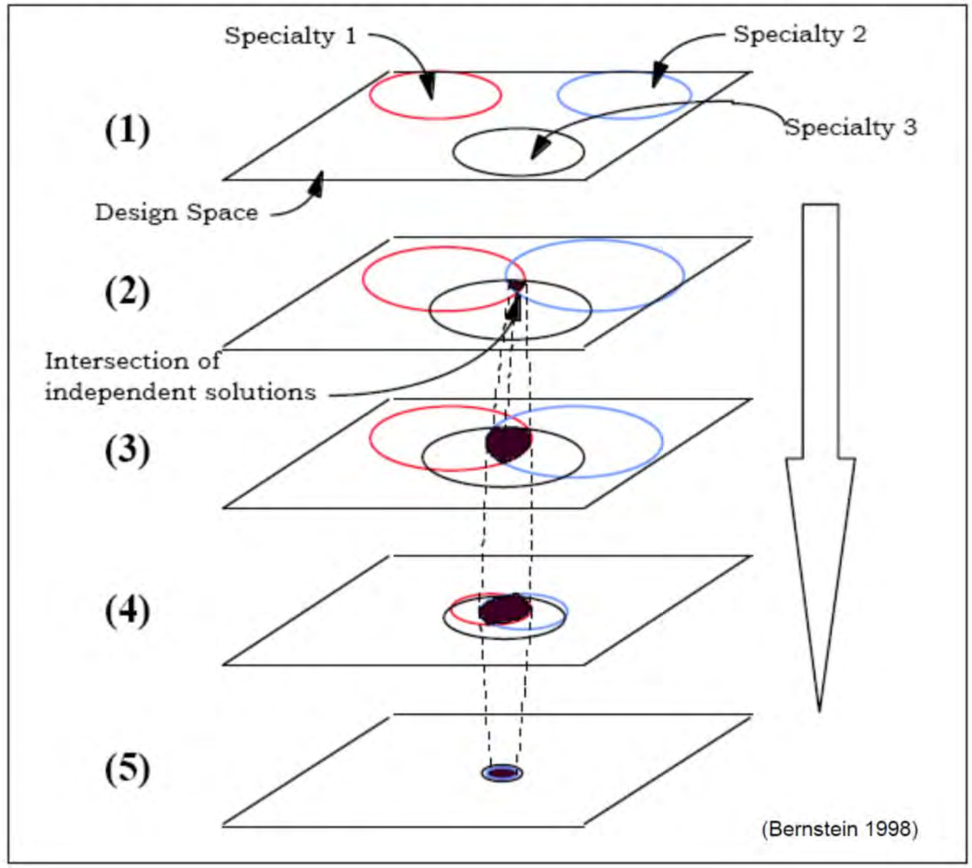
Set based design in the aerospace industry

Bernstein, J. I., 1998, Design Methods in the Aerospace Industry: Looking for Evidence of Set-Based Practices, Master of Science Thesis, Massachusetts Institute of Technology, 1998.



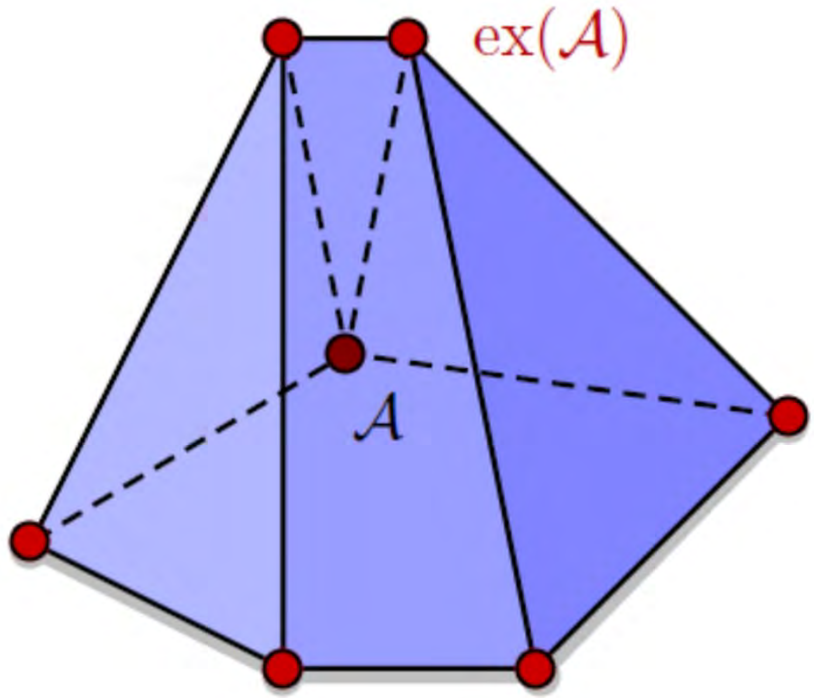
Bernstein JI (1998) *Design methods in the aerospace industry: looking for evidence of* ***set-based practices***. Master's thesis. Massachusetts Institute of Technology, Cambridge, MA.

Set based design/analysis

David J. Singer, PhD., Captain Norbert Doerry, PhD., and Michael E. Buckley," *What is* ***Set-Based Design****?* ," Presented at ASNE DAY 2009, National Harbor, MD., April 8-9, 2009. Also published in ASNE Naval Engineers Journal, 2009 Vol 121 No 4, pp. 31-43.

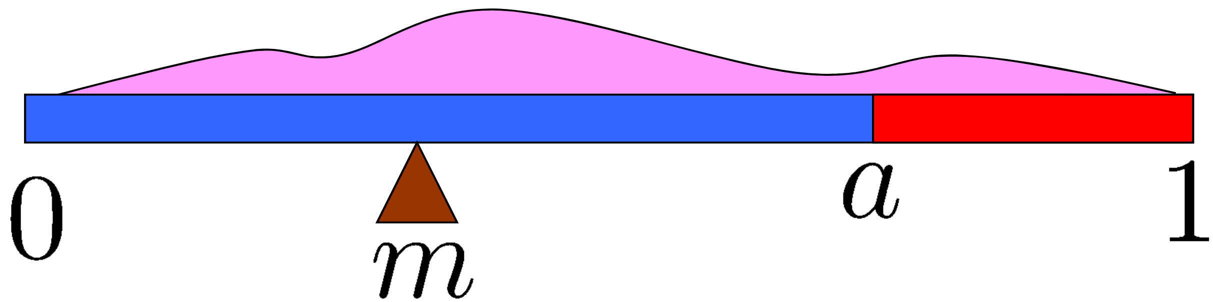
B. Rustem and Howe M. ***Algorithms for Worst-Case Design and Applications to Risk Management***. Princeton University Press, Princeton, 2002.

$$\boxed{\sup_{(f,\mu)\in\mathcal{A}} \mu[f(X) \geq a]}$$



Optimization problems are a priori infinite dimensional, non-convex and highly constrained but as in linear programming, under general conditions, they can be reduced to finite dimensional families of extremal scenarios of $\mathcal{A}$ and the dimension of the reduced problem is proportional to the number of probabilistic inequalities describing $\mathcal{A}$

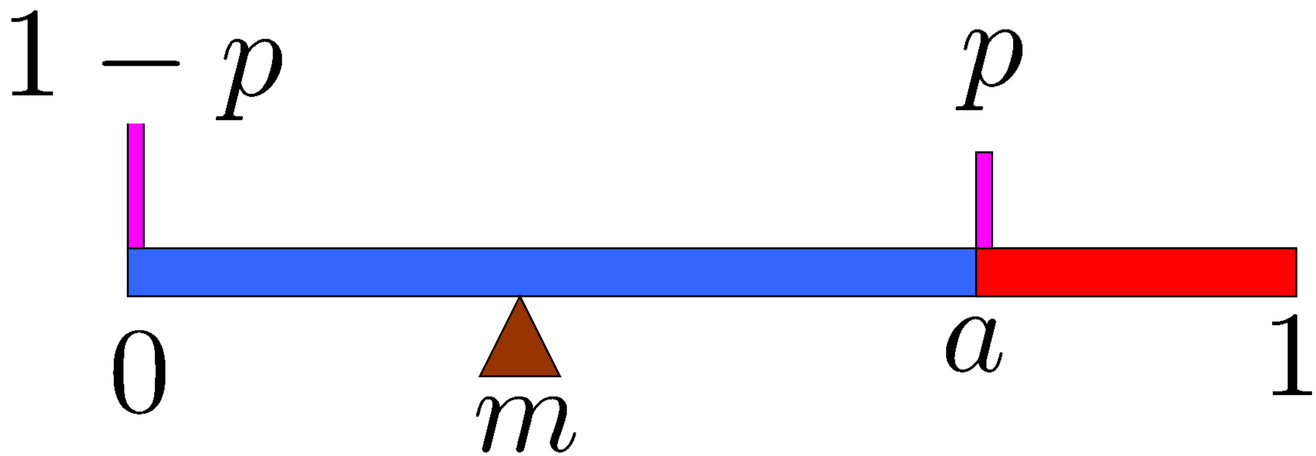
You are given one pound of playdoh,
how much mass can you put above a
while keeping the seesaw balanced around m?



P. L. Chebyshev
1821-1894

A. A. Markov
1856-1922

M. G. Krein
1907-1989



$$\begin{cases} \max p \\ \text{subject to } a\,p \le m \end{cases}$$

Answer $\boxed{\dfrac{m}{a}}$

What is the least upper bound on $\mathbb{P}[X \geq a]$ if all that you know is that $\mathbb{P}$ is an unknown distribution on $[0,1]$ having mean less than m

$$\mathcal{A} = \{\mu \in \mathcal{M}([0,1]) \,|\, \mathbb{E}_\mu[X] \leq m\}$$

Markov's inequality

Answer

$$\boxed{\sup_{\mu \in \mathcal{A}} \mu[X \geq a] = \frac{m}{a}}$$

$$\boxed{\sup_{(f,\mu)\in\mathcal{A}} \mu[f(X) \geq a]}$$

Can be considered as a generalization of classical Chebyshev inequalities

History of classical inequalities

S. Karlin and W. J. Studden. ***Tchebycheff Systems: With Applications in Analysis and Statistics***. Pure and Applied Mathematics, Vol. XV. Interscience Publishers John Wiley & Sons, New York-London-Sydney, 1966.

Classical Markov-Krein theorem and classical works of Krein, Markov and Chebyshev

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Theory of majorization

A. W. Marshall and I. Olkin. ***Inequalities: Theory of Majorization and its Applications***, volume 143 of *Mathematics in Science and Engineering*. Academic Press Inc. [Harcourt Brace Jovanovich Publishers], New York, 1979

Connections between Chebyshev inequalities and optimization theory

H. J. Godwin. **On generalizations of Tchebychef's inequality**. *J. Amer. Statist. Assoc.*, 50(271):923–945, 1955.

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Stochastic linear programming and Stochastic Optimization

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Optimal Uncertainty Quantification

H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz. **Optimal Uncertainty Quantification**. *SIAM Review*, 55(2):271–345, 2013.

T. J. Sullivan, M. McKerns, D. Meyer, F. Theil, H. Owhadi, and M. Ortiz. **Optimal uncertainty quantification for legacy data observations of Lipschitz functions.** *ESAIM Math. Model. Numer. Anal.*, 47(6):1657–1689, 2013.

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H. Owhadi, C. Scovel and T. Sullivan. Brittleness of Bayesian Inference under Finite Information in a Continuous World. Electronic Journal of Statistics, vol 9, pp 1-79, 2015. arXiv:1304.6772

H. Owhadi and Clint Scovel. Extreme points of a ball about a measure with finite support (2015). arXiv:1504.06745

Our proof relies on

- Winkler (1988, Extreme points of moment sets)
- Follows from an extension of Choquet theory (Phelps 2001, lectures on Choquet's theorem) by Von Weizsacker & Winkler (1979, Integral representation in the set of solutions of a generalized moment problem)
- Kendall (1962, Simplexes & Vector lattices)

G. Winkler. On the integral representation in convex noncompact sets of tight measures. *Mathematische Zeitschrift*, 158(1):71–77, 1978

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H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz.
Optimal Uncertainty Quantification. *SIAM Review*, 55(2):271–345, 2013.

$$\mathcal{A} = \left\{ (f,\mu) \,\middle|\, \begin{array}{c} f\colon \mathcal{X}_1 \times \cdots \times \mathcal{X}_m \to \mathbb{R}, \\ \mu = \mu_1 \otimes \cdots \otimes \mu_m, \\ \mathcal{G}(f,\mu) \leq 0 \end{array} \right\}$$

$$\mathcal{G}(f,\mu) \leq 0 \Leftrightarrow \begin{cases} n' \text{ generalized moment constraints on } \mu, & \mathbb{E}_\mu[\varphi_j^f] \leq 0 \\ n_k \text{ generalized moment constraints on } \mu_k, & \mathbb{E}_{\mu_k}[\psi_{k,j}^f] \leq 0 \end{cases}$$

Theorem

$$\sup_{(f,\mu)\in\mathcal{A}} \mathbb{E}_\mu[q_f] = \sup_{(f,\mu)\in\mathcal{A}_\Delta} \mathbb{E}_\mu[q_f]$$

$$\mathcal{A}_\Delta = \left\{ (f,\mu) \in \mathcal{A} \,\middle|\, \begin{array}{c} \mu_k \text{ is a sum of at most} \\ n' + n_k + 1 \text{ weighted} \\ \text{Dirac measures on } \chi_k \end{array} \right\}$$

Further Reduction of optimization variables

$$\{f : \mathcal{X} \to \mathbb{R},\ \mu \in \mathcal{P}(\mathcal{X})\}$$

$$\downarrow$$

$$\left\{ f : \mathcal{X} \to \mathbb{R},\ \mu \in \mathcal{P}(\mathcal{X}) \,\middle|\, \mu = \sum_{i=1}^{k} \alpha_k \delta_{x_k} \right\}$$

$$\downarrow$$

$$\{f : \{1, 2, \ldots, n\} \to \mathbb{R},\ \mu \in \mathcal{P}(\{1, 2, \ldots, n\})\}$$

$$\downarrow$$

$$\{\{1, 2, \ldots, q\},\ \mu \in \mathcal{P}(\{1, 2, \ldots, n\})\}$$

Another example: Optimal concentration inequality

H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz. Optimal Uncertainty Quantification. *SIAM Review*, 55(2):271–345, 2013.

$$\mathcal{A}_{MD} := \left\{ (f,\mu) \;\middle|\; \begin{array}{c} f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_m \to \mathbb{R}, \\ \mu \in \mathcal{M}(\mathcal{X}_1) \otimes \cdots \otimes \mathcal{M}(\mathcal{X}_m), \\ \mathbb{E}_\mu[f] \le 0, \\ \operatorname{Osc}_i(f) \le D_i \end{array} \right\}$$

$$\operatorname{Osc}_i(f) := \sup_{(x_1,\ldots,x_m)\in\mathcal{X}} \sup_{x_i'\in\mathcal{X}_i} \big(f(\ldots,x_i,\ldots) - f(\ldots,x_i',\ldots) \big).$$

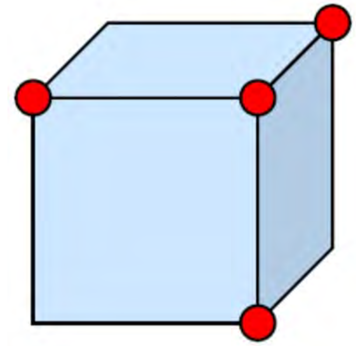
$$\boxed{\mathcal{U}(\mathcal{A}_{MD}) := \sup_{(f,\mu)\in\mathcal{A}_{MD}} \mu[f(X) \ge a]}$$

McDiarmid inequality's

$$\boxed{\mathcal{U}(\mathcal{A}_{MD}) \le \exp\left(-2 \frac{a^2}{\sum_{i=1}^m D_i^2} \right)}$$

Reduction of optimization variables

$$\mathcal{A}_{\mathcal{C}} := \left\{ (C,\alpha) \;\middle|\; \begin{array}{c} C \subset \{0,1\}^m, \\ \alpha \in \otimes_{i=1}^m \mathcal{M}(\{0,1\}), \\ \mathbb{E}_\alpha[h^C] \le 0 \end{array} \right\}$$



$$h^C : \{0,1\}^m \longrightarrow \mathbb{R}$$

$$t \longrightarrow a - \min_{s \in C} \sum_{i:\, s_i \neq t_i} D_i$$

$$\boxed{\mathcal{U}(\mathcal{A}_{\mathcal{C}}) := \sup_{(C,\alpha)\in\mathcal{A}_{\mathcal{C}}} \alpha[h^C \ge a]}$$

Theorem

$$\boxed{\mathcal{U}(\mathcal{A}_{MD}) = \mathcal{U}(\mathcal{A}_{\mathcal{C}})}$$

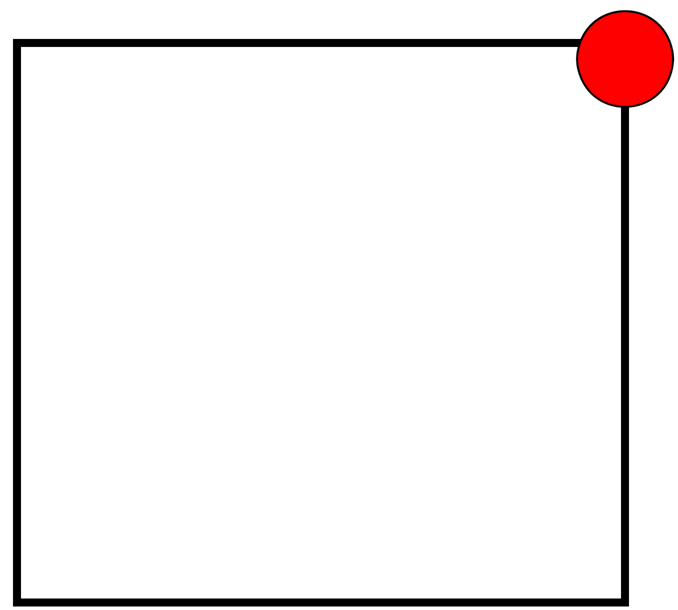
Explicit Solution m=2

Theorem $m = 2$

$$\mathcal{U}(\mathcal{A}_{MD}) = \begin{cases} 0 & \text{if} \quad D_1 + D_2 \leq a \\ \frac{(D_1+D_2-a)^2}{4D_1D_2} & \text{if} \quad |D_1 - D_2| \leq a \leq D_1 + D_2 \\ 1 - \frac{a}{\max(D_1,D_2)} & \text{if} \quad 0 \leq a \leq |D_1 - D_2| \end{cases}$$

$$C = \{(1,1)\}$$

$$h^C(s) = a - (1 - s_1)D_1 - (1 - s_2)D_2$$



Explicit Solution m=2

Theorem $m = 2$

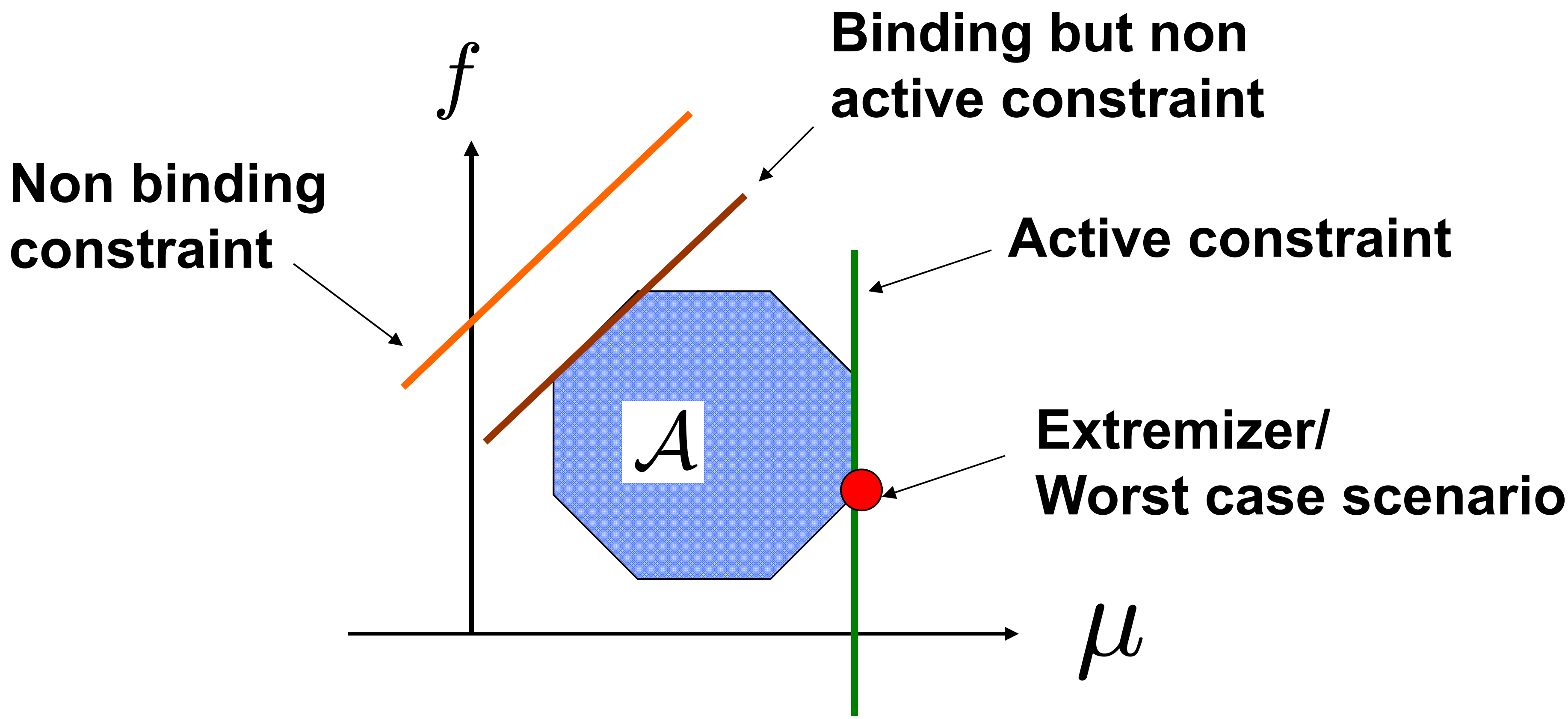
$$\mathcal{U}(\mathcal{A}_{MD}) = \begin{cases} 0 & \text{if} \quad D_1 + D_2 \le a \\ \frac{(D_1+D_2-a)^2}{4D_1 D_2} & \text{if} \quad |D_1 - D_2| \le a \le D_1 + D_2 \\ 1 - \frac{a}{\max(D_1, D_2)} & \text{if} \quad 0 \le a \le |D_1 - D_2| \end{cases}$$

Corollary If $D_1 \ge a + D_2$, then

$$\mathcal{U}(\mathcal{A}_{MD})(a, D_1, D_2) = \mathcal{U}(\mathcal{A}_{MD})(a, D_1, 0)$$

Each piece of information is a constraint on an optimization problem.

Optimization concepts (binding, active) transfer to UQ concepts



Optimal Hoeffding= Optimal McDiarmid for m=2

$$\mathcal{A}_{MD} := \left\{ (f,\mu) \,\middle|\, \begin{array}{c} f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_m \to \mathbb{R}, \\ \mu \in \mathcal{M}(\mathcal{X}_1) \otimes \cdots \otimes \mathcal{M}(\mathcal{X}_m), \\ \mathbb{E}_\mu[f] \leq 0, \\ \mathrm{Osc}_i(f) \leq D_i \end{array} \right\}$$

$$\mathcal{U}(\mathcal{A}_{\mathrm{MD}}) = \mathcal{U}(\mathcal{A}_{\mathrm{Hfd}})$$

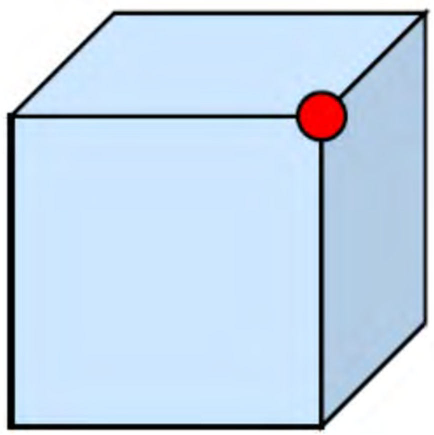
$$\mathcal{A}_{\mathrm{Hfd}} := \left\{ (f,\mu) \,\middle|\, \begin{array}{c} f = X_1 + \cdots + X_m, \\ \mu \in \bigotimes_{i=1}^m \mathcal{M}([b_i - D_i, b_i]), \\ \mathbb{E}_\mu[f] \leq 0 \end{array} \right\}$$

Explicit Solution m=3

Theorem $m = 3$

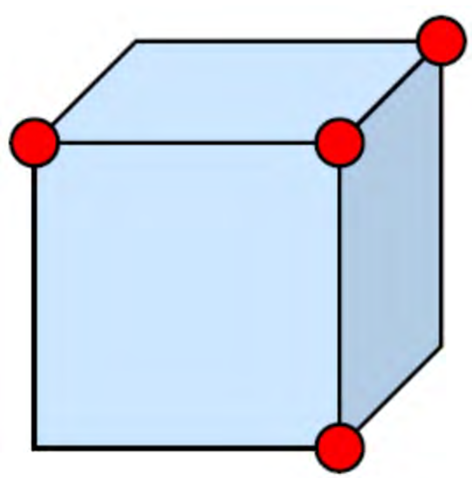
$$\boxed{\mathcal{U}(\mathcal{A}_{MD}) = \max(\mathcal{F}_1, \mathcal{F}_2)}$$

$\mathcal{F}_1$



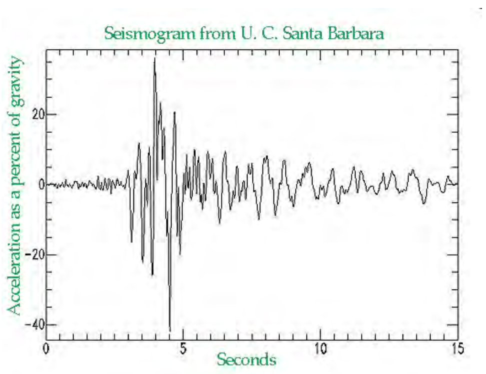
$$\boxed{\mathcal{U}(\mathcal{A}_{\mathrm{MD}}) = \mathcal{U}(\mathcal{A}_{\mathrm{Hfd}})}$$

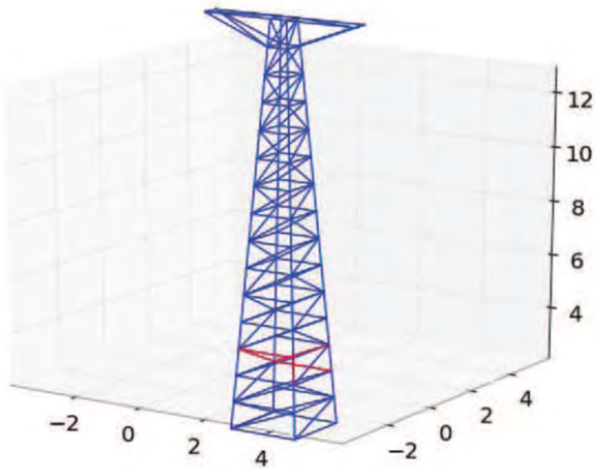
$\mathcal{F}_2$

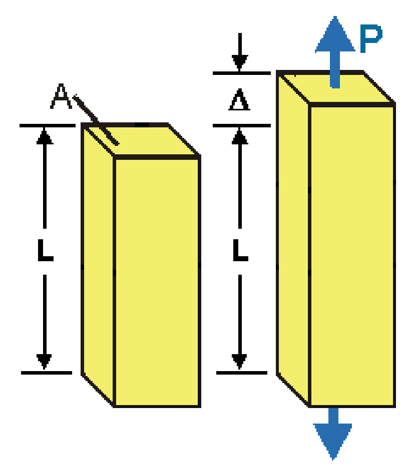


$$\boxed{\mathcal{U}(\mathcal{A}_{\mathrm{MD}}) > \mathcal{U}(\mathcal{A}_{\mathrm{Hfd}})}$$

Seismic Safety Assessment of a Truss Structure







$$a(t) \longrightarrow F(a)$$

Ground Acceleration

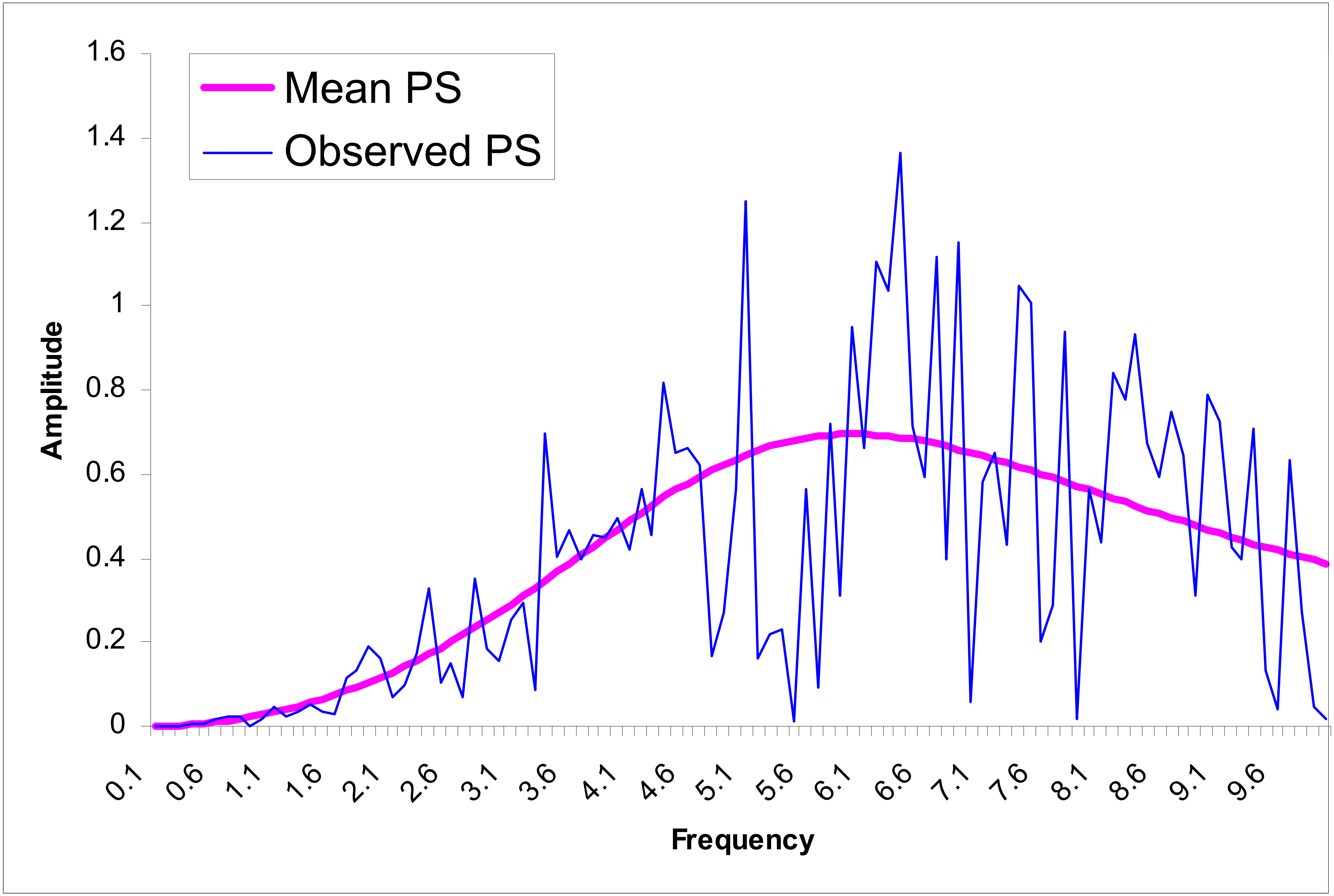
F

min(Yield Strain - Axial Strain)

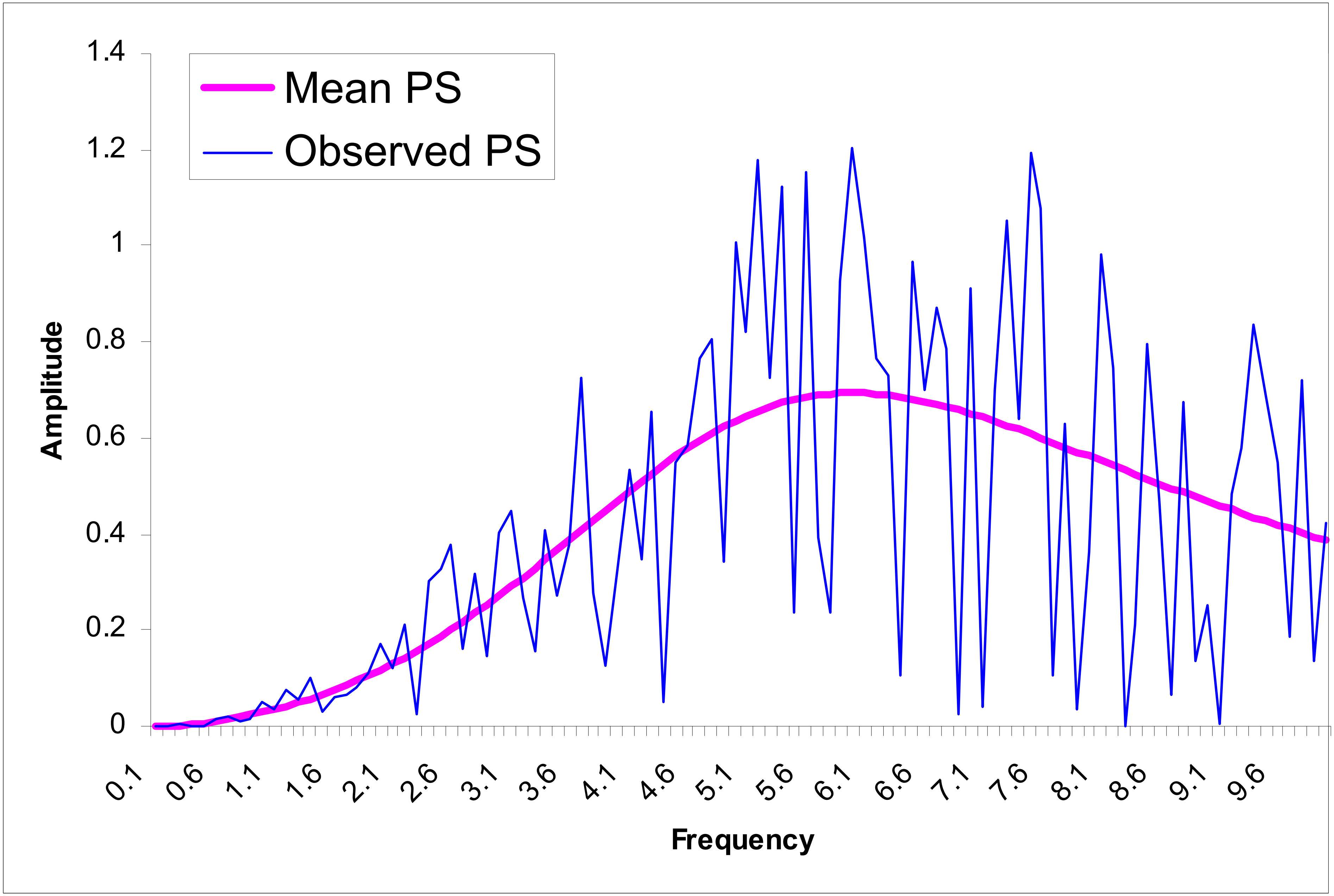
We want to certify that

$$\boxed{\mathbb{P}\left[F(a) \leq 0\right] \leq \epsilon}$$

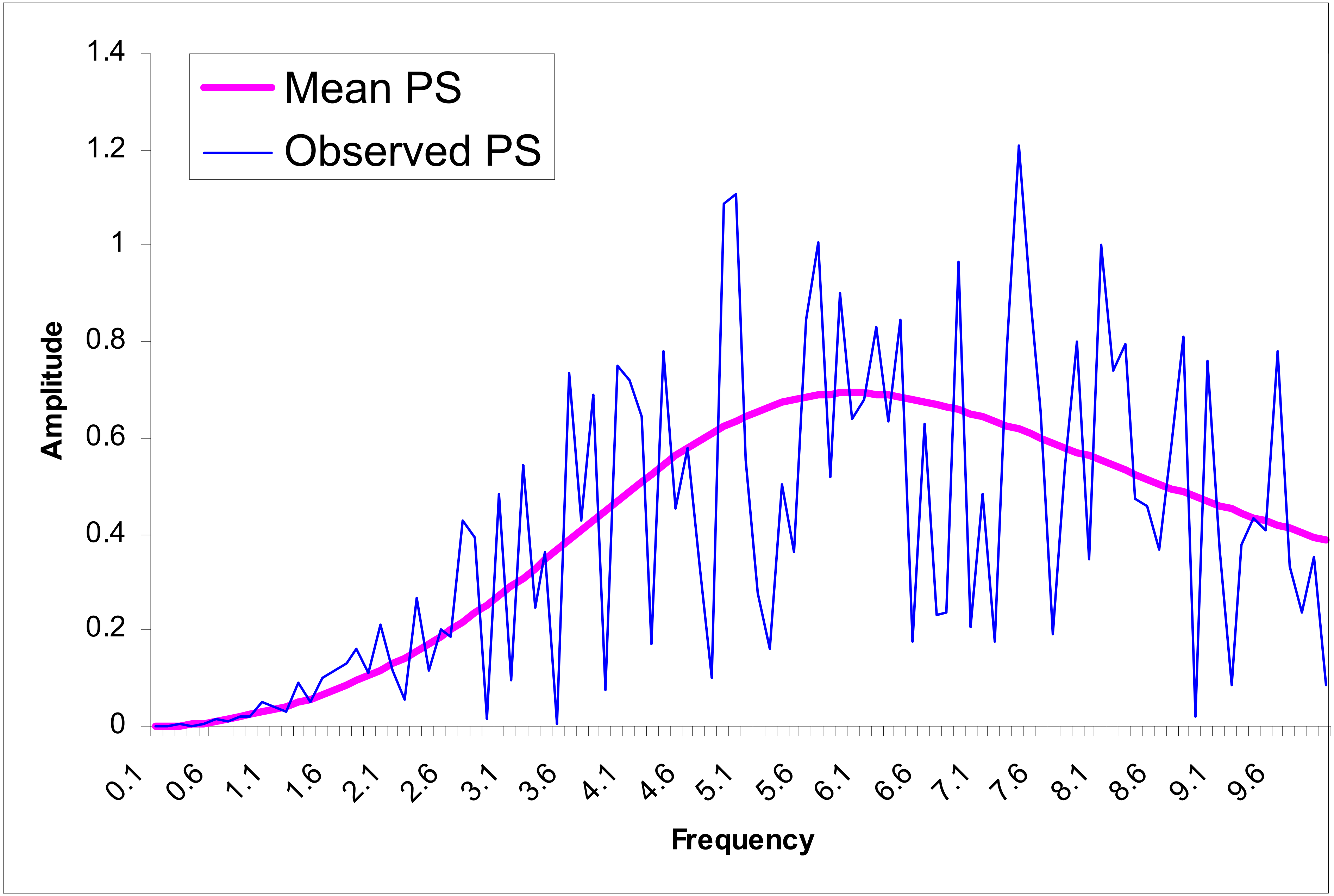
Power Spectrum



Power Spectrum

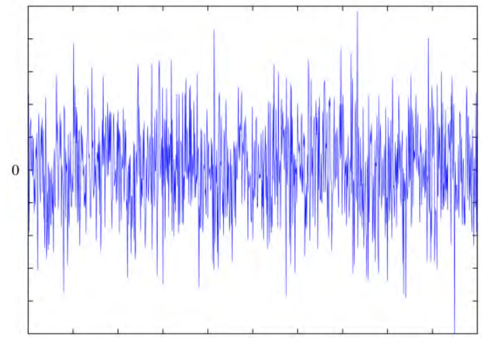


Power Spectrum

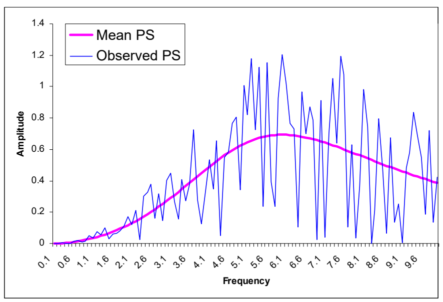


Filtered White Noise Model

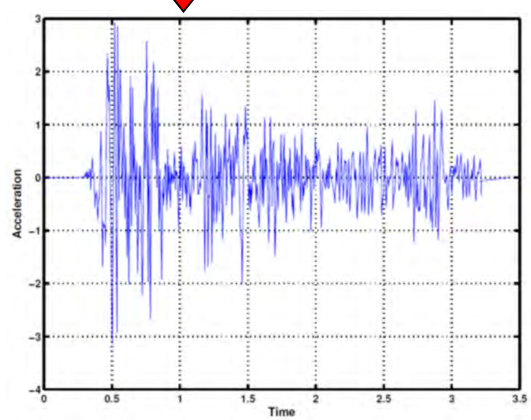
White noise



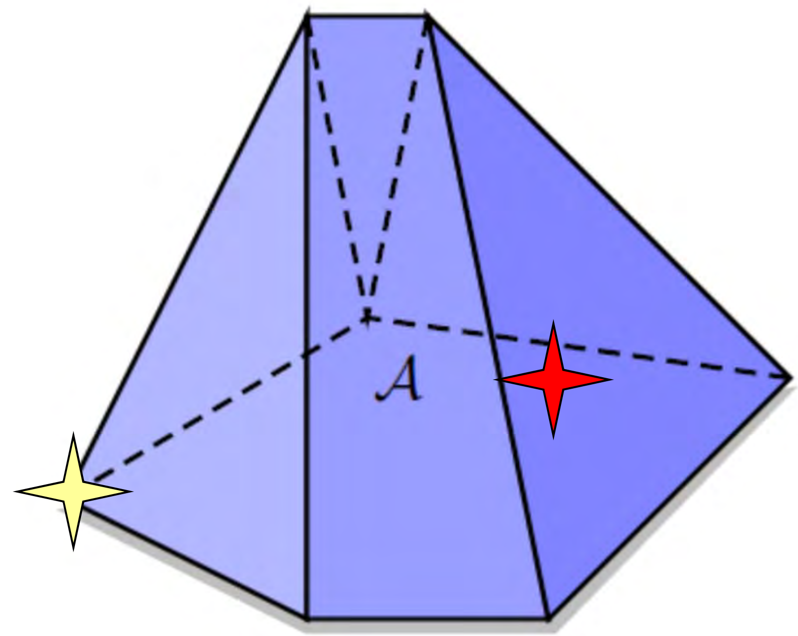
Filter



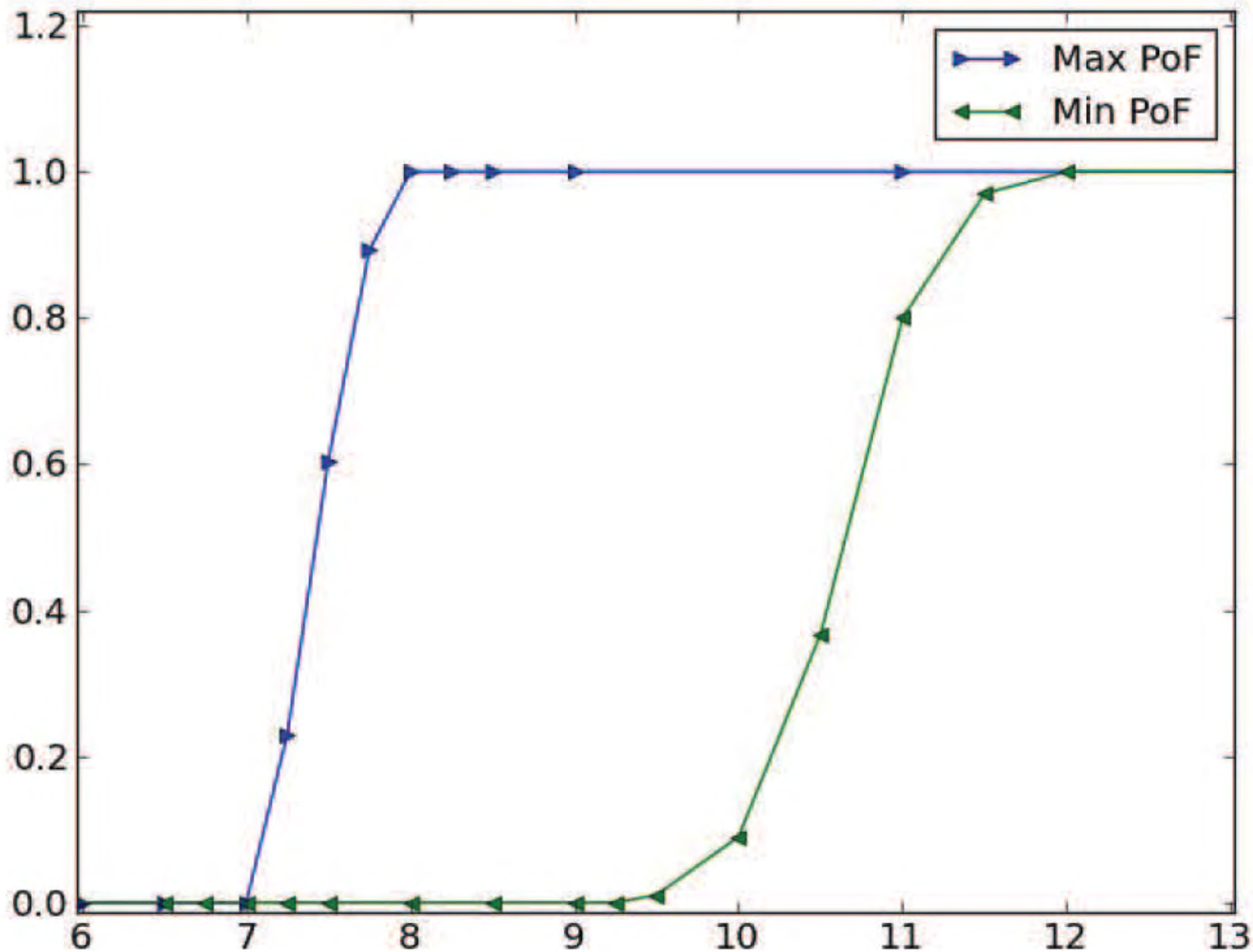
Ground acceleration



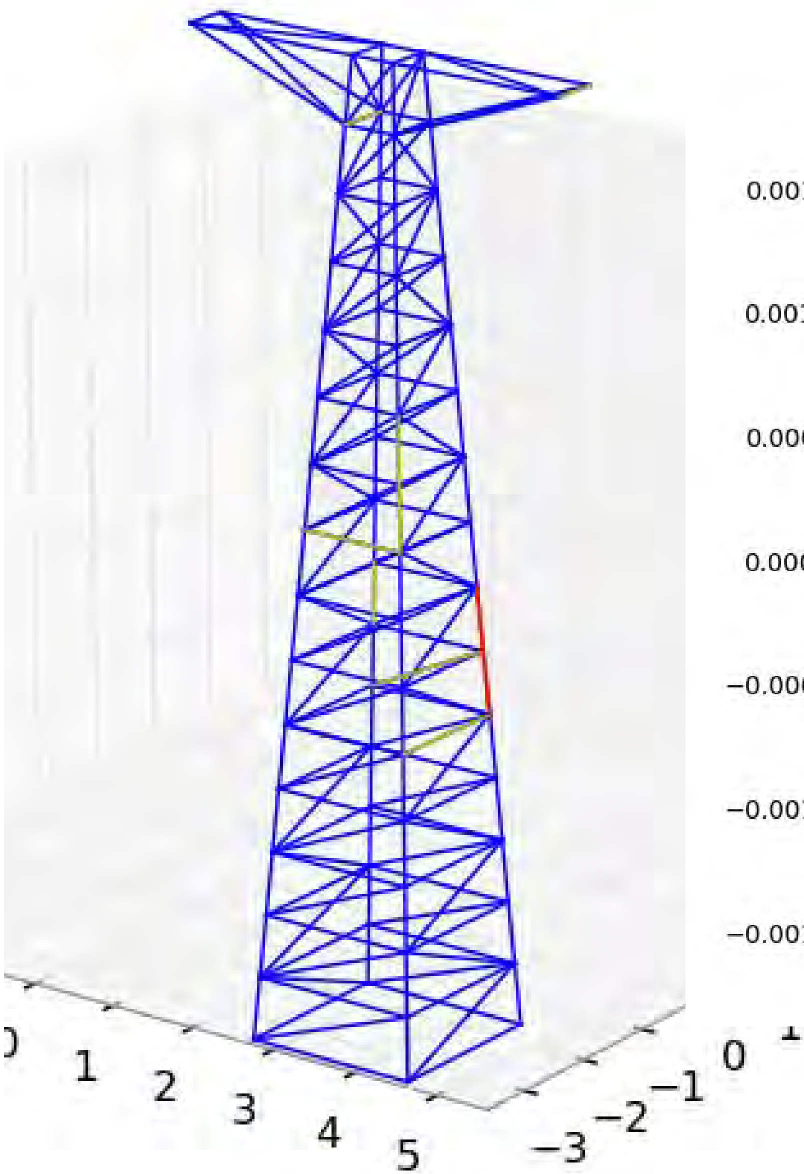
N. Lama, J. Wilsona, and G. Hutchinsona. Generation of synthetic earthquake accelograms using seismological modeling: a review. Journal of Earthquake Engineering, 4(3):321–354, 2000.

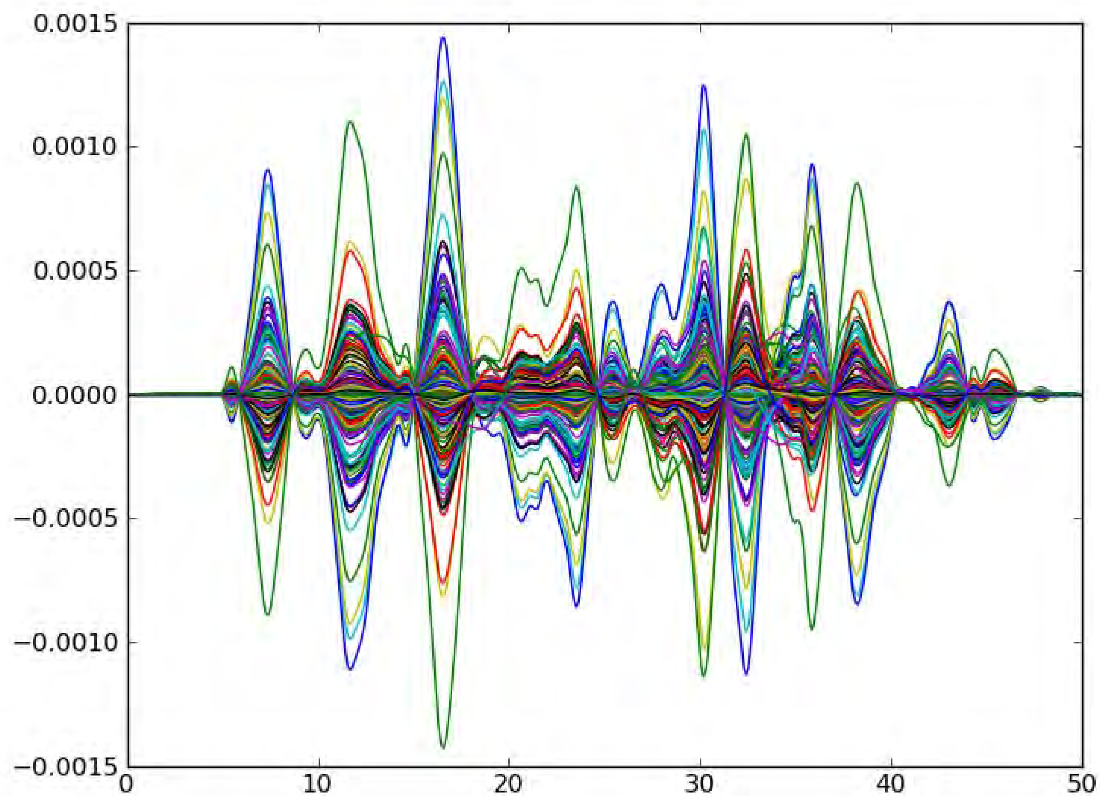


Vulnerability Curves (vs earthquake magnitude)



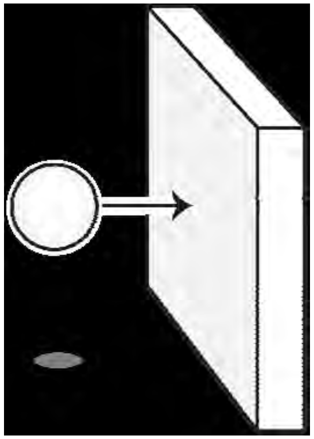
Identification of the weakest elements

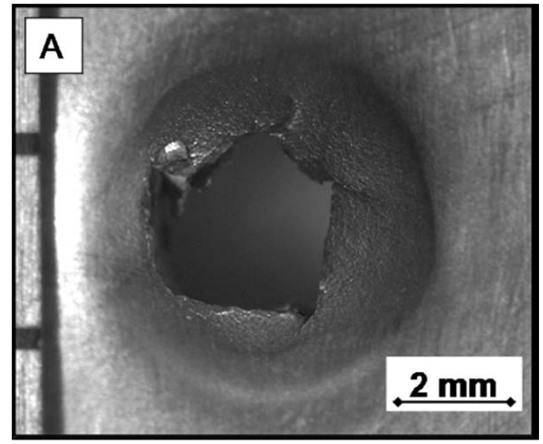




H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz. **Optimal Uncertainty Quantification**. SIAM Review, 55(2):271–345, 2013.

Caltech Small Particle Hypervelocity Impact Range





$$(h, \alpha, v) \xrightarrow{\quad \mathbf{G} \quad} G(h, \alpha, v)$$

Plate thickness

Plate Obliquity

Projectile velocity

Perforation area

We want to certify that

$$\boxed{\mathbb{P}[G = 0] \leq \epsilon}$$

Problem We don't know G nor $\mathbb{P}$.

What do we know?

Plate thickness $h \in \mathcal{X}_1 := [1.524, 2.667]\,\mathrm{mm},$

Plate Obliquity $\alpha \in \mathcal{X}_2 := [0, \frac{\pi}{6}],$

Projectile velocity $v \in \mathcal{X}_3 := [2.1, 2.8]\,\mathrm{km}\cdot\mathrm{s}^{-1}.$

Thickness, obliquity, velocity: independent random variables

Mean perforation area: in between 5.5 and 7.5 mm^2

$$m_1 \le \mathbb{E}[G] \le m_2$$

Bounds on the sensitivity of the response function w.r. to each variable

$$\mathrm{Osc}_i\, G \le D_i$$

$$\mathrm{Osc}_i\, G := \sup\left\{ |G(x) - G(x')| \;\middle|\; x_j = x'_j \text{ for } j \neq i \right\}$$

We only know

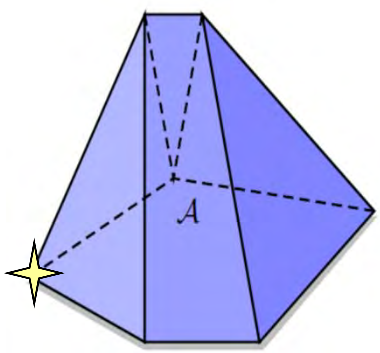
$$\boxed{(G, \mathbb{P}) \in \mathcal{A}}$$

$$\mathcal{A} := \left\{ (f, \mu) \,\middle|\, \begin{array}{c} \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ m_1 \leq \mathbb{E}_\mu[f] \leq m_2 \\ \mathrm{Osc}_i\, f \leq D_i \end{array} \right\}$$

Worst case bound

$$\mathbb{P}[G \leq 0] \leq \mathcal{U}(\mathcal{A}) := \sup_{(f,\mu) \in \mathcal{A}} \mu[f(X) \leq 0]$$

Reduction calculus



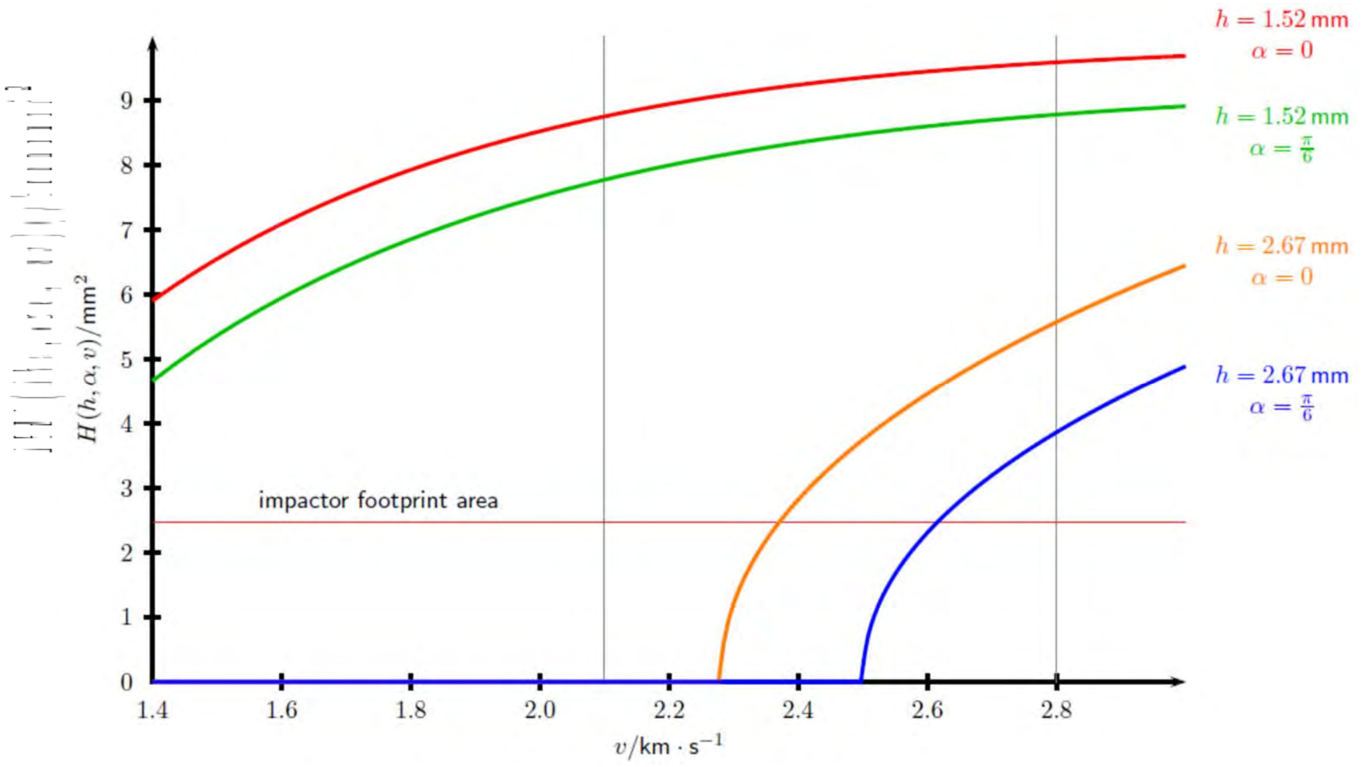
$$\mathcal{U}(\mathcal{A}) = 43.7\%$$

What if we know the response function?

What if we know $G = H$?

Deterministic surrogate model for the perforation area (in mm^2)

$$\boxed{H(h,\alpha,v) = K\left(\frac{h}{D_\mathrm{p}}\right)^{p} (\cos\alpha)^{u} \left(\tanh\left(\frac{v}{v_\mathrm{bl}} - 1\right)\right)_{+}^{m},}$$



Optimal bound on the probability of non perforation

$$\mathcal{U}(\mathcal{A}) := \sup_{(f,\mu)\in\mathcal{A}} \mu[f(X) \leq 0]$$

$$\mathcal{A} := \left\{ (f,\mu) \,\middle|\, \begin{array}{c} \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ 5.5\, mm^2 \leq \mathbb{E}_\mu[f] \leq 7.5\, mm^2, \\ f = H \end{array} \right\}$$

Application of the reduction calculus

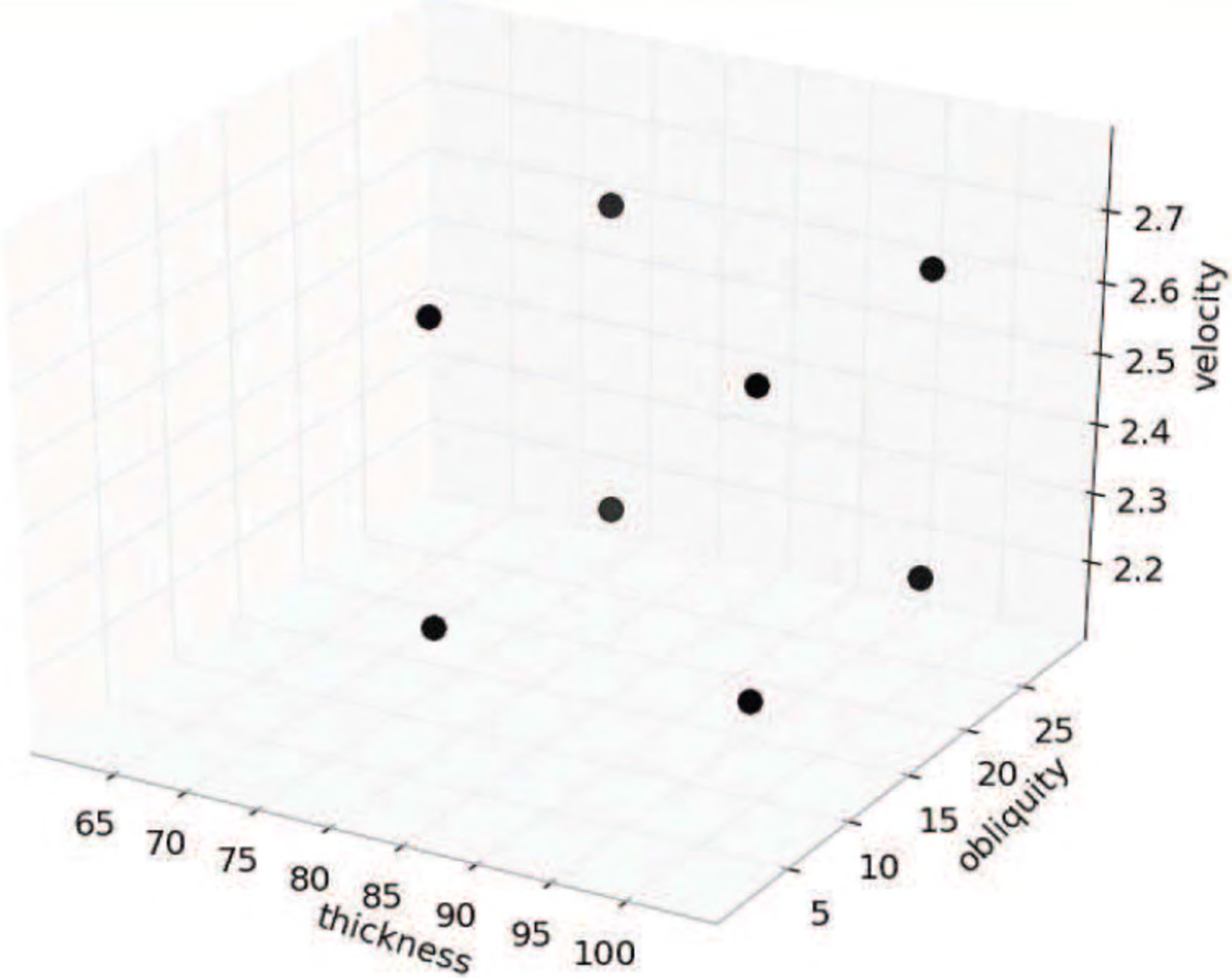
$$\mathcal{U}(\mathcal{A}) = \mathcal{U}(\mathcal{A}_\Delta)$$

$$\mathcal{A}_\Delta := \{(f,\mu) \in \mathcal{A} | \mu_k \text{ has support at only 2 points}\}$$

The measure of probability can be reduced to the tensorization of 2 Dirac masses on thickness, obliquity and velocity

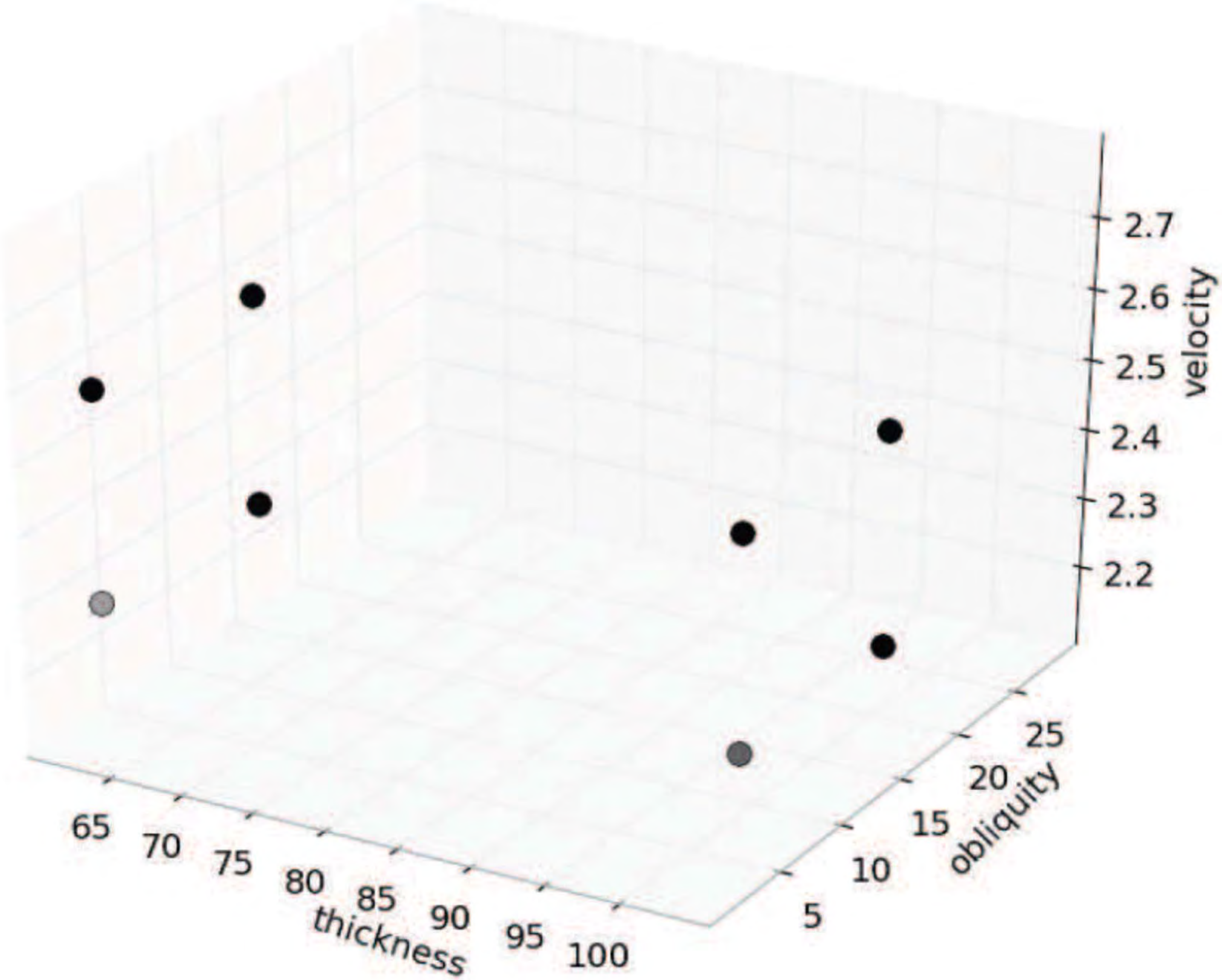
$$\mathcal{U}(\mathcal{A}) \overset{\text{num}}{=} 37.9\%$$

The optimization variables can be reduced to the tensorization of 2 Dirac masses on thickness, obliquity and velocity



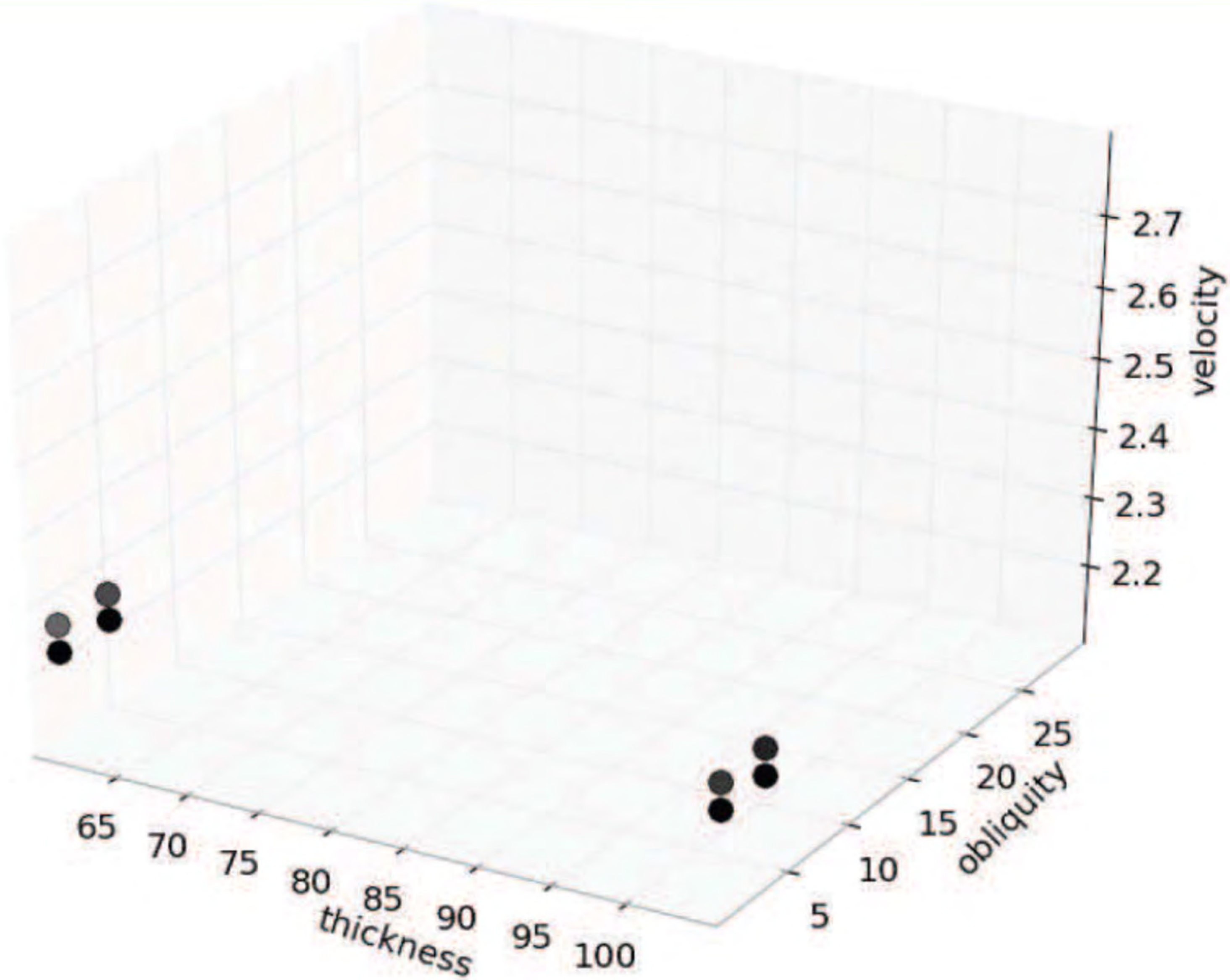
Support Points at iteration 0

Numerical optimization



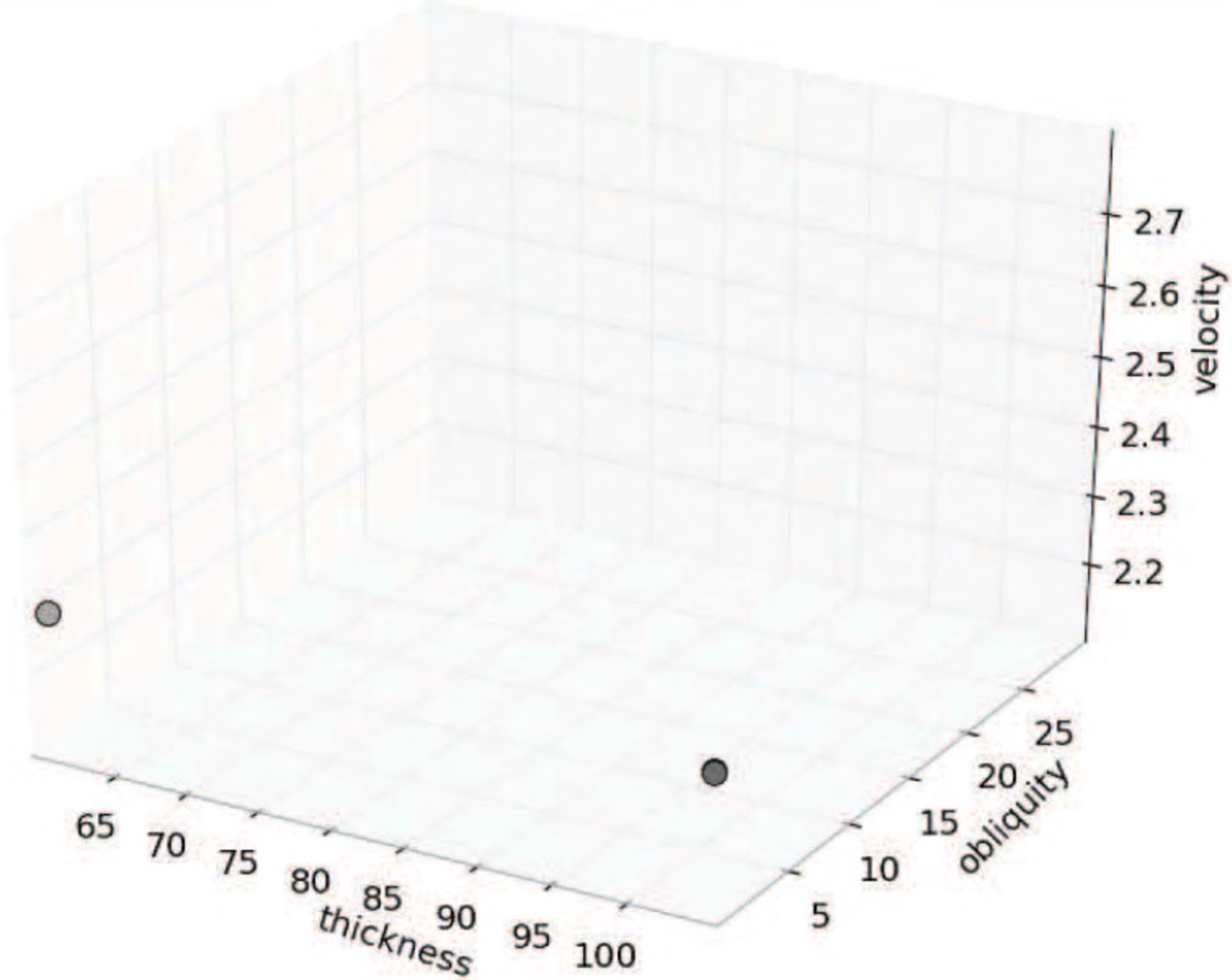
Support Points at iteration 150

Numerical optimization



Support Points at iteration 200

Velocity and obliquity marginals each collapse to a single Dirac mass. The plate thickness marginal collapses to have support on the extremes of its range.



Iteration 1000

Probability non-perforation maximized by distribution supported on minimal, not maximal, impact obliquity. Dirac on velocity at a non extreme value.

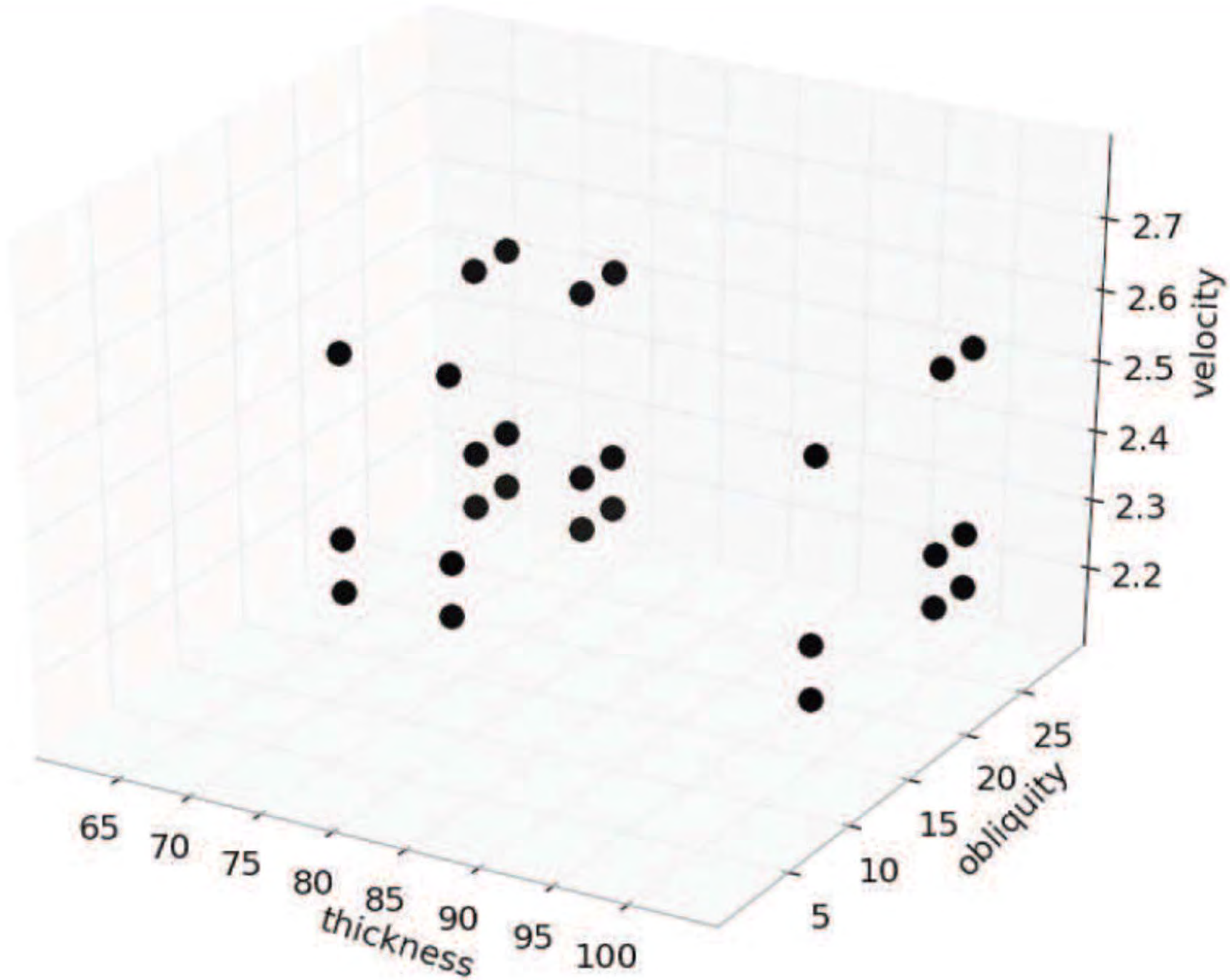
Important observations

Extremizers are singular

They identify key players
i.e. vulnerabilities of the physical system

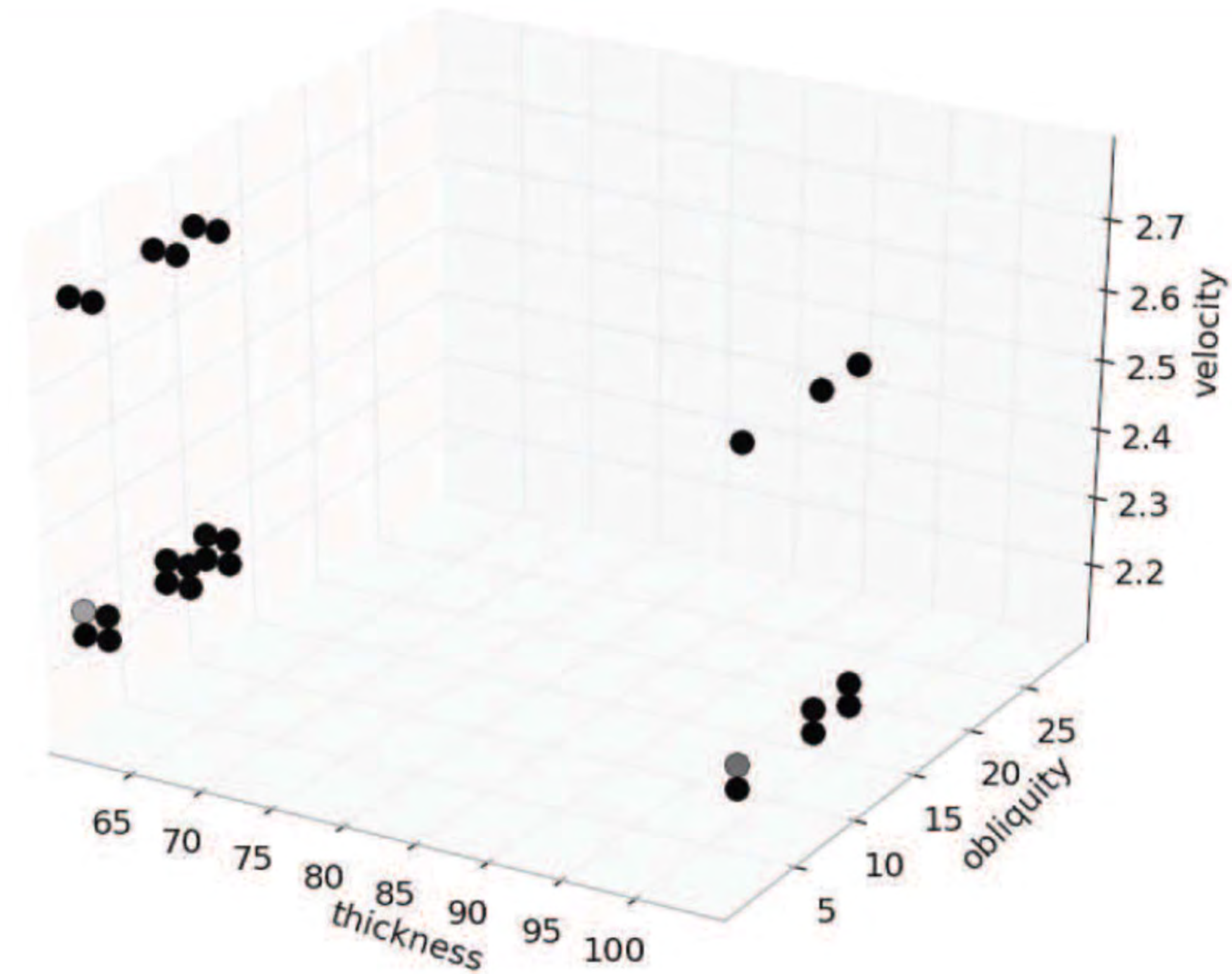
Extremizers are attractors

Initialization with 3 support points per marginal



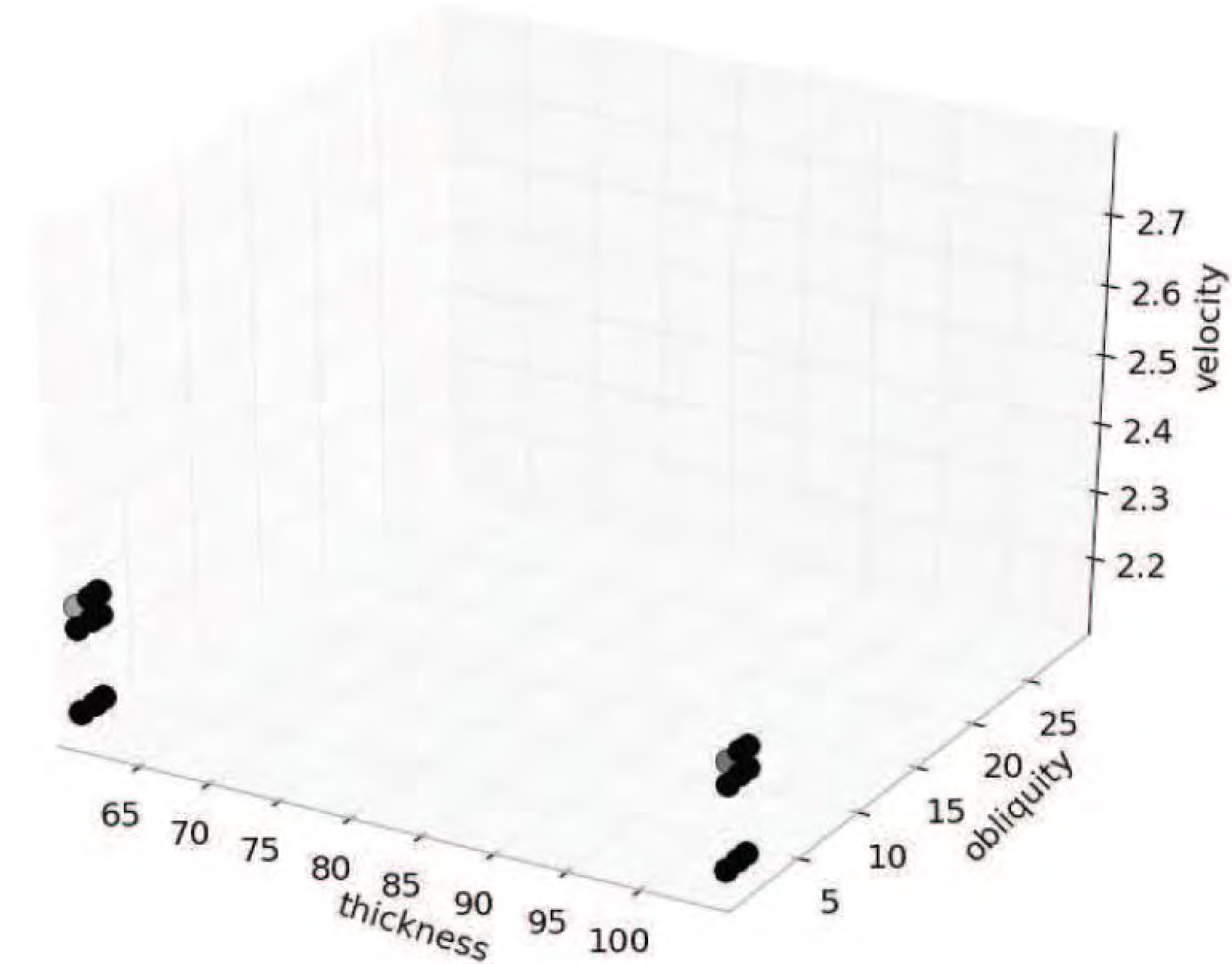
Support Points at iteration 0

Initialization with 3 support points per marginal



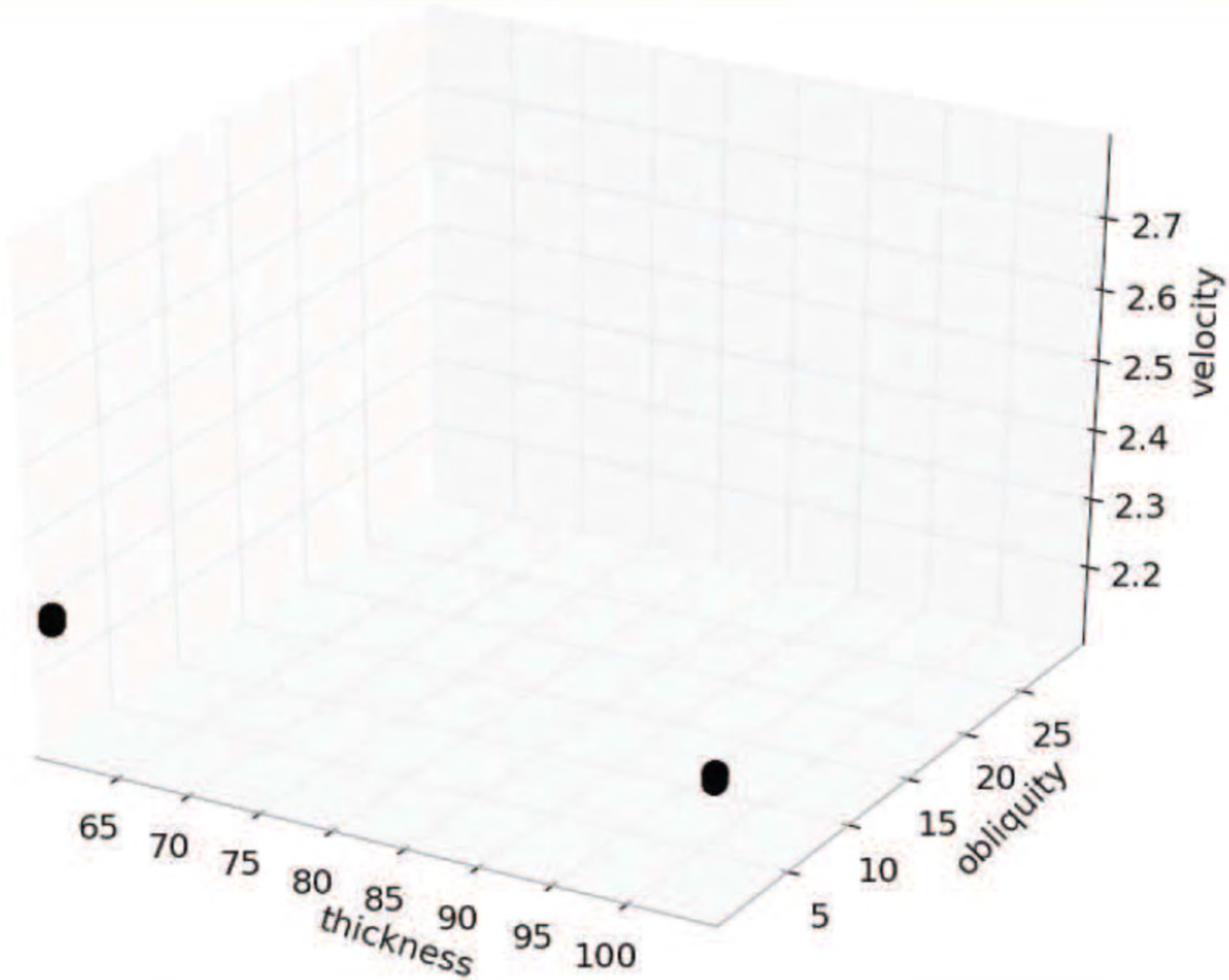
Support Points at iteration 500

Initialization with 3 support points per marginal



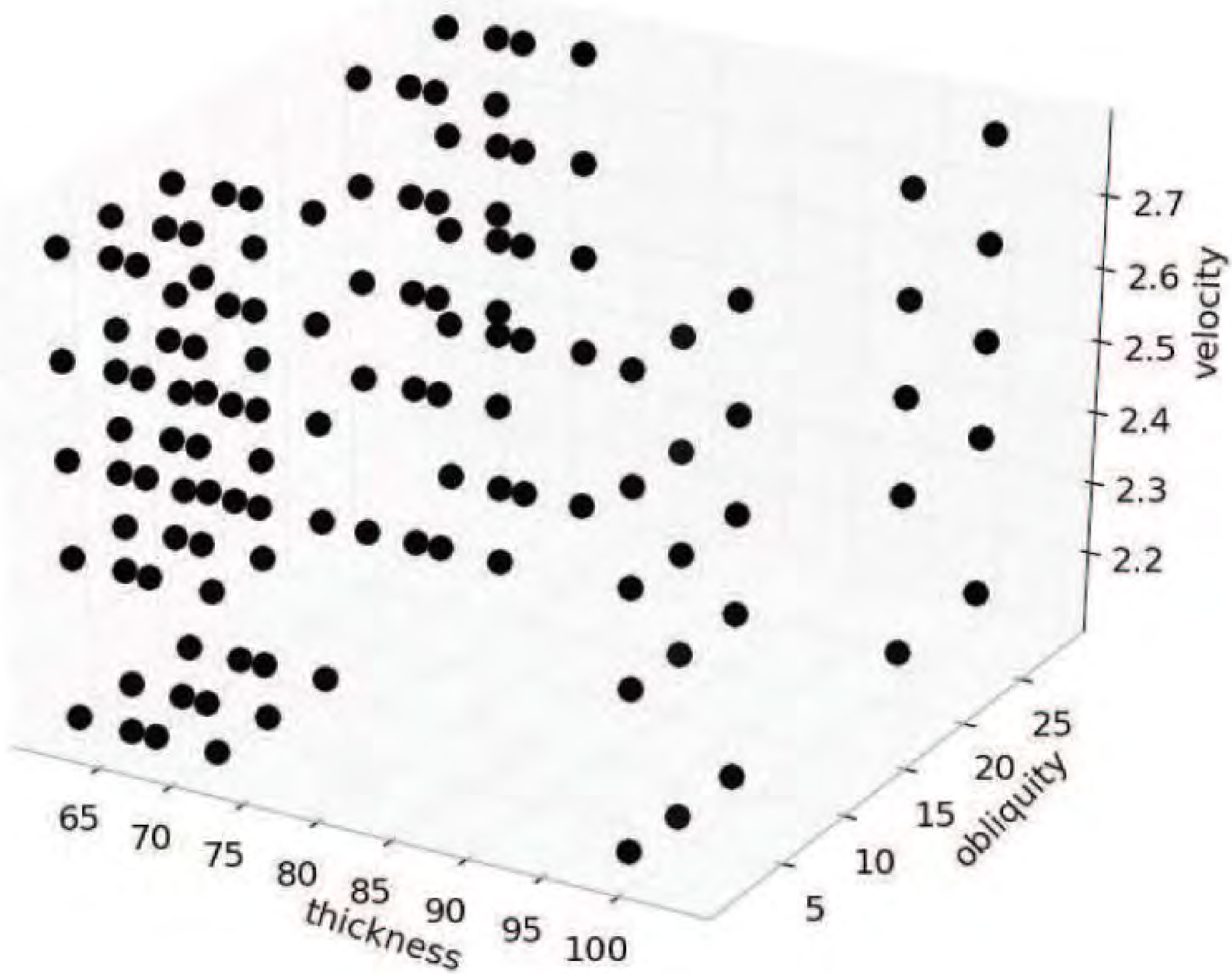
Support Points at iteration 1000

Initialization with 3 support points per marginal



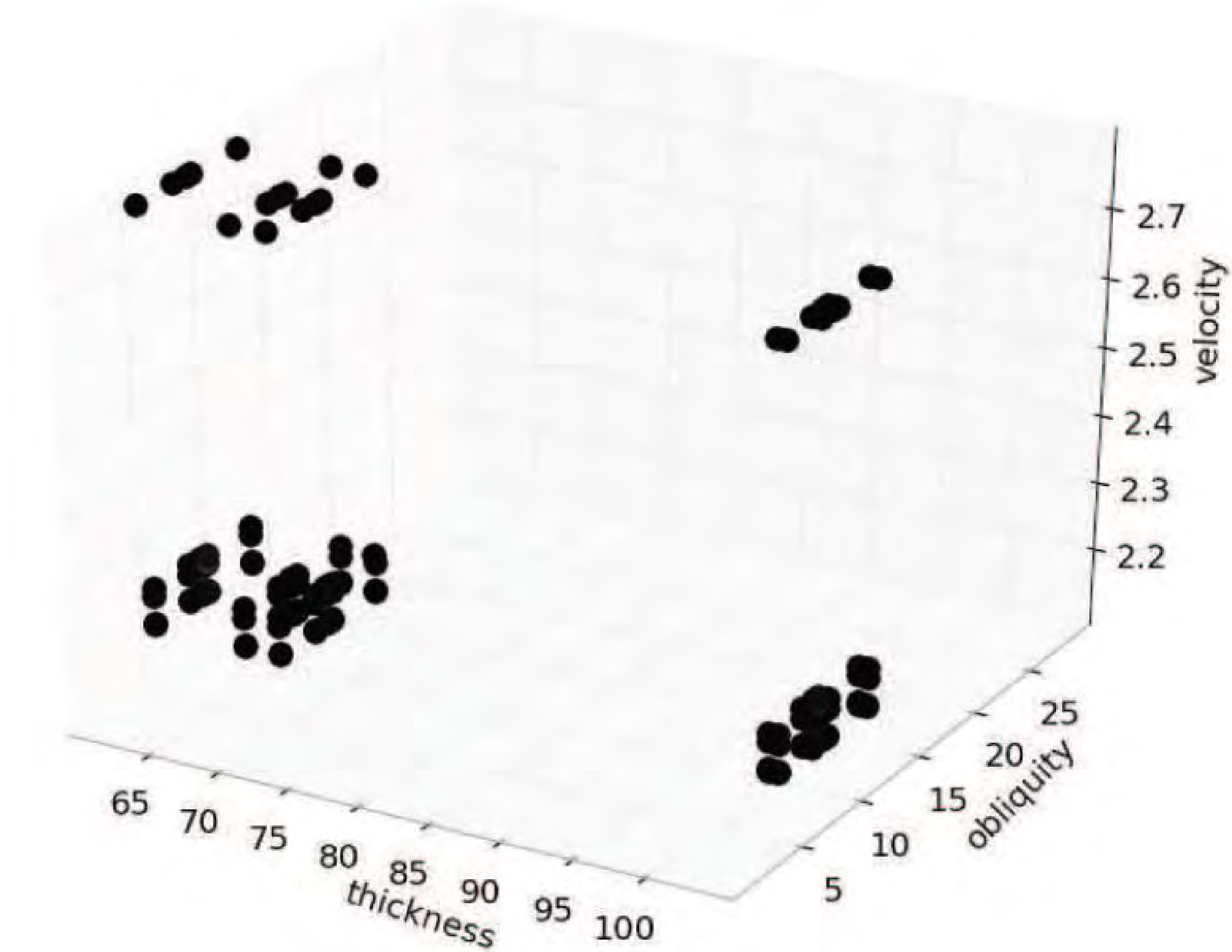
Support Points at iteration 2155

Initialization with 5 support points per marginal



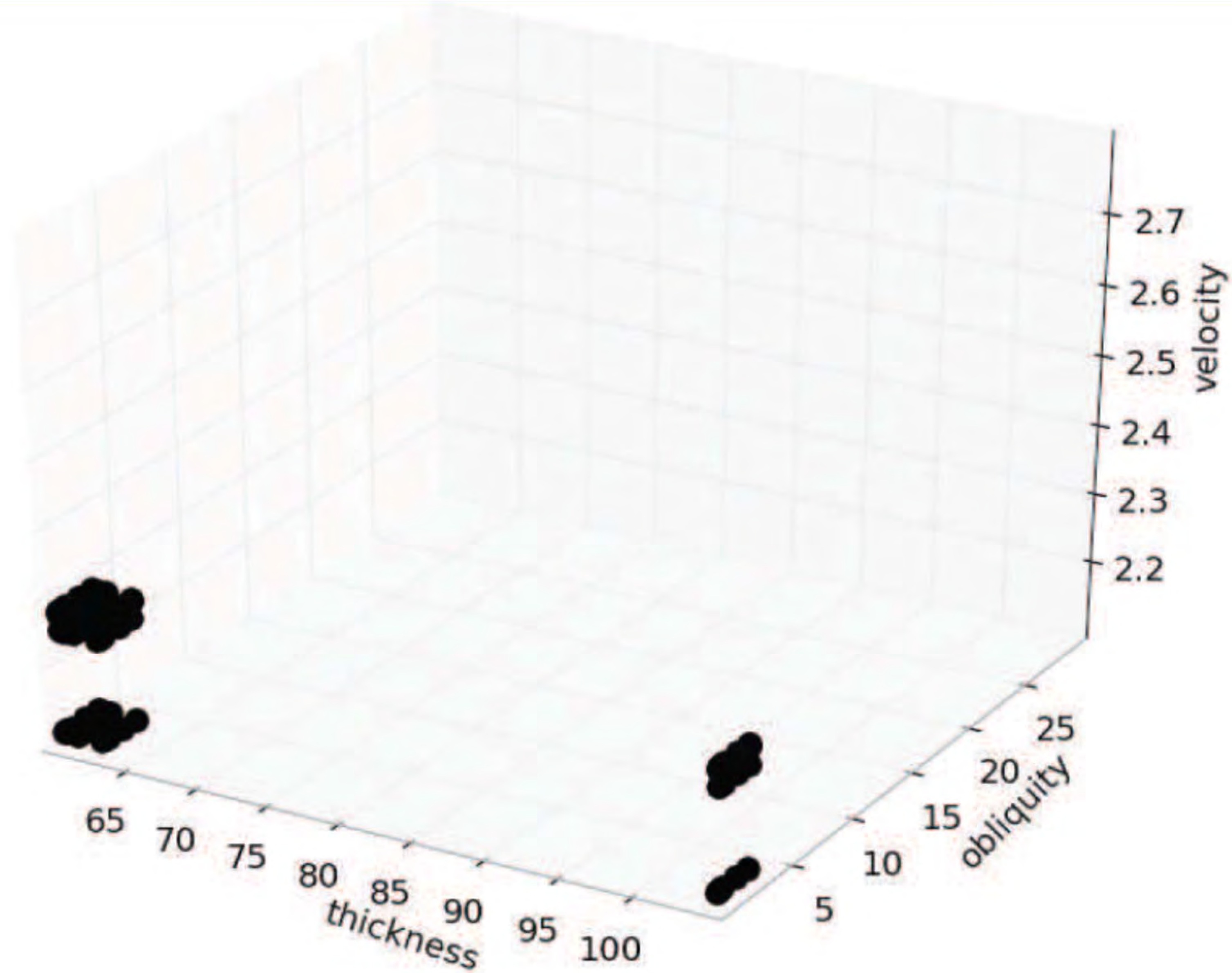
Support Points at iteration 0

Initialization with 5 support points per marginal



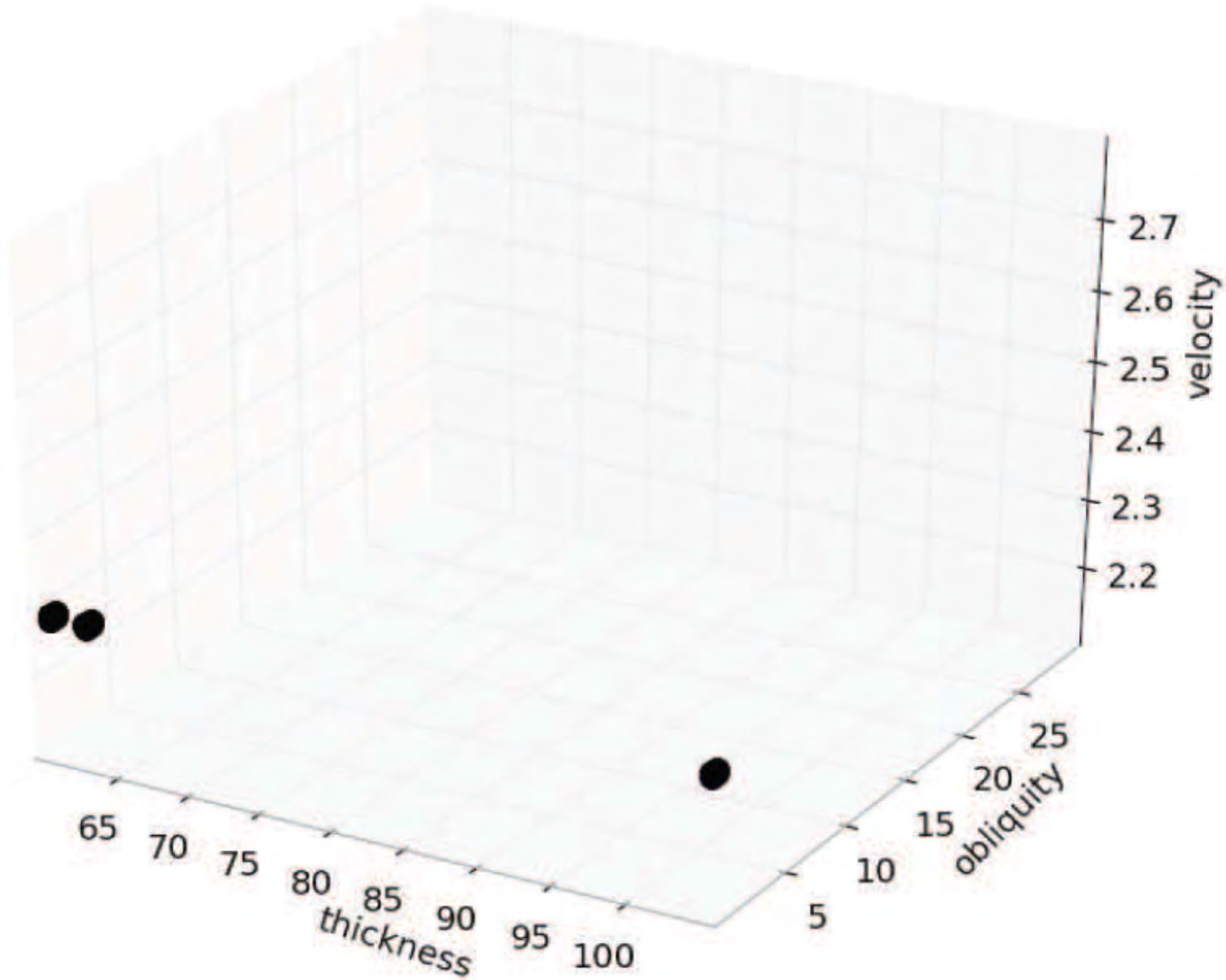
Support Points at iteration 1000

Initialization with 5 support points per marginal



Support Points at iteration 3000

Initialization with 5 support points per marginal



Support Points at iteration 7100

Unknown response function G + Legacy data

Objective

We want least upper bound on $\mathbb{P}[G(h,\alpha,v) \leq \theta]$

Constraints on input variables

$$h, \alpha, v\colon \text{ independent}$$

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

Constraint on the mean perf. area

$$\boxed{\mathbb{E}[G(h,\alpha,v)] \geq 11.0\,\text{mm}^2}$$

Modified Lipschitz continuity constraints on response function

$$|G(h,\alpha,v) - G(h',\alpha',v')| \leq d_L((h,\alpha,v),(h',\alpha',v')) + T,$$

$$d_L((h,\alpha,v),(h',\alpha',v')) := L_h|h-h'| + L_\alpha|\alpha-\alpha'| + L_v|v-v'|$$

$$L := (L_h, L_\alpha, L_v), \qquad T := 1.0\,\text{mm}^2,$$

$$L_h := 175.0\,\text{mm}^2/\text{in}, \quad L_\alpha := 0.075\,\text{mm}^2/\text{deg}, \quad L_v := 0.1\,\text{mm}^2/(\text{m/s}).$$

Legacy Data

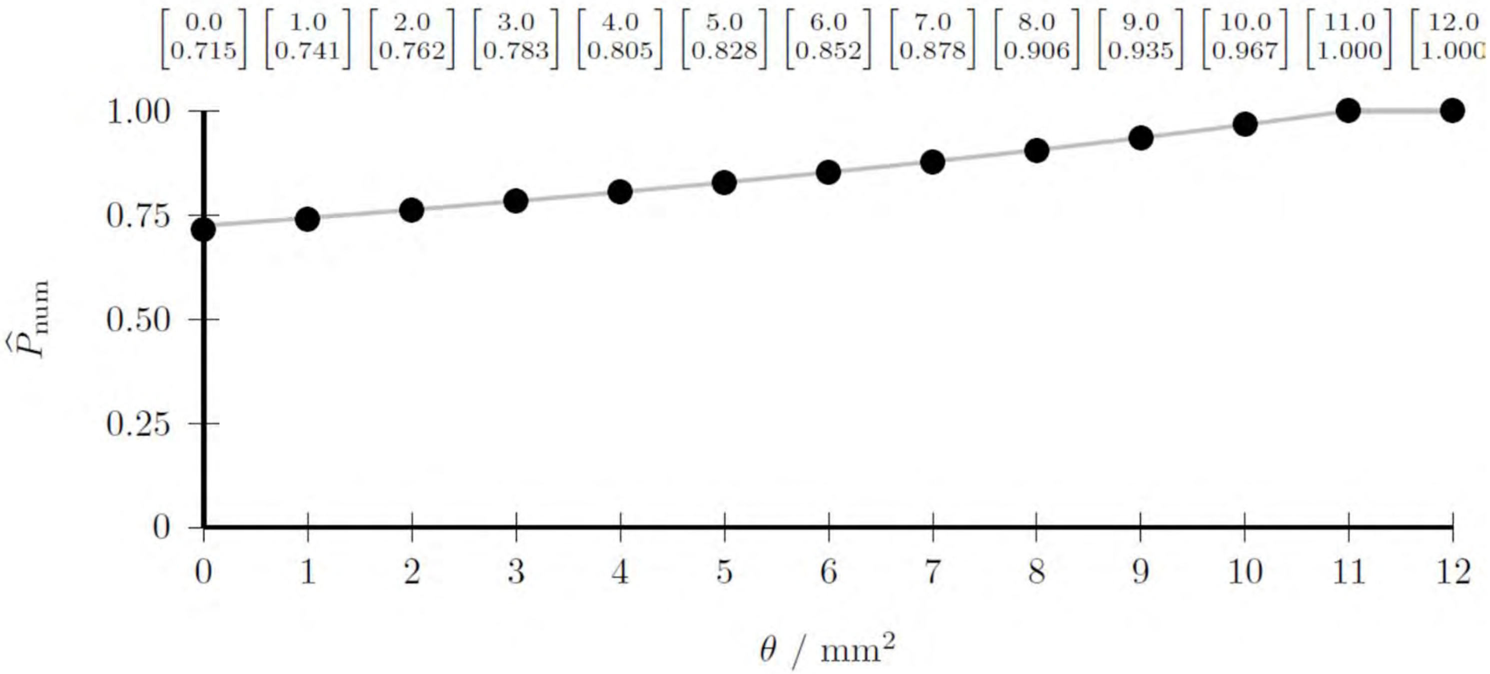
32 data points

(steel-on-aluminium shots A48–A81) from summer 2010 at Caltech's SPHIR facility:

These constrain the value of G at 32 points

T. J. Sullivan, M. McKerns, D. Meyer, F. Theil, H. Owhadi, and M. Ortiz. Optimal uncertainty quantification for legacy data observations of Lipschitz functions. *ESAIM Math. Model. Numer. Anal.*, 47(6):1657–1689, 2013.

ID	h (inches)	α (degrees)	v (m/s)	$G(h, \alpha, v)$ (mm^2)
A48	0.062	0.0	2288.0	7.73
A49	0.125	30.0	2840.0	13.38
A50	0.125	0.0	2556.0	11.83
A51	0.062	30.0	2329.0	6.31
A52	0.062	0.0	2363.0	7.78
A53	0.125	0.0	2326.0	9.26
A54	0.125	30.0	3235.0	15.98
A55	0.062	0.0	2686.0	9.86
A56	0.062	30.0	2728.0	11.35
A57	0.062	30.0	2627.0	12.09
A58	0.125	30.0	2531.0	11.24
A60	0.125	0.0	2363.0	9.93
A61	0.062	0.0	2707.0	9.96
A62	0.062	30.0	2756.0	11.07
A63	0.062	0.0	2614.0	9.02
A64	0.125	0.0	2439.0	10.52
A65	0.062	0.0	2485.0	8.56
A66	0.125	0.0	2607.0	12.46
A67	0.125	30.0	3036.0	15.36
A68	0.125	30.0	2325.0	8.15
A69	0.062	30.0	2702.0	10.81
A70	0.062	30.0	2473.0	9.52
A71	0.121	30.0	2520.0	9.47
A72	0.121	0.0	2439.0	10.19
A73	0.121	30.0	2366.0	9.42
A74	0.121	30.0	2402.0	8.68
A75	0.062	30.0	2413.0	9.19
A77	0.062	30.0	2756.0	11.32
A78	0.121	30.0	2432.0	10.00
A79	0.062	30.0	2393.0	9.29
A80	0.121	30.0	2479.0	9.53
A81	0.060	30.0	2356.0	8.27



Least upper bound on $\mathbb{P}[G(h, \alpha, v) \leq \theta]$

The numerical results demonstrate agreement with the Markov bound

$$\mathbb{P}[G(h, \alpha, v) \leq \theta] \leq \frac{M - m}{M - \theta},$$

$$M := \sup_{(h,\alpha,v)\in\mathcal{X}} \inf_{z\in\mathcal{O}} \left(G(z) + d_L(z, (h, \alpha, v)) + T\right) \approx 39.895\,\mathrm{mm}^2$$

Only 2 data points out of 32 carry information about the optimal bound

Legacy Data

32 data points

(steel-on-aluminium shots A48–A81) from summer 2010 at Caltech's SPHIR facility:

Only A54 and A67 carry information

The other 30 data points carry no information about least upper bound and could have be ignored.

T. J. Sullivan, M. McKerns, D. Meyer, F. Theil, H. Owhadi, and M. Ortiz. Optimal uncertainty quantification for legacy data observations of Lipschitz functions. *ESAIM Math. Model. Numer. Anal.*, 47(6):1657–1689, 2013.

ID	h (inches)	α (degrees)	v (m/s)	$G(h,\alpha,v)$ (mm^2)
A48	0.062	0.0	2288.0	7.73
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A51	0.062	30.0	2329.0	6.31
A52	0.062	0.0	2363.0	7.78
A53	0.125	0.0	2326.0	9.26
A54	0.125	30.0	3235.0	15.98
A55	0.062	0.0	2686.0	9.86
A56	0.062	30.0	2728.0	11.35
A57	0.062	30.0	2627.0	12.09
A58	0.125	30.0	2531.0	11.24
A60	0.125	0.0	2363.0	9.93
A61	0.062	0.0	2707.0	9.96
A62	0.062	30.0	2756.0	11.07
A63	0.062	0.0	2614.0	9.02
A64	0.125	0.0	2439.0	10.52
A65	0.062	0.0	2485.0	8.56
A66	0.125	0.0	2607.0	12.46
A67	0.125	30.0	3036.0	15.36
A68	0.125	30.0	2325.0	8.15
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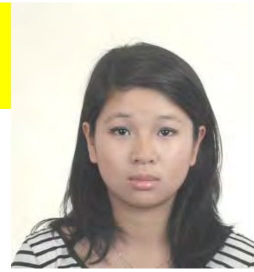
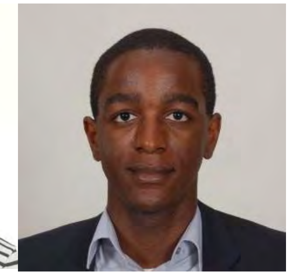
A71	0.121	30.0	2520.0	9.47
A72	0.121	0.0	2439.0	10.19
A73	0.121	30.0	2366.0	9.42
A74	0.121	30.0	2402.0	8.68
A75	0.062	30.0	2413.0	9.19
A77	0.062	30.0	2756.0	11.32
A78	0.121	30.0	2432.0	10.00
A79	0.062	30.0	2393.0	9.29
A80	0.121	30.0	2479.0	9.53
A81	0.060	30.0	2356.0	8.27

What if we have model uncertainty?





What do we want?

Least upper bound on $\mathbb{P}[G(h,v) \leq \theta]$

What do we know?

Numerical model $(h,v) \to F(h,v)$

59 noisy data/experimental points $G(h_i, v_i)$

Expert judgement (+data points):

$\mathbb{E}[G(h,v)] \geq 12\,\mathrm{mm}^2$

h and v are independent random variables

$(h,v) \in [0.5, 3.0]\mathrm{mm} \times [4.5, 7.0]\mathrm{km/s}$

PSAAP numerical model

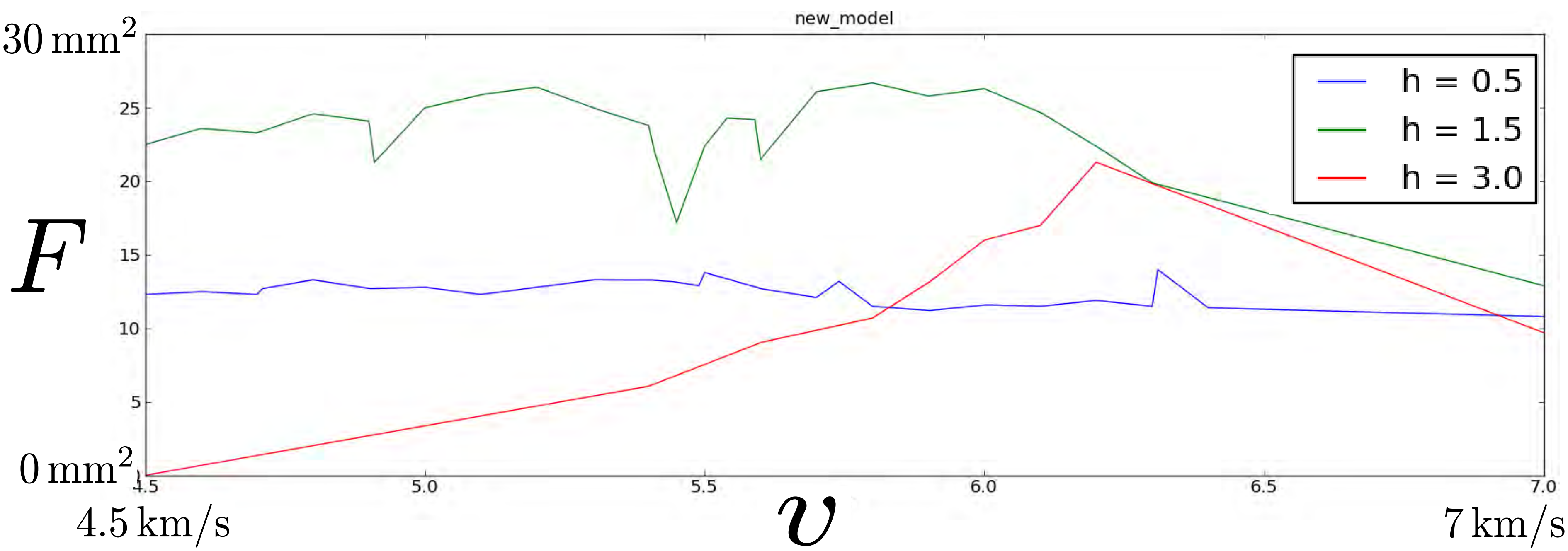
Plate Obliquity=0

$$(h, v) \xrightarrow{\mathbf{F}} F(h, v)$$

Plate thickness

Projectile velocity

Perforation area



59 data/experimental points

Plate Obliquity=0

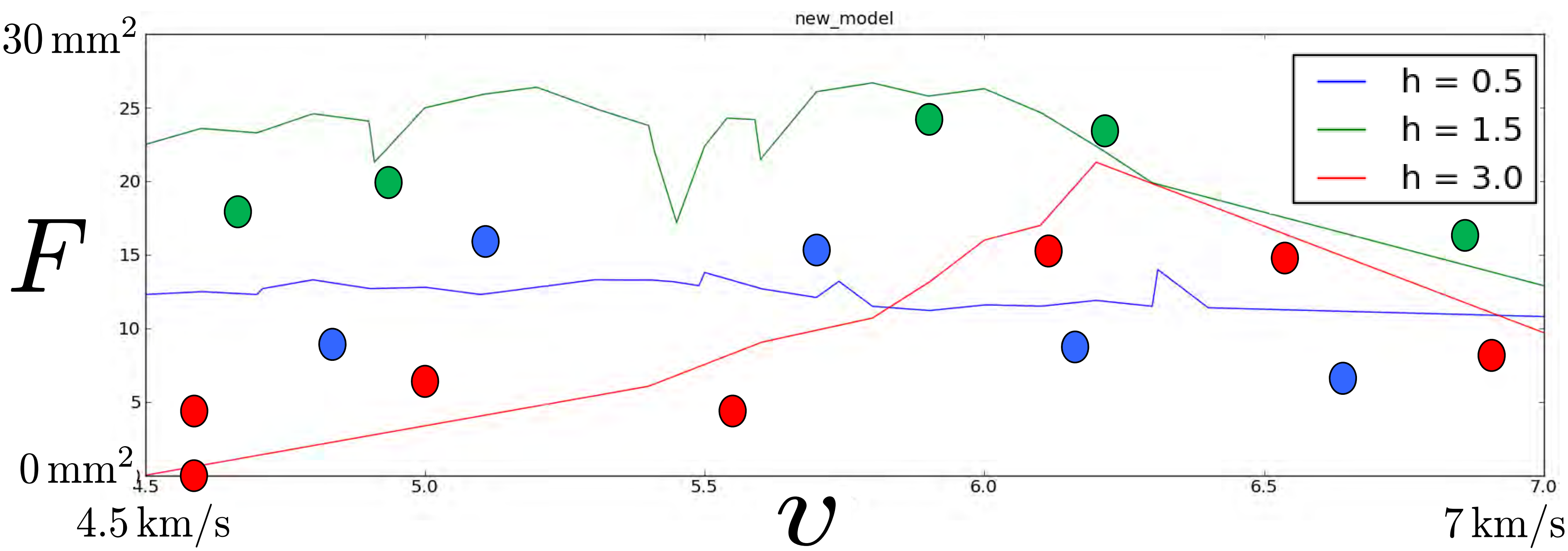
G

$$(h, v) \longrightarrow G(h, v)$$

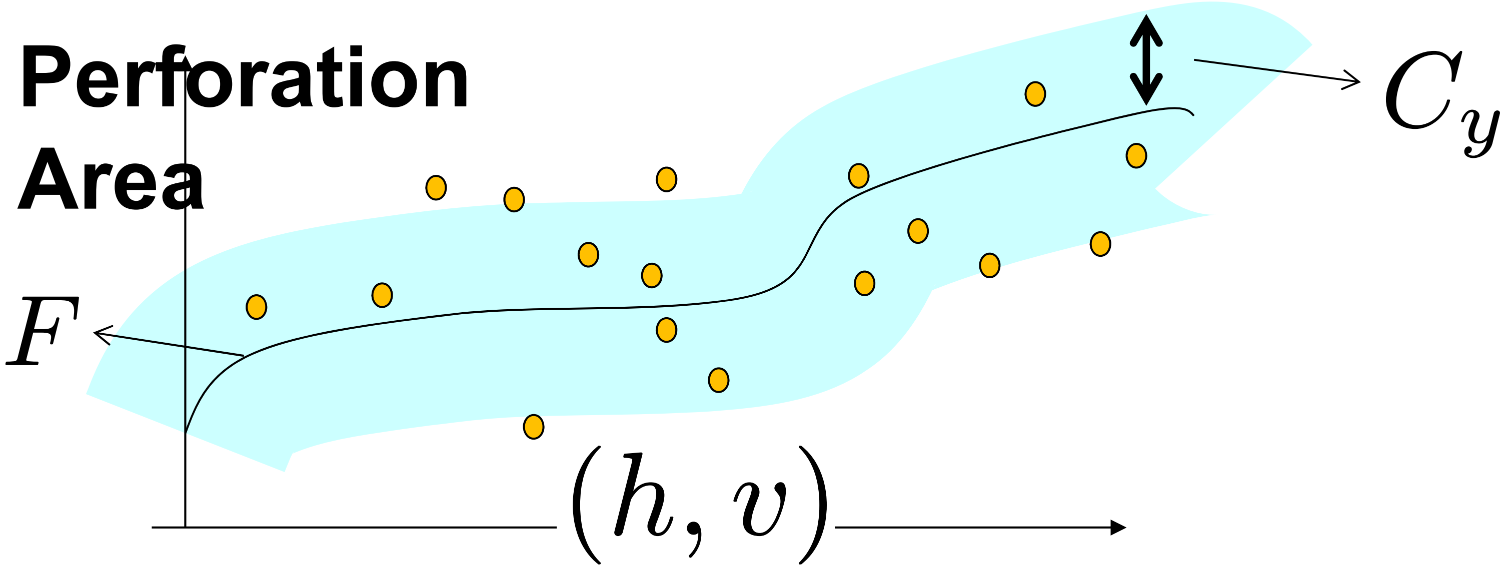
Plate thickness

Projectile velocity

Perforation area



Confidence sausage around the model



With probability $\boxed{p_1}$ we have

$$\mathbb{P}[|G - F| \leq \boxed{C_y}] \geq \boxed{p_2(p_1, C_y, data)}$$

Cy	at prob. 0.78	at prob. 0.85	at prob. 0.94
3	0.3991	0.3822	0.3483
5	0.5325	0.5155	0.4816
7	0.6325	0.6155	0.5816
9	0.8325	0.8155	0.7816

Admissible set

$$\mathcal{A} := \left\{ (g,\mu) \;\middle|\; \begin{array}{c} g\colon \mathcal{X} \to \mathcal{Y}, \\ \mu = \mu_h \otimes \mu_v, \\ \mathcal{X} := [0.5, 3.0]\mathrm{mm} \times [4.5, 7.0]\mathrm{km/s}, \\ \mathbb{E}_\mu[g(h,v,\alpha)] \geq 12.0\mathrm{mm}^2, \\ \|g - F\|_\infty \leq C_y \end{array} \right\}$$

Confidence sausage

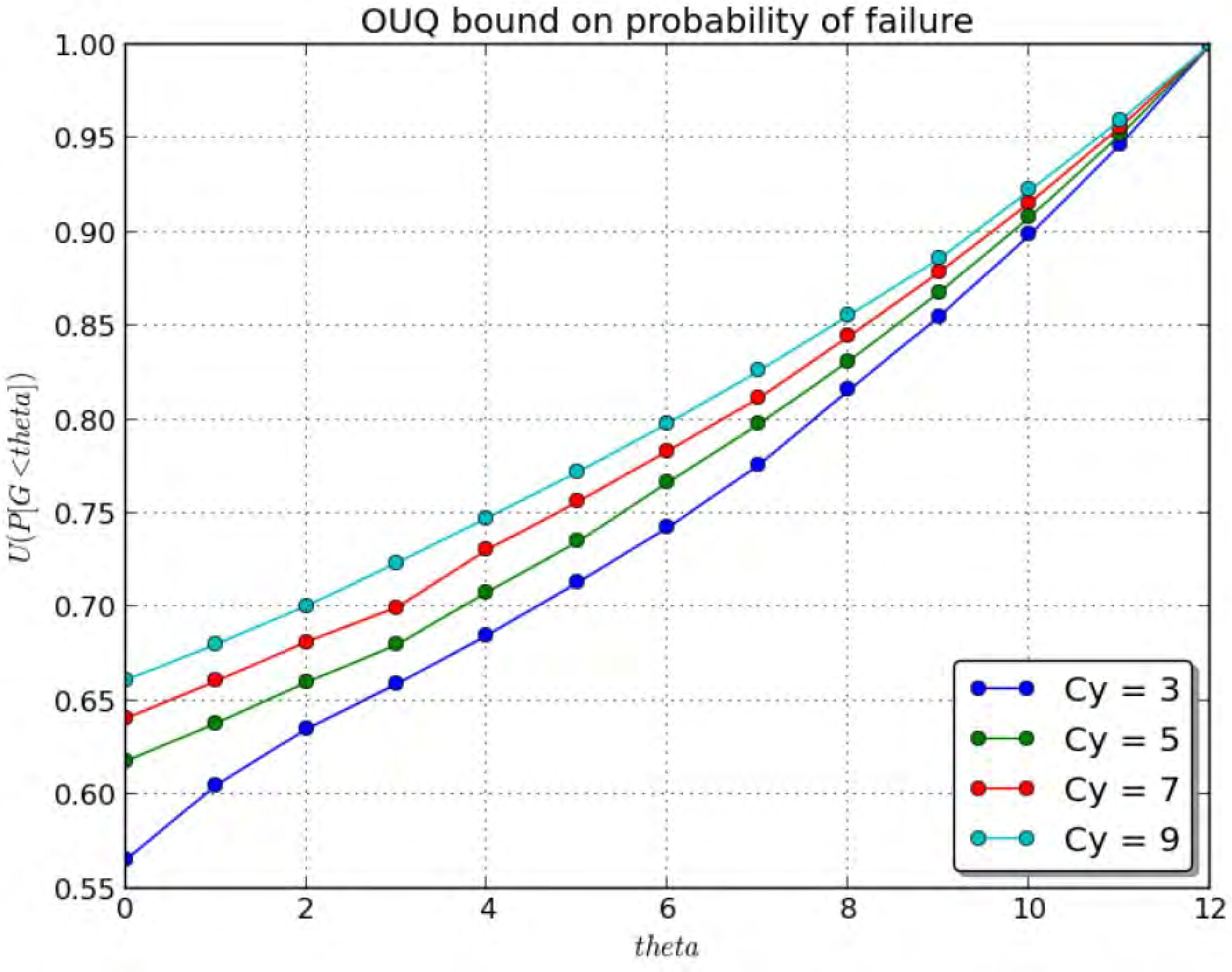
With probability $\boxed{p_1}$ we have

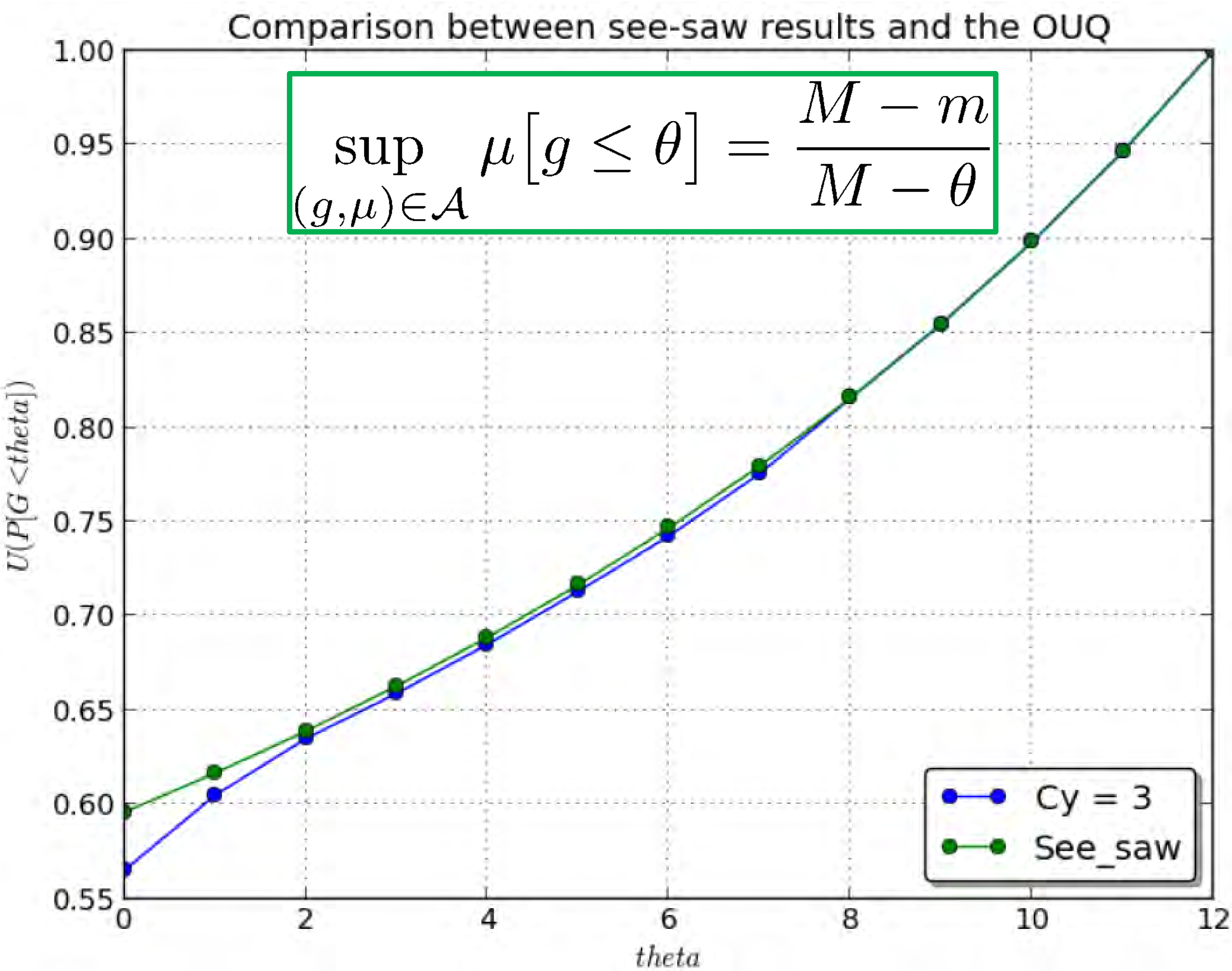
$$\mathbb{P}[|G - F| \leq \boxed{C_y}] \geq \boxed{p_2(p_1, C_y, data)}$$

For $C_y = \boxed{5}$ and $p_1 = \boxed{0.85}$ we have $p_2 = \boxed{0.51}$

What we compute

$$\sup_{(g,\mu)\in\mathcal{A}} \mu[g \leq \theta]$$


OUQ bound on probability of failure
$U(P[G < theta])$
$theta$
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0
2
4
6
8
10
12
Cy = 3
Cy = 5
Cy = 7
Cy = 9

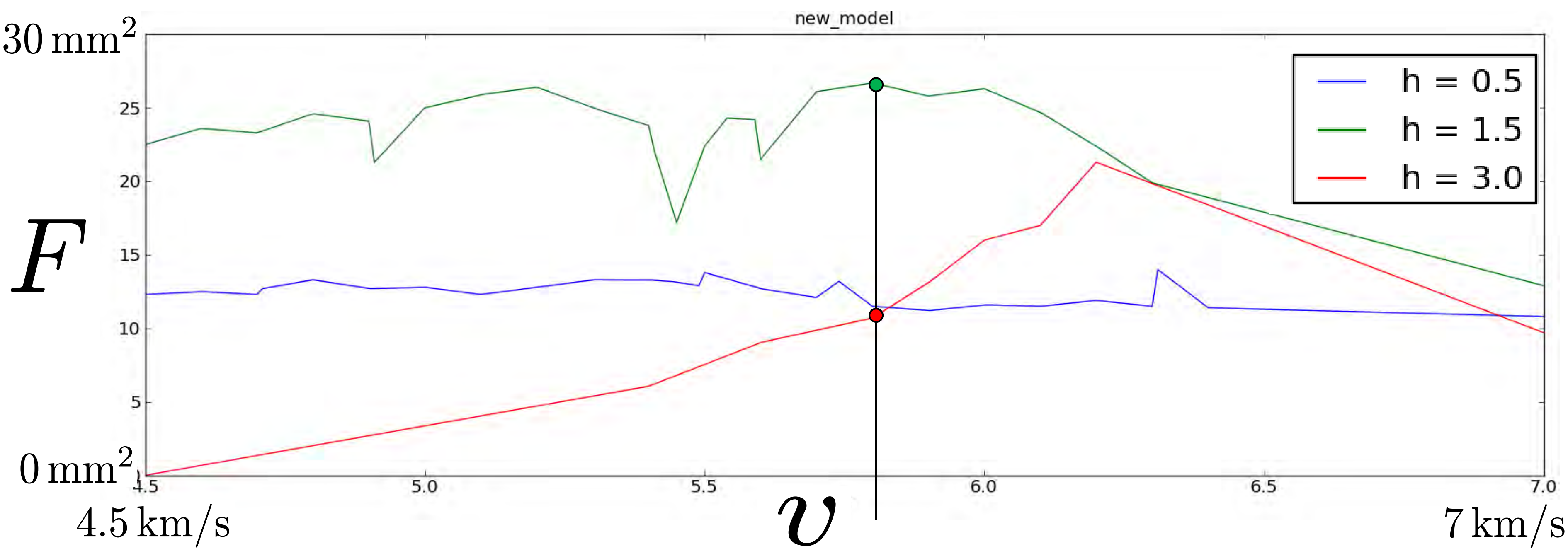

Comparison between see-saw results and the OUQ
$$\sup_{(g,\mu)\in\mathcal{A}} \mu[g \le \theta] = \frac{M-m}{M-\theta}$$
U(P[G<theta])
theta
Cy = 3
See_saw
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0
2
4
6
8
10
12

$$\boxed{\sup_{(g,\mu)\in\mathcal{A}} \mu[g \leq \theta] = \frac{M-m}{M-\theta}}$$

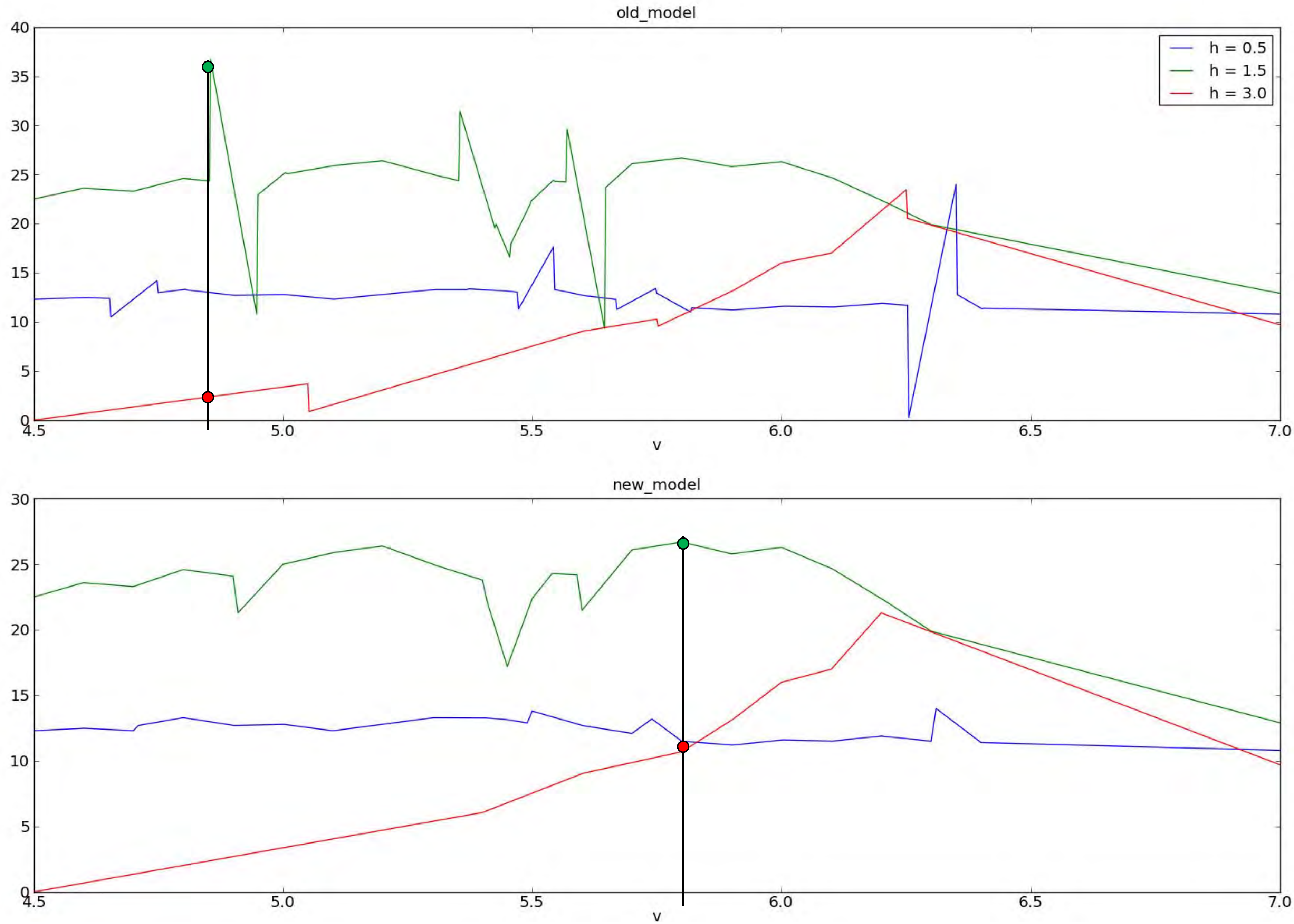
For $C_y = 3$ and $\theta \geq 8$ the model impacts the least upper bound only through its maximum value M

At the extremum

μ_v collapses to a single mass of Dirac



The extremizers led to the identification of a bug in an old model



Caltech PSAAP Center UQ analysis

L. J. Lucas, H. Owhadi, and M. Ortiz. Rigorous verification, validation, uncertainty quantification and certification through concentration-of-measure inequalities. *Comput. Methods Appl. Mech. Engrg.*, 197(51-52):4591–4609, 2008.

M. M. McKerns, L. Strand, T. J. Sullivan, A. Fang, and M. A. G. Aivazis. Building a framework for predictive science. In *Proceedings of the 10th Python in Science Conference (SciPy 2011)*, 2011.

P.-H. T. Kamga, B. Li, M. McKerns, L. H. Nguyen, M. Ortiz, H. Owhadi, and T. J. Sullivan. Optimal uncertainty quantification with model uncertainty and legacy data. *Journal of the Mechanics and Physics of Solids*, 72:1–19, 2014

A. A. Kidane, A. Lashgari, B. Li, M. McKerns, M. Ortiz, H. Owhadi, G. Ravichandran, M. Stalzer, and T. J. Sullivan. Rigorous model-based uncertainty quantification with application to terminal ballistics. Part I: Systems with controllable inputs and small scatter. *Journal of the Mechanics and Physics of Solids*, 60(5):983–1001, 2012.

T. J. Sullivan, M. McKerns, D. Meyer, F. Theil, H. Owhadi, and M. Ortiz. **Optimal uncertainty quantification for legacy data observations of Lipschitz functions.** *ESAIM Math. Model. Numer. Anal.*, 47(6):1657–1689, 2013.

H. Owhadi, C. Scovel, T. J. Sullivan, M. McKerns, and M. Ortiz. **Optimal Uncertainty Quantification**. *SIAM Review*, 55(2):271–345, 2013.

Reduced numerical optimization problems solved using

- **mystic: http://trac.mystic.cacr.caltech.edu/project/mystic**
  - **a highly-configurable optimization framework**
- **pathos: http://trac.mystic.cacr.caltech.edu/project/pathos**
  - **a distributed parallel graph execution framework providing a high-level programmatic interface to heterogeneous computing**

Mike McKerns

Important observations

In presence of incomplete information on the distribution of input variables the dependence of the least upper bound on the accuracy of the model is very weak

We need to extract as much information as possible from the sample/experimental data on the underlying distributions

How do we reason with the worst in presence of data sampled from an unknown distribution?

Quantity of Interest $\Phi(\mu^\dagger) = \mu^\dagger[X \geq a]$

$\mu^\dagger$: Unknown or partially known measure of probability on $\mathbb{R}$

You know $\mu^\dagger \in \mathcal{A}$

You observe $d = (d_1, \ldots, d_n) \in \mathbb{R}^n$

n i.i.d samples from $\mu^\dagger$

Problem:

Find the best estimate of $\Phi(\mu^\dagger)$

$$\theta(d)$$

Player I

Chooses

$\mu \in \mathcal{A}$

Max

Min

Player II

Sees $d \sim \mu^n$

Chooses θ

$$\mathcal{E}(\mu, \theta)$$

Mean squared error

$$\mathcal{E}(\mu, \theta) = \mathbb{E}_{d \sim \mu^n}\left[\left[\theta(d) - \Phi(\mu)\right]^2\right]$$

Confidence error

$$\mathcal{E}(\mu, \theta) = \mathbb{P}_{d \sim \mu^n}\left[\left|\theta(d) - \Phi(\mu)\right| \geq r\right]$$

Game theory and statistical decision theory

John Von Neumann

Abraham Wald

J. Von Neumann. Zur Theorie der Gesellschaftsspiele. *Math. Ann.*, 100(1):295–320, 1928

J. Von Neumann and O. Morgenstern. *Theory of Games and Economic Behavior*. Princeton University Press, Princeton, New Jersey, 1944.

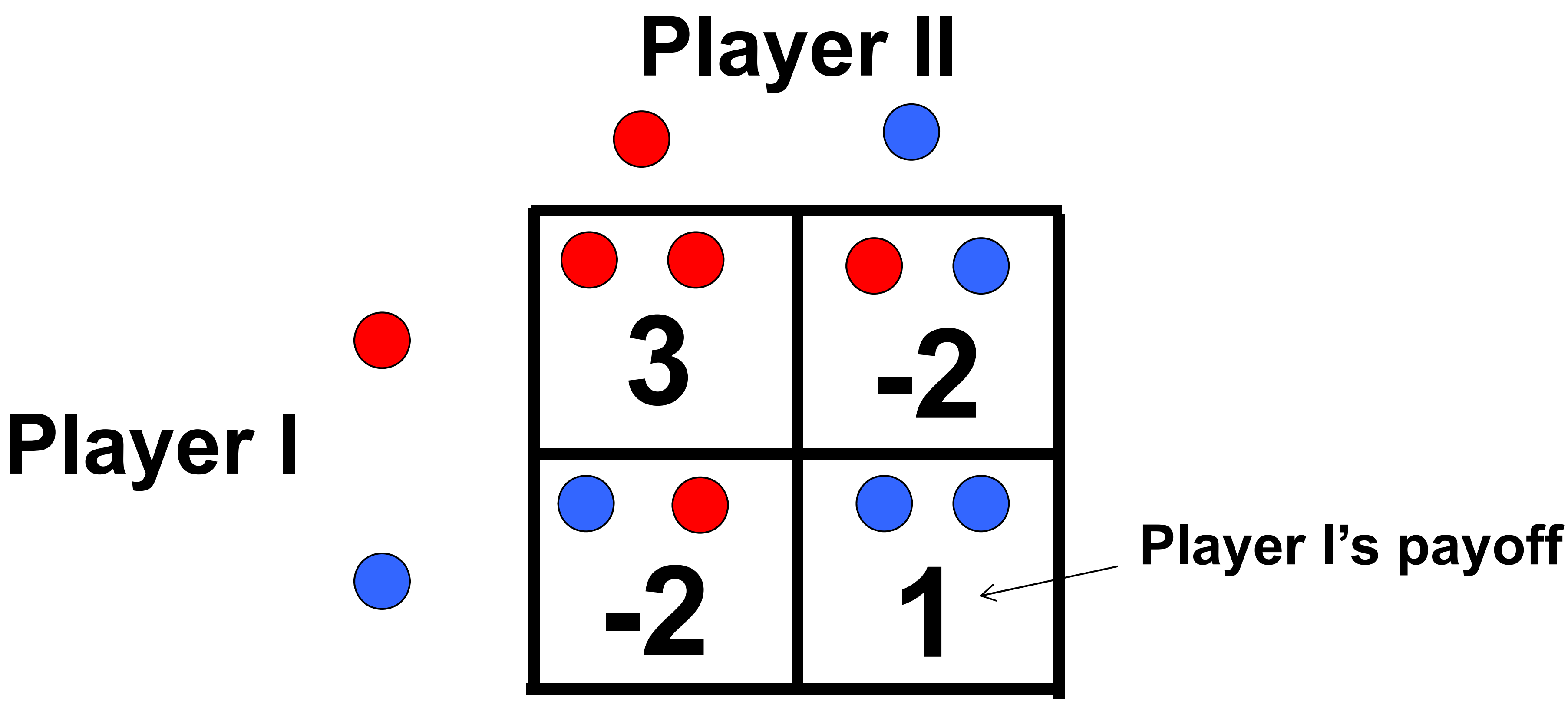
A. Wald. Contributions to the theory of statistical estimation and testing hypotheses. *Ann. Math. Statist.*, 10(4):299–326, 1939.

A. Wald. Statistical decision functions which minimize the maximum risk. *Ann. of Math. (2)*, 46:265–280, 1945.

A. Wald. An essentially complete class of admissible decision functions. *Ann. Math. Statistics*, 18:549–555, 1947.

A. Wald. Statistical decision functions. *Ann. Math. Statistics*, 20:165–205, 1949.

Deterministic zero sum game

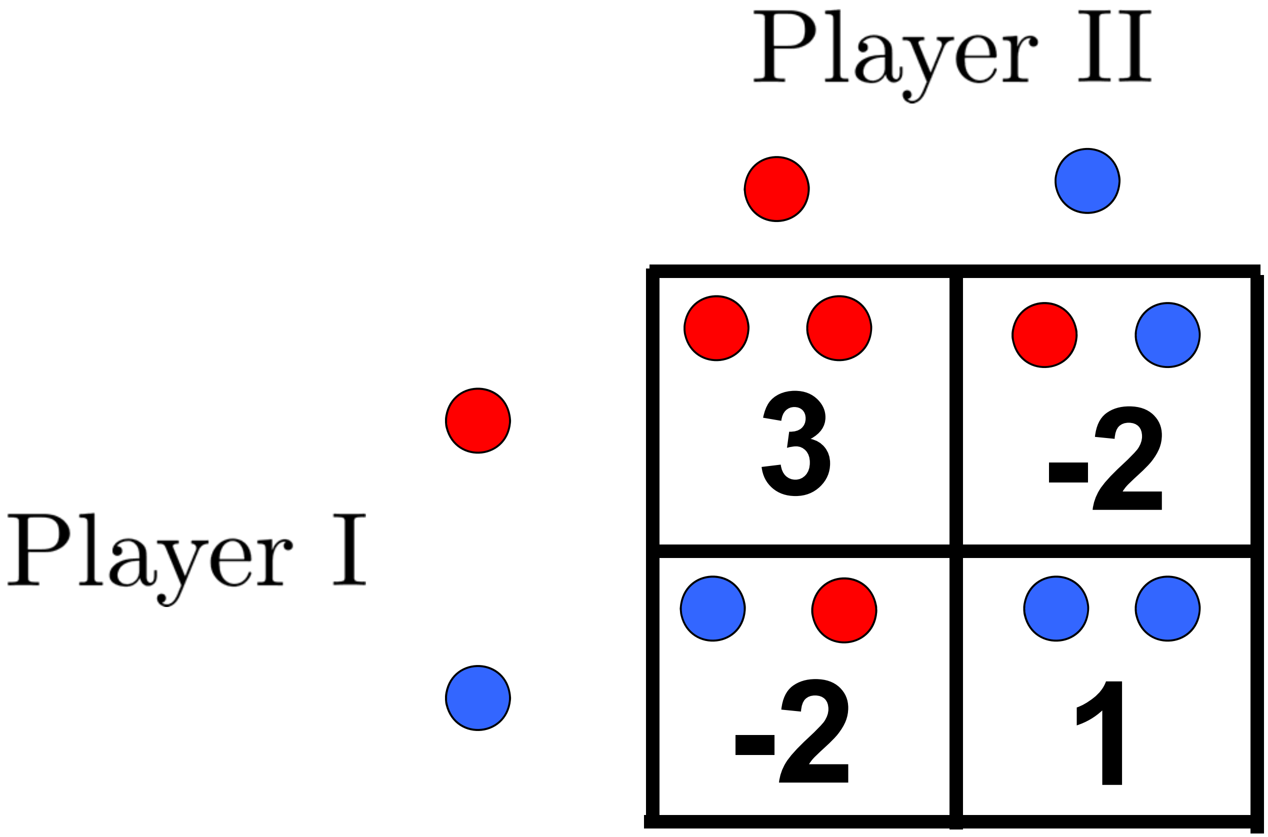


Player I & II both have a blue and a red marble

At the same time, they show each other a marble

How should I & II play the game?

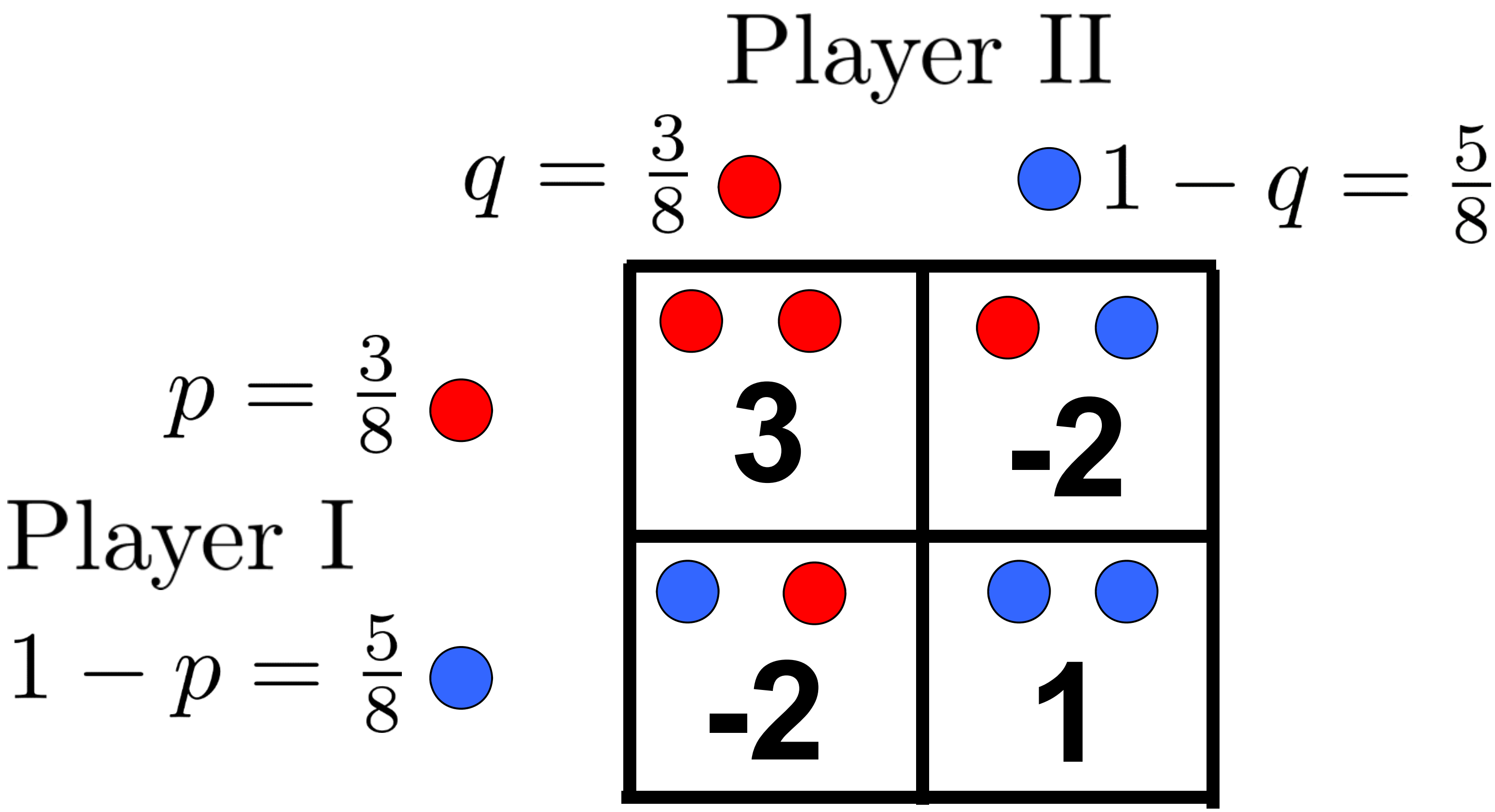
Pure strategy solution



II should play blue and loose 1 in the worst case

I should play red and loose 2 in the worst case

Mixed strategy (repeated game) solution



II should play red with probability 3/8 and win 1/8 on average

$$\text{Player } I\text{'s expected payoff} = 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)$$

$$= 1 - 3q + p(8q-3) = -\tfrac{1}{8} \text{ for } q = \tfrac{3}{8}$$

I should play red with probability 3/8 and loose 1/8 on average

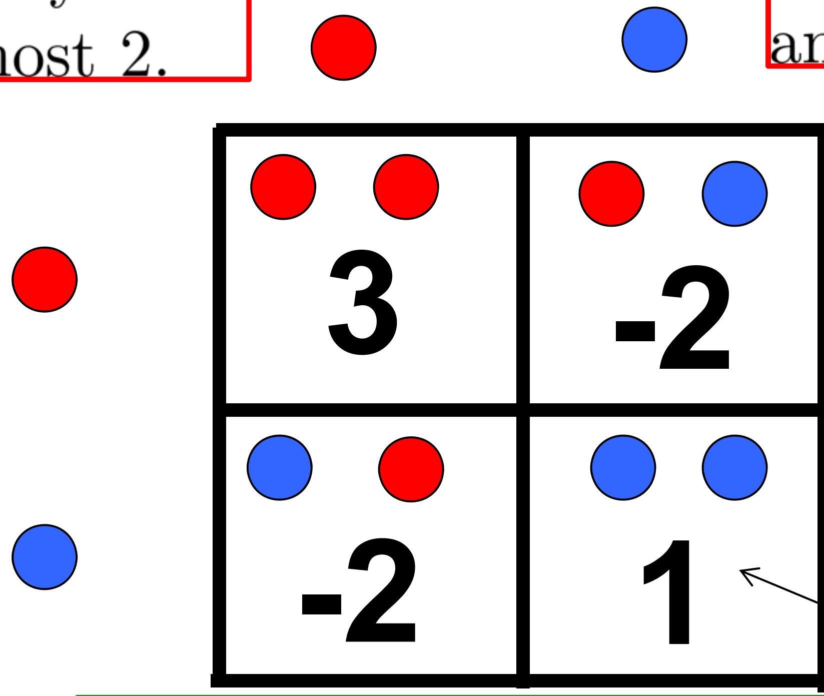
$$\max\min \neq \min\max$$

Maximin pure strategy for Player I: Play red and loose at most 2.

Player II

Minimax pure strategy for Player II: Play blue and loose at most 1.

Player I



J. Von Neumann

Player I's payoff

$$\max\min = \min\max$$

Maximin mixed strategy for Player I: Play red with probability $\frac{3}{8}$ and loose exactly $\frac{1}{8}$ on average.

Minimax mixed strategy for Player II: Play red with probability $\frac{3}{8}$ and win exactly $\frac{1}{8}$ on average.

Player I chooses $\mu \in \mathcal{A}$

Player II chooses θ

Max

Min

$$\mathcal{E}(\mu, \theta)$$

Pure strategy solution for Player II

Optimal bound on the statistical error

$$\max_{\mu \in \mathcal{A}} \mathcal{E}(\mu, \theta)$$

Optimal statistical estimators

$$\min_{\theta} \max_{\mu \in \mathcal{A}} \mathcal{E}(\mu, \theta)$$

Not a saddle point: $\min_{\theta} \max_{\mu \in \mathcal{A}} \mathcal{E}(\mu, \theta) \neq \max_{\mu \in \mathcal{A}} \min_{\theta} \mathcal{E}(\mu, \theta) = 0$

Player I chooses $\mu \in \mathcal{A}$

Player II chooses θ

$$\mathcal{E}(\mu, \theta)$$

Max

Min

Mixed strategy (repeated game) solution for Player I

$$\mu \sim \pi_I \in \mathcal{M}(\mathcal{A})$$

Mixed strategy (repeated game) solution for Player II

Choose θ at random and minimize

$$\mathbb{E}_{\mu \sim \pi_I,\, \hat{\theta}}\big[\mathcal{E}(\mu, \hat{\theta})\big]$$

Saddle point: $\min_{\hat{\theta}} \max_{\pi_I \in \mathcal{M}(\mathcal{A})} \mathbb{E}_{\mu \sim \pi_I, \hat{\theta}}\big[\mathcal{E}(\mu, \theta)\big] = \max_{\pi_I \in \mathcal{M}(\mathcal{A})} \min_{\hat{\theta}} \mathbb{E}_{\mu \sim \pi_I, \hat{\theta}}\big[\mathcal{E}(\mu, \theta)\big]$

Bayesian estimator (with prior $\pi \in \mathcal{M}(\mathcal{A})$)

$$\theta_\pi(d) = \mathbb{E}_{\mu \sim \pi,\, d' \sim \mu^n}\left[\Phi(\mu) \middle| d' = d\right]$$

Theorem If the loss is quadratic, i.e.

$$\mathcal{E}(\mu, \theta) = \mathbb{E}_{d \sim \mu^n}\left[\left[\theta(d) - \Phi(\mu)\right]^2\right]$$

then for all prior $\pi \in \mathcal{M}(\mathcal{A})$

$$\underbrace{\min_\theta \max_\mu \mathcal{E}(\mu, \theta)}_{\text{Minimal loss in non cooperative game}} \geq \underbrace{\mathbb{E}_{\mu \sim \pi}\left[\mathcal{E}(\mu, \theta_\pi)\right]}_{\text{Variance of Bayesian estimator}}$$

Can we have equality?

Theorem If the loss is quadratic, i.e.

$$\mathcal{E}(\mu,\theta) = \mathbb{E}_{d\sim\mu^n}\left[\left[\theta(d) - \Phi(\mu)\right]^2\right]$$

then the optimal $\hat{\theta}$ is non-random and lives in the (classical) Bayesian class of estimators

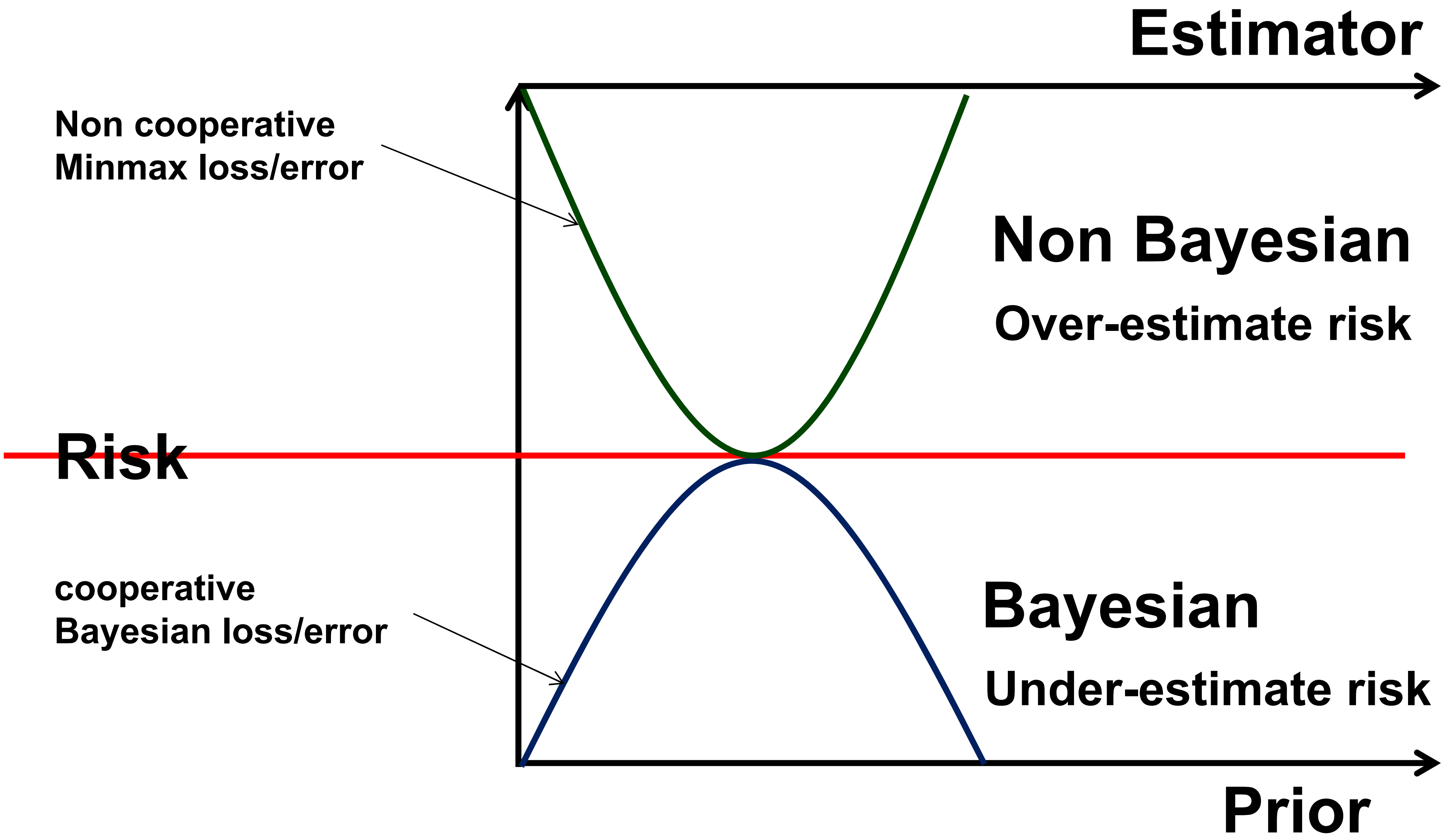
$$\min_{\theta}\max_{\mu}\mathcal{E}(\mu,\theta) = \max_{\pi}\mathbb{E}_{\mu\sim\pi}\left[\mathcal{E}(\mu,\theta_\pi)\right]$$

The best mixed strategy for I and II = worst prior for II

The best estimator is not random if the loss function is strictly convex

A. Dvoretzky, A. Wald, and J. Wolfowitz. Elimination of randomization in certain statistical decision procedures and zero-sum two-person games. *Ann. Math. Statist.*, 22(1):1–21, 1951.

Complete class theorem



Further generalization of Statistical decision theory

L. J. Savage. The theory of statistical decision. *Journal of the American Statistical Association*, 46:55–67, 1951.

L. Le Cam. An extension of Wald's theory of statistical decision functions. *Ann. Math. Statist.*, 26:69–81, 1955

L. D. Brown. Minimaxity, more or less. In *Statistical Decision Theory and Related Topics V*, pages 1–18. Springer, 1994.

L. D. Brown. An essay on statistical decision theory. *Journal of the American Statistical Association*, 95(452):1277–1281, 2000.

I. Gilboa and D. Schmeidler. Maxmin expected utility with non-unique prior. *Journal of Mathematical Economics*, 18(2):141–153, 1989

A. Shapiro and A. Kleywegt. Minimax analysis of stochastic problems. *Optim. Methods Softw.*, 17(3):523–542, 2002.

M. Sniedovich. The art and science of modeling decision-making under severe uncertainty. *Decis. Mak. Manuf. Serv.*, 1(1-2):111–136, 2007

M. Sniedovich. A classical decision theoretic perspective on worst-case analysis. *Appl. Math.*, 56(5):499–509, 2011.

Impact in econometrics and social sciences

O. Morgenstern. Abraham Wald, 1902-1950. *Econometrica: Journal of the Econometric Society*, pages 361–367, 1951.

G. Tintner. Abraham Wald's contributions to econometrics. *Ann. Math. Statistics*, 23:21–28, 1952.

R. Leonard. ***Von Neumann, Morgenstern, and the Creation of Game Theory: From Chess to Social Science,*** *1900–1960*. Cambridge University Press, 2010.

If we want to make decision theory practical for UQ we need to introduce computational complexity constraints

H. Owhadi and C. Scovel. Towards Machine Wald. *Handbook for Uncertainty Quantication*, 2016. arXiv:1508.02449.

How do we do that?

Is there a natural relation between game theory, computational complexity and numerical approximations?

A simple approximation problem

Approximate solution x of

$$\boxed{Ax = b}$$

A: Known $n \times n$ symmetric positive definite matrix

b: Unknown element of $\mathbb{R}^n$

Based on the information that

$$\boxed{\Phi x = y}$$

Φ: Known $m \times n$ rank m matrix $(m < n)$

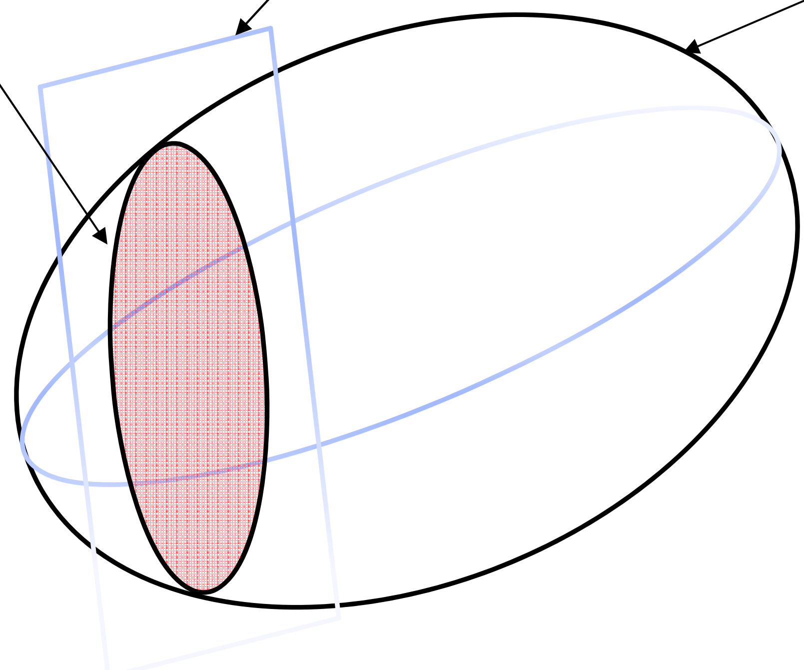
$$\boxed{b^T Q^{-1} b \leq 1}$$

y: Known element of $\mathbb{R}^m$

Q: Known $n \times n$ symmetric positive definite matrix

Set of candidates (ambiguity set) for x

$$\mathcal{A} = \left\{ z \in \mathbb{R}^n \mid \Phi z = y, \text{ and } |Az|_{Q^{-1}} \leq 1 \right\}$$



$$|b|_{Q^{-1}} := \sqrt{b^T Q^{-1} b}$$

Classical numerical analysis minimax solution

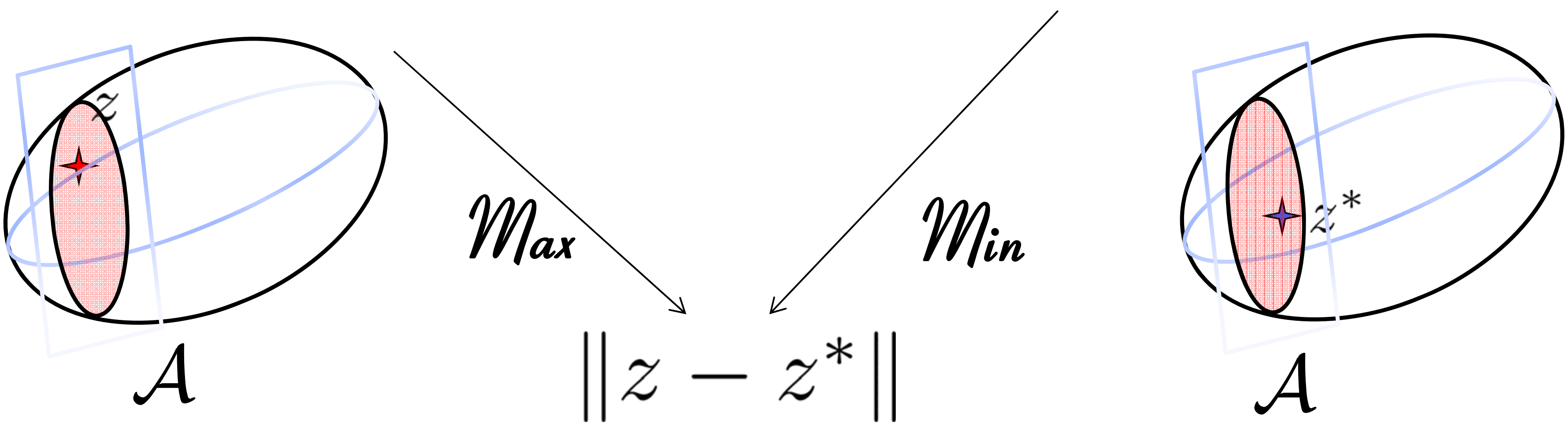
z^* minimizing

$$\boxed{\min_{z^* \in \mathcal{A}} \max_{z \in \mathcal{A}} \|z - z^*\|}$$

Looks like a game

Player I: Chooses $z \in \mathcal{A}$

Player II: Chooses $z^* \in \mathcal{A}$



Classical numerical analysis minimax solution

z^* minimizing

$$\boxed{\min_{z^* \in \mathcal{A}} \max_{z \in \mathcal{A}} \|z - z^*\|}$$

No saddle point in the numerical analysis formulation!

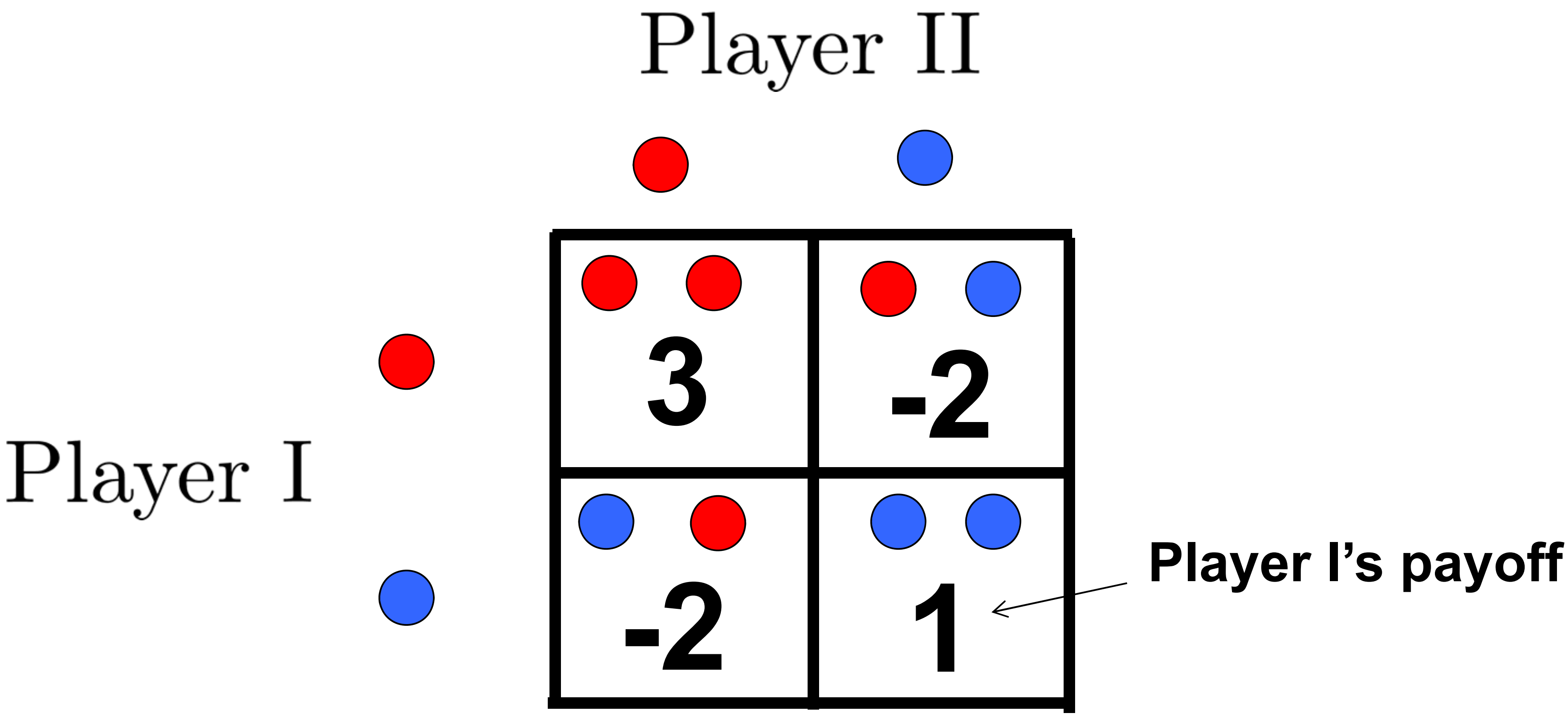
$$\max_{z^* \in \mathcal{A}} \min_{z \in \mathcal{A}} \|z - z^*\| = 0$$

$$\Downarrow$$

$$\boxed{\min_{z^* \in \mathcal{A}} \max_{z \in \mathcal{A}} \|z - z^*\| \neq \max_{z^* \in \mathcal{A}} \min_{z \in \mathcal{A}} \|z - z^*\|}$$

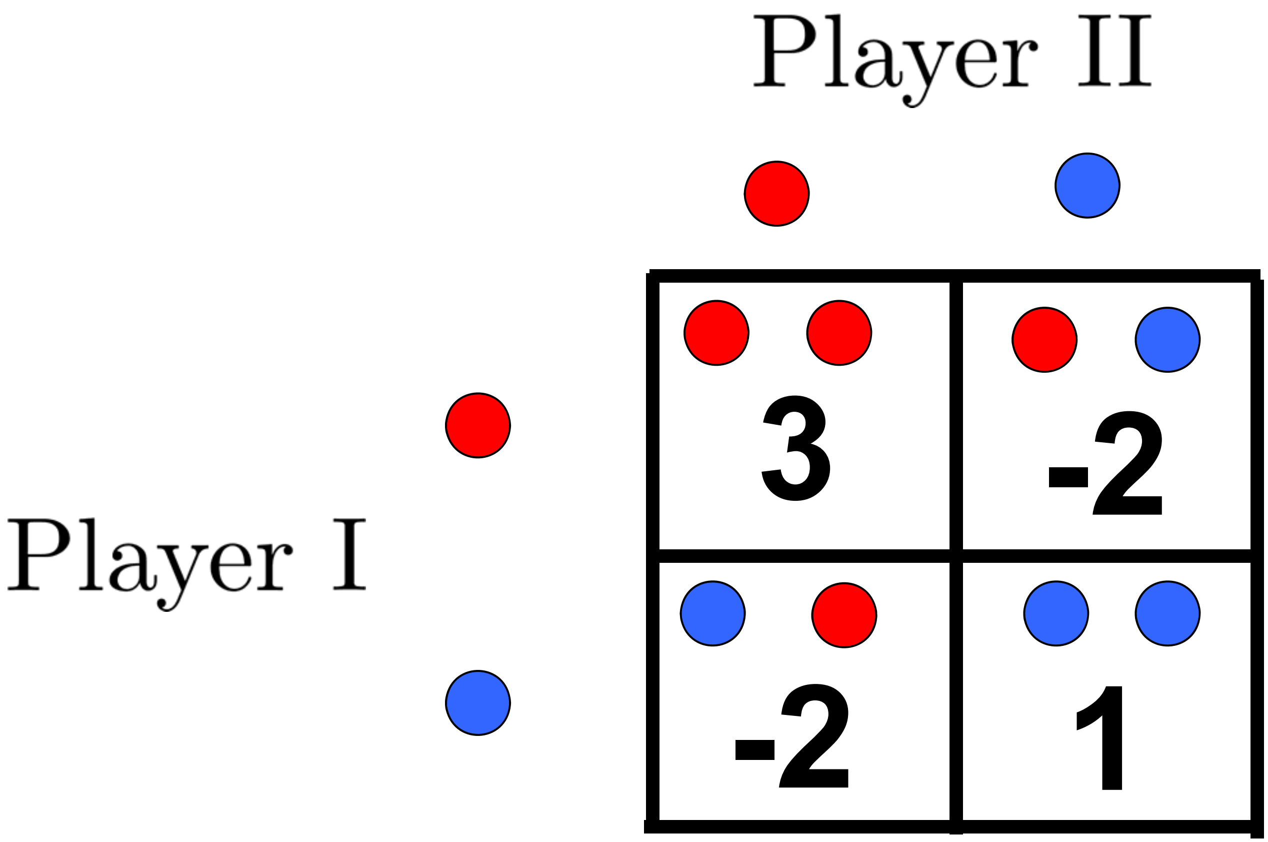
Why should we care?

Deterministic zero sum game



How should I and II play the game?

Pure strategy (classical numerical analysis) solution



II should play blue and loose 1 in the worst case

I should play red and loose 2 in the worst case

Mixed strategy (repeated game) solution

Player II

		$q = \frac{3}{8}$	$1 - q = \frac{5}{8}$
	$p = \frac{3}{8}$	**3**	**-2**
Player I	$1 - p = \frac{5}{8}$	**-2**	**1**

II should play red with probability 3/8 and win 1/8 on average

$$\text{Player } I\text{'s expected payoff} = 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)$$

$$= 1 - 3q + p(8q - 3) = -\tfrac{1}{8} \text{ for } q = \tfrac{3}{8}$$

I should play red with probability 3/8 and loose 1/8 on average

Maximin pure strategy for Player I: Play red and loose at most 2.

$$\min\max \neq \max\min$$

Minimax pure strategy for Player II: Play blue and loose at most 1.

Player II

Player I

3	-2
-2	1

Player I's payoff

J. Von Neumann

Maximin mixed strategy for Player I: Play red with probability $\frac{3}{8}$ and loose exactly $\frac{1}{8}$ on average.

Minimax mixed strategy for Player II: Play red with probability $\frac{3}{8}$ and win exactly $\frac{1}{8}$ on average.

$$\min\max = \max\min$$

Game theoretic formulation

$$\boxed{Ax = b}$$

Player I

chooses

$b \in \mathbb{R}^n$

$b^T Q^{-1} b \leq 1$

Player II

sees $y = \Phi x$

chooses x^*

$$\xrightarrow{Max} \|x - x^*\| \xleftarrow{Min}$$

Abraham Wald

Continuous game but as in decision theory under compactness it can be approximated by a finite game

Best strategy: lift minimax to measures

$$\boxed{Ax = b}$$

Player I

chooses

$b \in \mathbb{R}^n$

$b^T Q^{-1} b \leq 1$

Player II

sees $y = \Phi x$

chooses x^*

$$\text{Player I} \xrightarrow{Max} \|x - x^*\| \xleftarrow{Min} \text{Player II}$$

The best strategy for I is to play at random

Player II's best strategy live
in the Bayesian class of estimators

Player II's mixed strategy

$$\boxed{Ax = b} \Leftrightarrow \boxed{AX = \xi}$$

$$\boxed{\xi \sim \mathcal{N}(0, Q)}$$

Player II's bet

$$x^* = \mathbb{E}\big[X \big| \Phi X = \Phi x\big]$$

Player II's recovery error on x_i

$$\big|x_i - \mathbb{E}[X_i|\Phi X = \Phi x]\big| \quad \text{unknown}$$

Player II's stochastic error assuming that Player I is selecting x at random with the same prior distribution

$$\big|X_i - \mathbb{E}[X_i|\Phi X]\big|$$

random variable with known distribution

Player II's mixed strategy

$$\boxed{Ax = b} \Longleftrightarrow \boxed{AX = \xi}$$

$$\boxed{\xi \sim \mathcal{N}(0, Q)}$$

Theorem

$$\left|\underbrace{x_i - \mathbb{E}[X_i|\Phi X = y]}_{\text{unknown deterministic error}}\right| \leq \sqrt{\underbrace{\mathbb{E}\left[\left|X_i - \mathbb{E}[X_i|\Phi X]\right|^2\right]}_{\text{known Standard Deviation of stochastic error}}\ \underbrace{b^T Q^{-1} b}_{\text{known compactness bound on } b}}$$

Owhadi 2015, Multi-grid with rough coefficients and Multiresolution PDE decomposition from Hierarchical Information Games, arXiv:1503.03467, SIAM Review (to appear)

Main Question

Can we turn the process of discovery of a scalable numerical method into a UQ problem and, to some degree, solve it as such in an automated fashion?

Can we use a computer, not only to implement a numerical method but also to find the method itself?

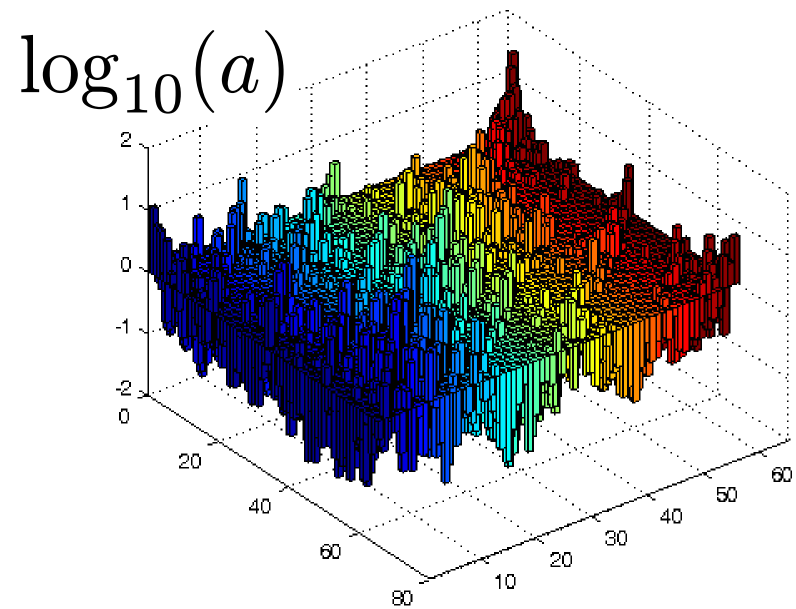
Example: Find a method for solving (1) as fast as possible to a given accuracy

$$(1)\quad \boxed{\begin{cases} -\operatorname{div}(a\nabla u) = g, & x\in\Omega,\\ u=0, & x\in\partial\Omega,\end{cases}}$$

$\Omega\subset\mathbb{R}^d$ $\qquad$ $\partial\Omega$ is piec. Lip.

a unif. ell.

$a_{i,j}\in L^\infty(\Omega)$



Multigrid Methods

Multigrid: [Fedorenko, 1961, Brandt, 1973, Hackbusch, 1978]

Multiresolution/Wavelet based methods

[Brewster and Beylkin, 1995, Beylkin and Coult, 1998, Averbuch et al., 1998]

- **Linear complexity with smooth coefficients**

Problem **Severely affected by lack of smoothness**

Robust/Algebraic multigrid

[Mandel et al., 1999,Wan-Chan-Smith, 1999,
Xu and Zikatanov, 2004, Xu and Zhu, 2008], [Ruge-Stüben, 1987]
[Panayot - 2010]

Stabilized Hierarchical bases, Multilevel preconditioners

[Vassilevski - Wang, 1997, 1998]

[Panayot - Vassilevski, 1997]

[Chow - Vassilevski, 2003]

[Aksoylu- Holst, 2010]

- Some degree of robustness but problem remains open with rough coefficients

Why? **Interpolation operators are unknown**

Don't know how to bridge scales with rough coefficients!

Low Rank Matrix Decomposition methods

Fast Multipole Method: [Greengard and Rokhlin, 1987]

Hierarchical Matrix Method: [Hackbusch et al., 2002]

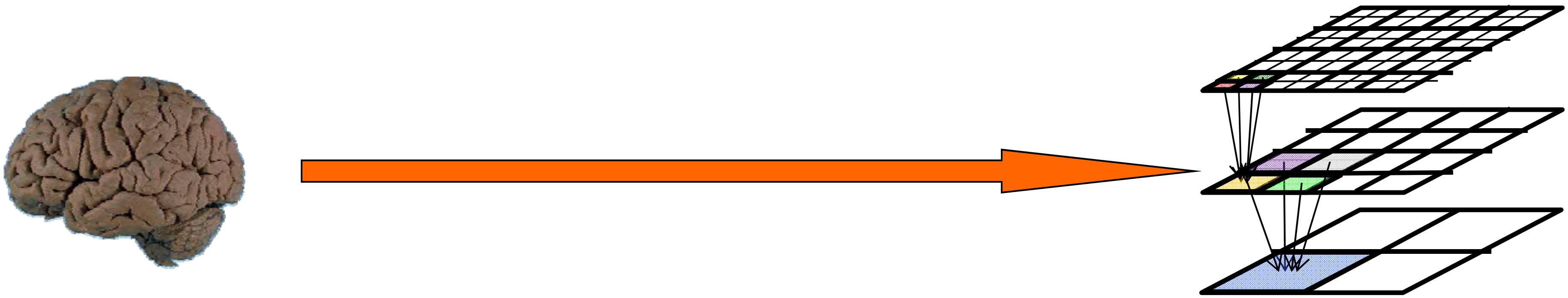
[Bebendorf, 2008]:

$$\boxed{N \ln^{2d+8} N \text{ complexity}}$$

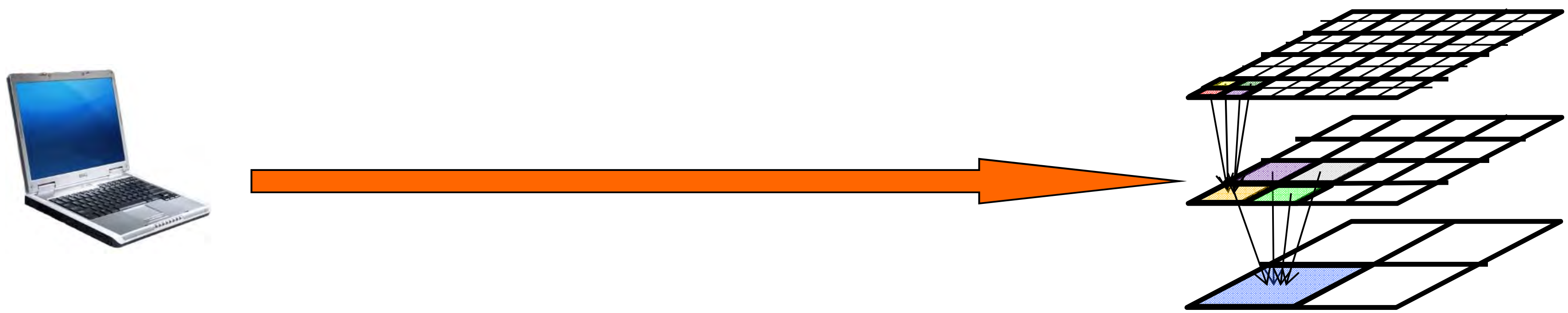
To achieve grid-size accuracy in L^2-norm

Common theme between these methods

Their process of discovery is based on intuition, brilliant insight, and guesswork



Can we turn this process of discovery into an algorithm?



Answer: YES

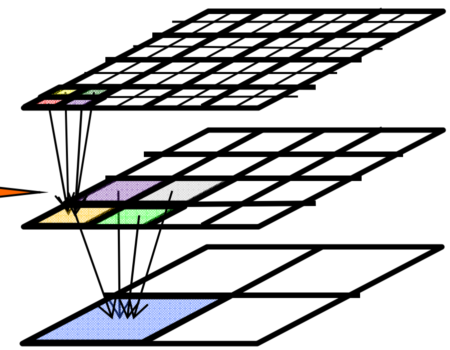
Compute fast

Play adversarial Information game

Compute with partial information

Identify game

Find optimal strategy



Owhadi 2015, Multi-grid with rough coefficients and Multiresolution PDE decomposition from Hierarchical Information Games, arXiv:1503.03467, SIAM Review (to appear)

Resulting method:

This is a theorem

$\boxed{N \ln^{3d} N \text{ complexity}}$

To achieve grid-size accuracy in H^1-norm

Subsequent solves: $\boxed{N \ln^{d+1} N \text{ complexity}}$

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ \qquad\qquad u = 0 \text{ on } \partial\Omega, \end{cases}$$

Resulting method:

$$\boxed{H_0^1(\Omega) = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots}$$

$$< \psi, \chi >_a := \int_\Omega (\nabla\psi)^T a \nabla\chi = 0 \text{ for } (\psi, \chi) \in \mathfrak{W}^{(i)} \times \mathfrak{W}^{(j)},\ i \neq j$$

Theorem For $v \in \mathfrak{W}^{(k)}$

$$\boxed{\frac{C_1}{2^k} \leq \frac{\|v\|_a}{\|\operatorname{div}(a\nabla v)\|_{L^2(\Omega)}} \leq \frac{C_2}{2^k}}$$

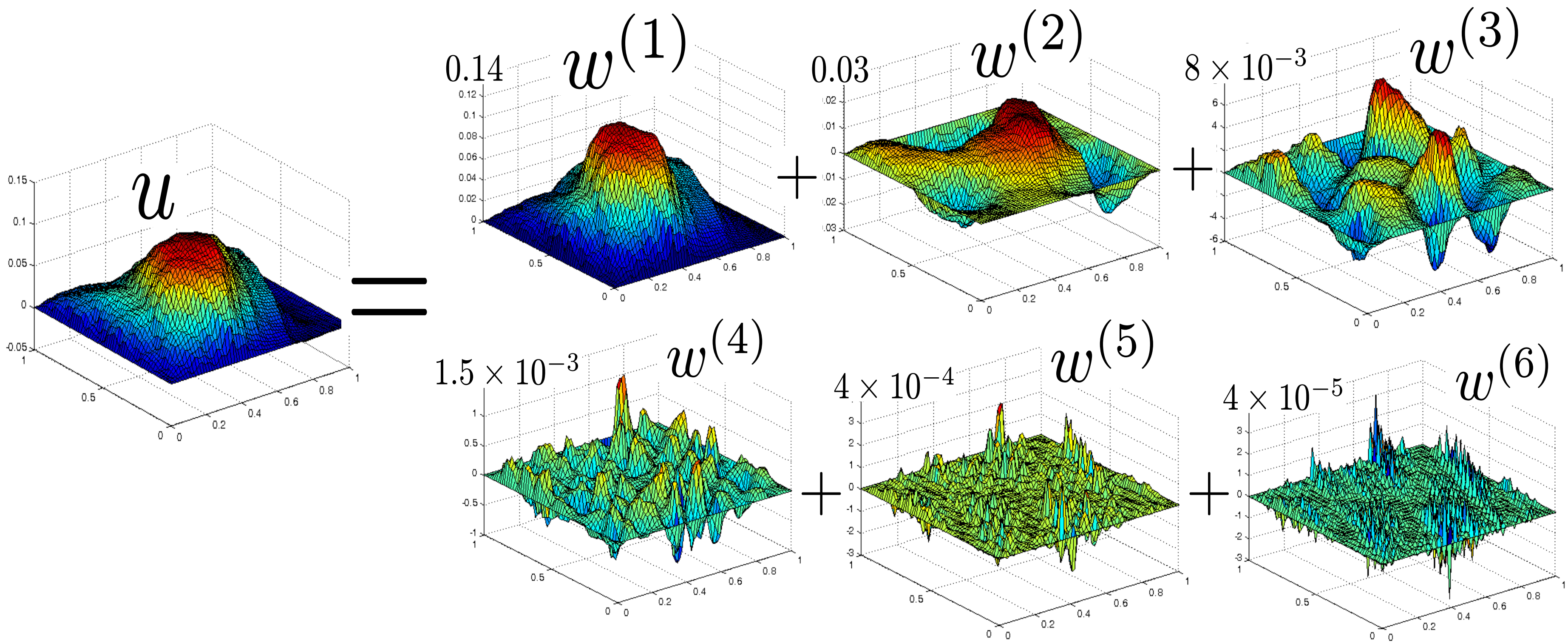
$$\|v\|_a^2 := < v, v >_a = \int_\Omega (\nabla v)^T a \nabla v$$

Looks like an eigenspace decomposition

$$\boxed{u = w^{(1)} + w^{(2)} + \cdots + w^{(k)} + \cdots}$$

$$w^{(k)} = \text{F.E. sol. of PDE in } \mathfrak{W}^{(k)}$$

Can be computed independently



Multiresolution decomposition of solution space

$$\boxed{u = w^{(1)} + w^{(2)} + \cdots + w^{(k)} + \cdots}$$

$w^{(k)} =$ F.E. sol. of PDE in $\mathfrak{W}^{(k)}$

Can be computed independently

$B^{(k)}$: Stiffness matrix of PDE in $\mathfrak{W}^{(k)}$

Theorem

$$\boxed{\frac{\lambda_{\max}(B^{(k)})}{\lambda_{\min}(B^{(k)})} \leq C}$$

Just relax in $\mathfrak{W}^{(k)}$ to find $w^{(k)}$

Quacks like an eigenspace decomposition

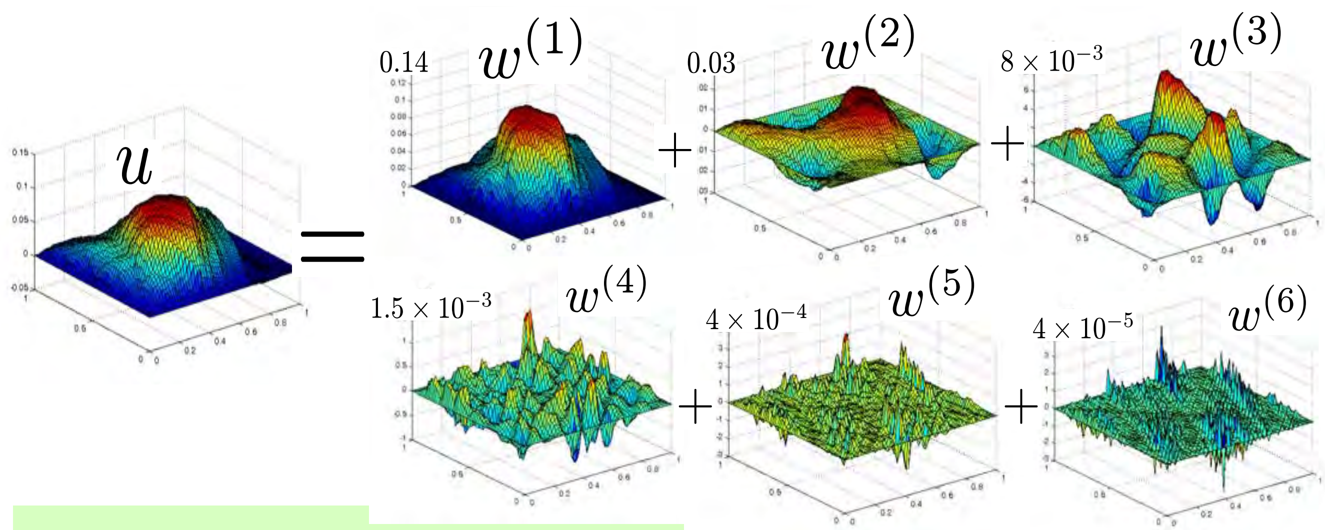
Application to time dependent problems

[Owhadi-Zhang 2016, From gamblets to near FFT-complexity solvers for wave and parabolic PDEs with rough coefficients]

$$\boxed{\mu(x)\partial_t^2 u - \operatorname{div}(a\nabla u) = g(x,t)}$$

$$\boxed{\mu(x)\partial_t u - \operatorname{div}(a\nabla u) = g(x,t)}$$

Hyperbolic and parabolic PDEs with rough coefficients can be solved in $\mathcal{O}(N \ln^{3d} N)$ (near FFT) complexity



Swims like an eigenspace decomposition

$\boxed{\mathfrak{V}\text{: F.E. space of } H^1_0(\Omega) \text{ of dim. } N}$

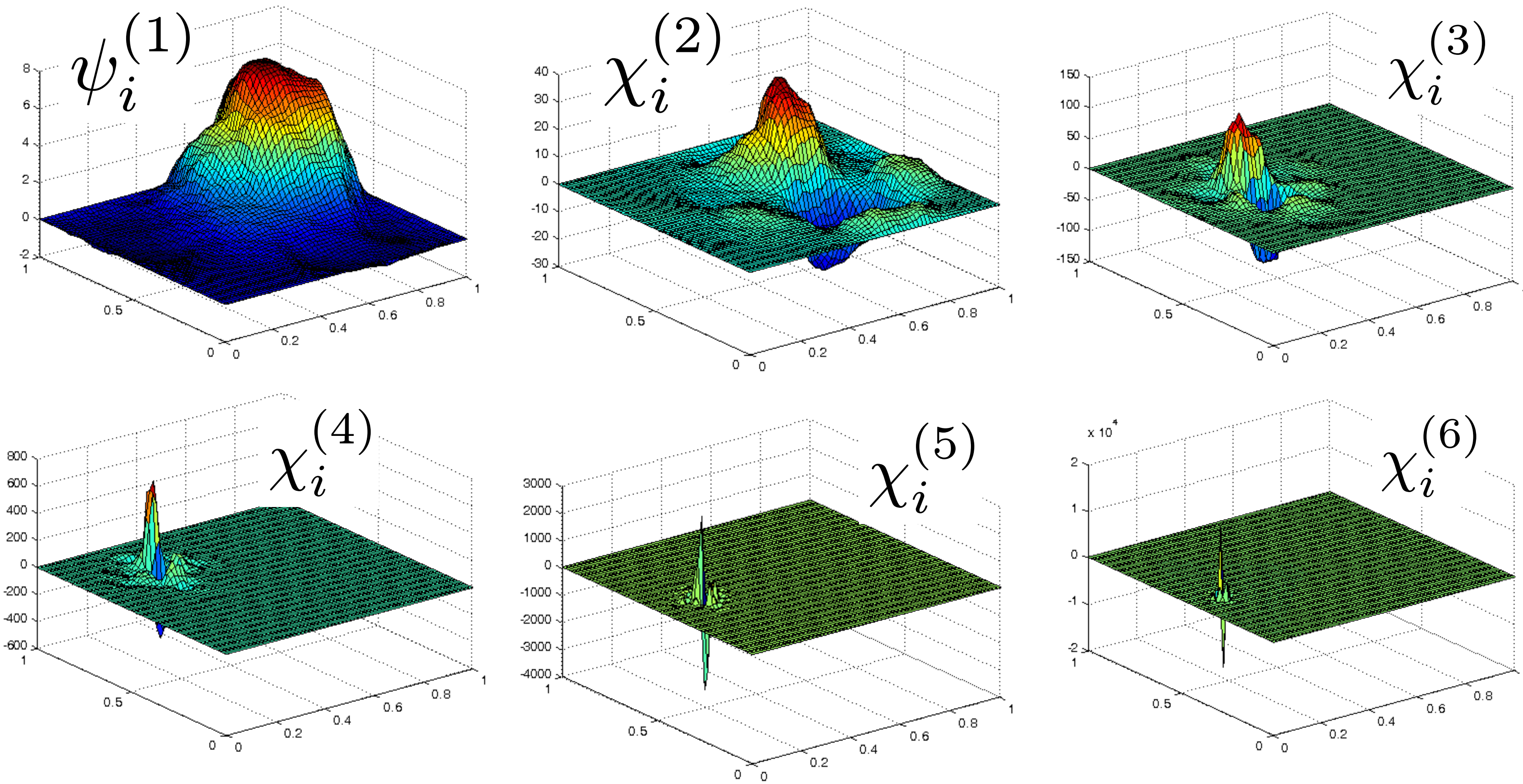
Theorem The decomposition

$$\boxed{\mathfrak{V} = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)}}$$

Can be performed and stored in

$$\boxed{\mathcal{O}(N \ln^{3d} N) \text{ operations}}$$

Doesn't have the complexity of an eigenspace decomposition



Basis functions look like and behave like wavelets: Localized and can be used to compress the operator and locally analyze the solution space

$$
\begin{tikzcd}
H_0^1(\Omega) \arrow[rr, "\mathrm{div}(a\nabla\cdot)"] & & H^{-1}(\Omega) \\
u & & g \arrow[d] \\
\mathbb{R}^m \ni u_m \arrow[u] \arrow[rr, bend left, "\text{Reduced operator}"] & & g_m \in \mathbb{R}^m \arrow[ll, "\textbf{Inverse Problem}"]
\end{tikzcd}
$$

Numerical implementation requires computation with partial information.

$$\phi_1, \ldots, \phi_m \in L^2(\Omega)$$

$$u_m = \left(\int_\Omega \phi_1 u, \ldots, \int_\Omega \phi_m u\right)$$

$$u_m \in \mathbb{R}^m \xrightarrow{\boxed{\text{Missing information}}} u \in H_0^1(\Omega)$$

Discovery process

Identify underlying information game

$$\boxed{\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases}}$$

Measurement functions: $\phi_1, \ldots, \phi_m \in L^2(\Omega)$

Player I

Chooses
$g \in L^2(\Omega)$
$\|g\|_{L^2(\Omega)} \leq 1$

Player II

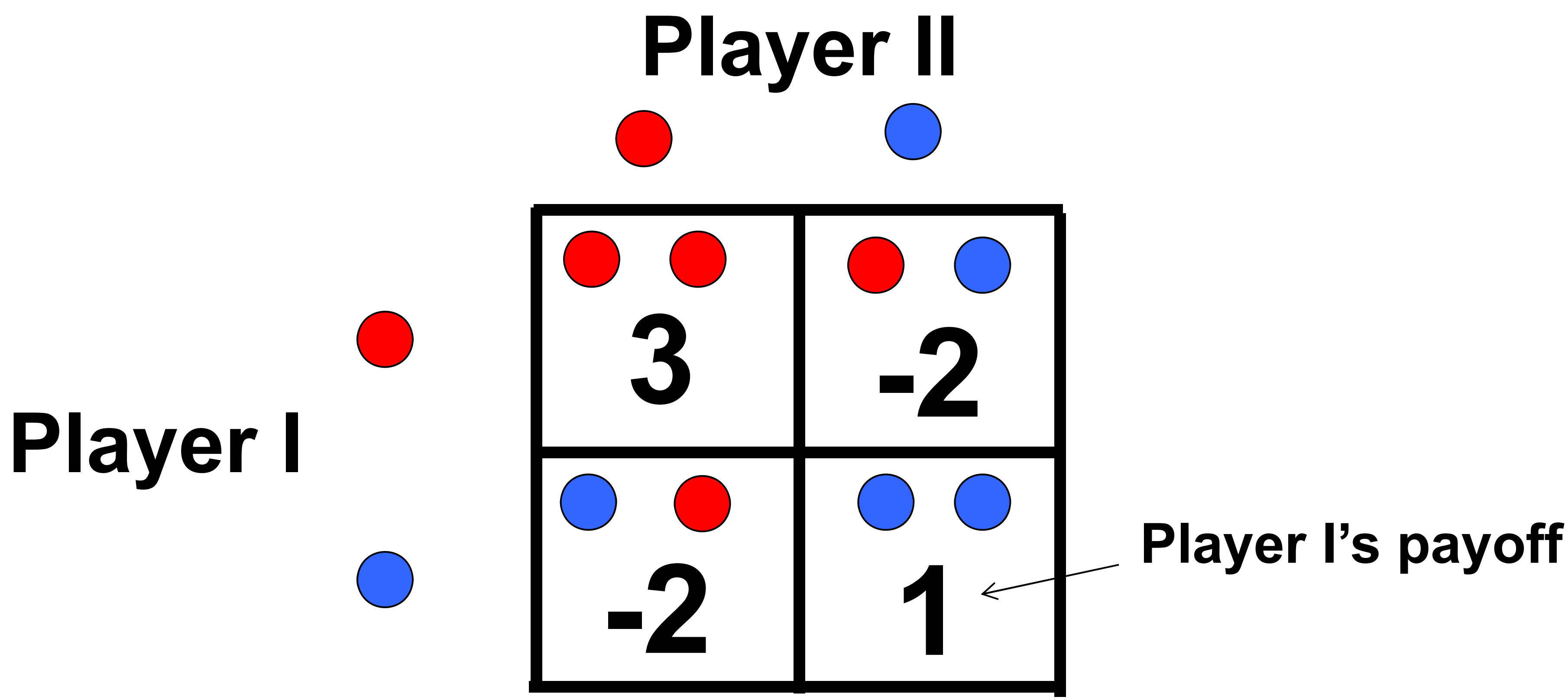
Sees $\int_\Omega u\phi_1, \ldots, \int_\Omega u\phi_m$
Chooses $u^* \in L^2(\Omega)$

Max *Min*

$$\|u - u^*\|_a$$

$\|f\|_a^2 := \int_\Omega (\nabla f)^T a \nabla f$

Deterministic zero sum game



Player I & II both have a blue and a red marble

At the same time, they show each other a marble

How should I & II play the (repeated) game?

Game theory

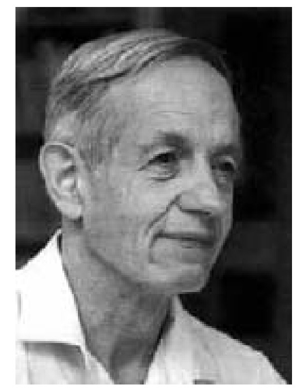
Optimal strategies are mixed strategies

Optimal way to play is at random

Player II

		q	$1-q$
Player I	p	**3**	**-2**
	$1-p$	**-2**	**1**

John Von Neumann



John Nash

$$\text{Player } I\text{'s expected payoff}$$

$$= 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)$$

$$= 1 - 3q + p(8q-3) \;\; = -\frac{1}{8} \qquad \text{for } q = \frac{3}{8}$$

Player A

Chooses
$g \in L^2(\Omega)$
$\|g\|_{L^2(\Omega)} \leq 1$

Player B

Sees $\int_\Omega u\phi_1, \ldots, \int_\Omega u\phi_m$
Chooses $u^* \in L^2(\Omega)$

$$\left\| u - u^* \right\|_a$$

Continuous game but as in decision theory under compactness it can be approximated by a finite game

Abraham Wald

The best strategy for A is to play at random

Player B's best strategy live in the Bayesian class of estimators

Player II's class of mixed strategies

Pretend that player I is choosing g at random

$$g \in L^2(\Omega) \iff \xi\text{: Random field}$$

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases} \iff \begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{cases}$$

Player II's bet

$$\boxed{u^*(x) := \mathbb{E}\Big[v(x)\Big| \int_\Omega v(y)\phi_i(y)\,dy = \int_\Omega u(y)\phi_i(y)\,dy, \forall i\Big]}$$

Player II's optimal strategy?

Player II's best bet? $\iff$ min max problem over distribution of ξ

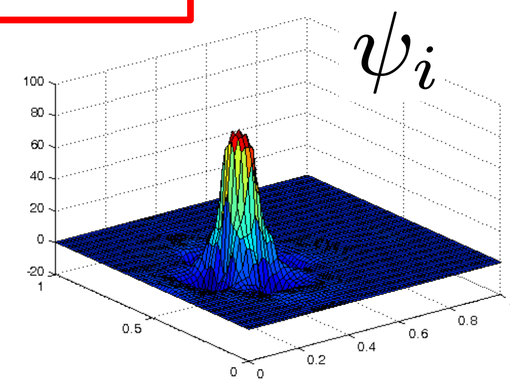
Computational efficiency → $\boxed{\xi \sim \mathcal{N}(0,\Gamma)}$

Elementary gambles form deterministic basis functions for player B's bet

Theorem

$$\boxed{u^*(x) = \sum_{i=1}^{m} \psi_i(x) \int_\Omega u(y)\phi_i(y)\,dy}$$

Gamblets



ψ_i: Elementary gambles/bets

Player II's bet if $\int_\Omega u\phi_j = \delta_{i,j}$, $j = 1, \ldots, m$

$$\boxed{\psi_i(x) := \mathbb{E}_{\xi\sim\mathcal{N}(0,\Gamma)}\Big[v(x)\Big|\int_\Omega v(y)\phi_j(y)\,dy = \delta_{i,j},\ j\in\{1,\ldots,m\}}$$

What are these gamblets?

Depend on

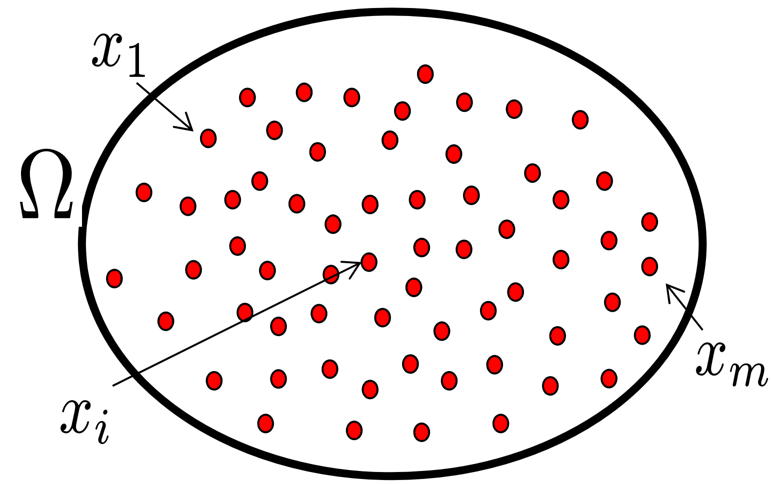
- Γ: Covariance function of ξ (Player B's decision)
- $(\phi_i)_{i=1}^m$: Measurements functions (rules of the game)

Example

[Owhadi, SIAM MMS, 2015]
Bayesian Numerical Homogenization

$$\Gamma(x,y) = \delta(x-y)$$

$$\phi_i(x) = \delta(x-x_i)$$



$a = I_d \Longleftrightarrow \psi_i$: Polyharmonic splines

[Harder-Desmarais, 1972] [Duchon 1976, 1977,1978]

$a_{i,j} \in L^\infty(\Omega) \Longleftrightarrow \psi_i$: Rough Polyharmonic splines

[Owhadi-Zhang-Berlyand 2013]

What is Player II's best strategy?

What is Player II's best choice for

$$\Gamma(x,y)=\mathbb{E}\big[\xi(x)\xi(y)\big] \quad \textbf{?}$$

$$\boxed{\Gamma=\mathcal{L}} \longleftrightarrow \int_\Omega \xi(x)f(x)\,dx \sim \mathcal{N}(0,\|f\|_a^2)$$

$$\|f\|_a^2 := \int_\Omega (\nabla f)^T a \nabla f$$

$$\Updownarrow$$

$$\boxed{\mathcal{L}=-\operatorname{div}(a\nabla\cdot)}$$

Why? $\longleftrightarrow$ **See algebraic generalization**

The recovery is optimal (Galerkin projection)

Theorem If $\Gamma = \mathcal{L}$ then

$u^*(x)$ is the F.E. solution of (1) in $\text{span}\{\mathcal{L}^{-1}\phi_i | i = 1, \ldots, m\}$

$$\boxed{\|u - u^*\|_a = \inf_{\psi \in \text{span}\{\mathcal{L}^{-1}\phi_i : i \in \{1,\ldots,m\}\}} \|u - \psi\|_a}$$

$$\boxed{\mathcal{L} = -\operatorname{div}(a\nabla\cdot)}$$

(1) $$\boxed{\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}}$$

Optimal variational properties

Theorem

$\sum_{i=1}^{m} w_i \psi_i$ minimizes $\|\psi\|_a$
over all ψ such that $\int_\Omega \phi_j \psi = w_j$ for $j = 1, \ldots, m$

Variational characterization

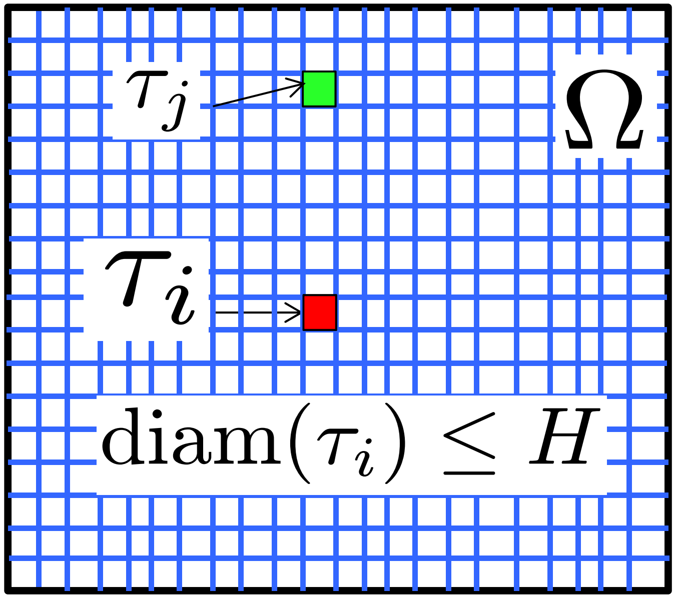
Theorem ψ_i: Unique minimizer of

$$\begin{cases} \text{Minimize} & \|\psi\|_a \\ \text{Subject to} & \psi \in H_0^1(\Omega) \text{ and } \int_\Omega \phi_j \psi = \delta_{i,j}, \quad j = 1, \ldots, m \end{cases}$$

Selection of measurement functions

Example Indicator functions of a Partition of Ω of resolution H

$$\boxed{\phi_i = 1_{\tau_i}}$$

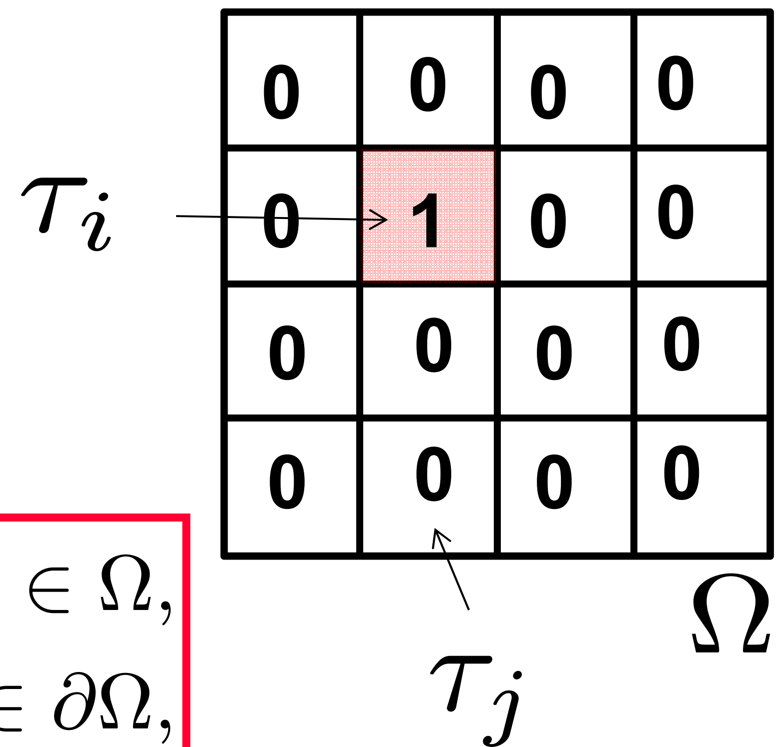


Theorem

$$\boxed{\|u - u^*\|_a \leq \frac{H}{\lambda_{\min}(a)} \|g\|_{L^2(\Omega)}}$$

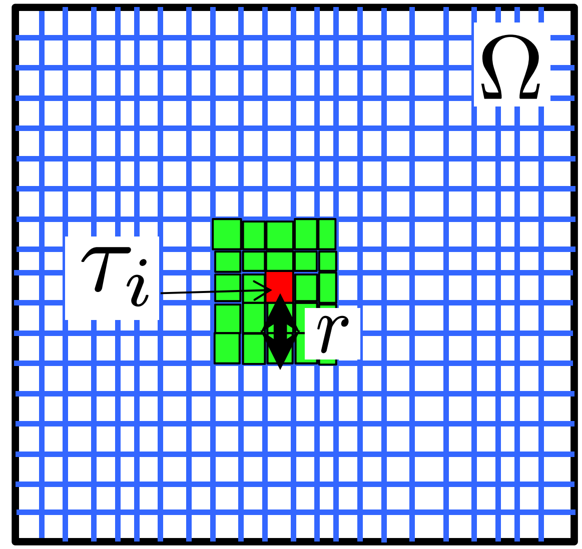
Elementary gamble

$\boxed{\psi_i}$ Your best bet on the value of u given the information that $\int_{\tau_i} u = 1$ and $\int_{\tau_j} u = 0$ for $j \neq i$



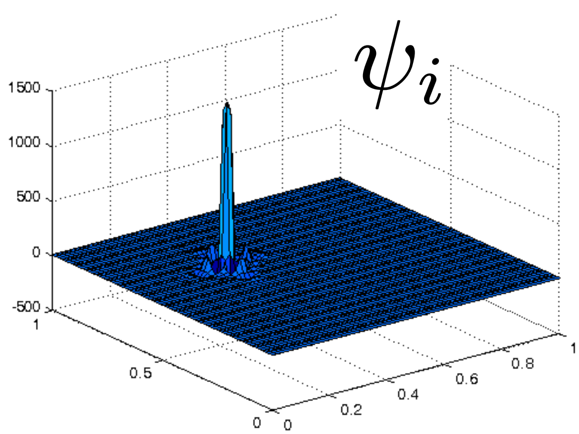
$$\text{(1)} \quad \boxed{\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}}$$

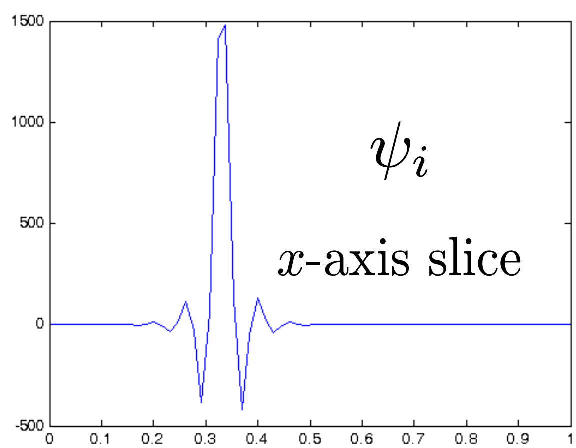
Exponential decay of gamblets

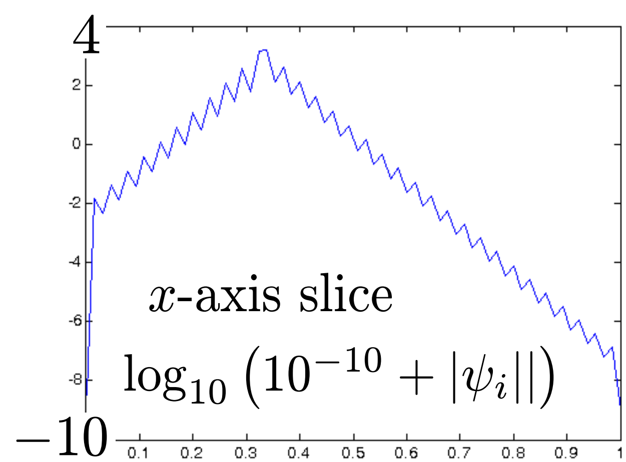


Theorem

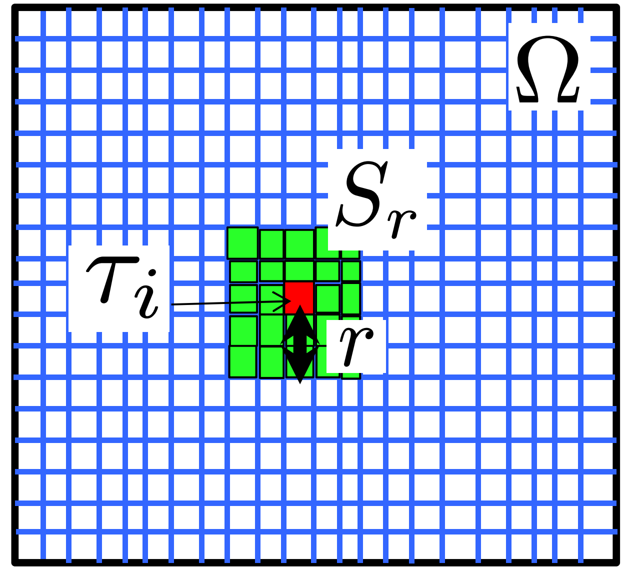
$$\boxed{\int_{\Omega\cap(B(\tau_i,r))^c}(\nabla\psi_i)^T a\nabla\psi_i \leq e^{-\frac{r}{lH}}\|\psi_i\|_a^2}$$







Localization of the computation of gamblets



$\psi_i^{\mathrm{loc},r}$: Minimizer of

$$\begin{cases} \text{Minimize} & \|\psi\|_a \\ \text{Subject to} & \psi \in H^1_0(S_r) \text{ and } \int_{S_r} \phi_j \psi = \delta_{i,j} \\ & \qquad \text{for } \tau_j \in S_r \end{cases}$$

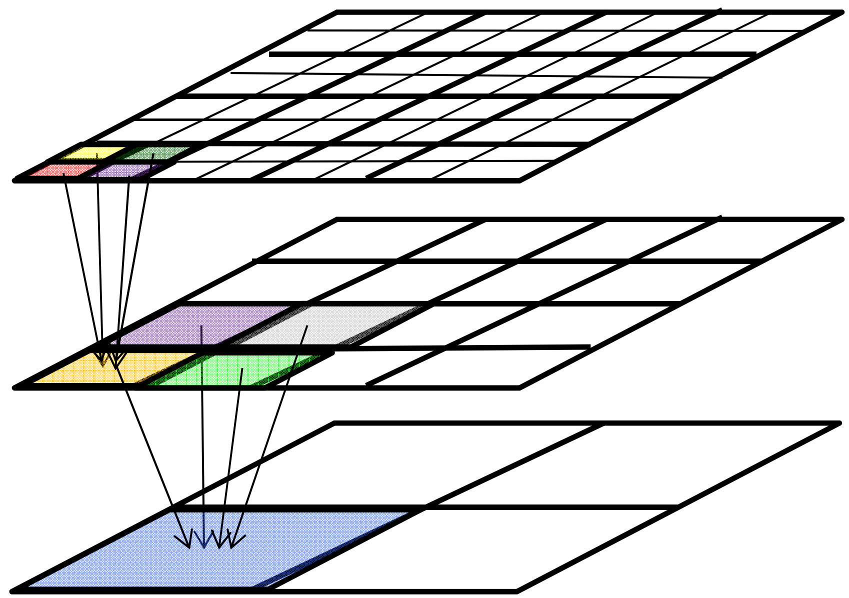
$$\boxed{\text{No loss of accuracy if localization} \sim H \ln \frac{1}{H}}$$

$$u^{*,\mathrm{loc}}(x) = \sum_{i=1}^m \psi_i^{\mathrm{loc,r}}(x) \int_\Omega u(y)\phi_i(y)\,dy$$

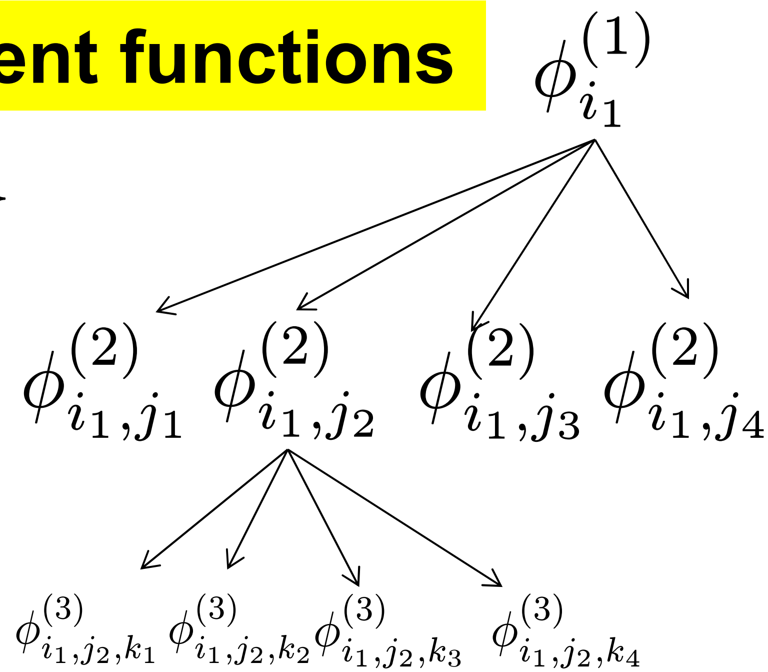
Theorem If $r \geq CH \ln \frac{1}{H}$

$$\|u - u^{*,\mathrm{loc}}\|_a \leq \frac{1}{\sqrt{\lambda_{\min}(a)}} H \|g\|_{L^2(\Omega)}$$

Formulation of the hierarchical game



Hierarchy of nested Measurement functions

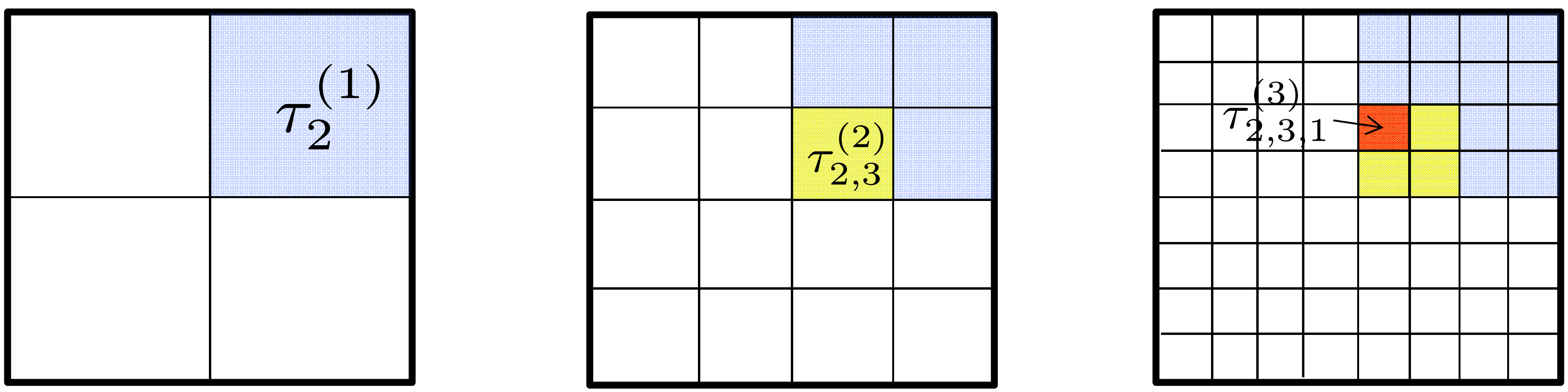


$$\phi^{(k)}_{i_1,\ldots,i_k} \quad \text{with } k \in \{1,\ldots,q\}$$

$$\boxed{\phi^{(k)}_i = \sum_j c_{i,j}\phi^{(k+1)}_{i,j}}$$

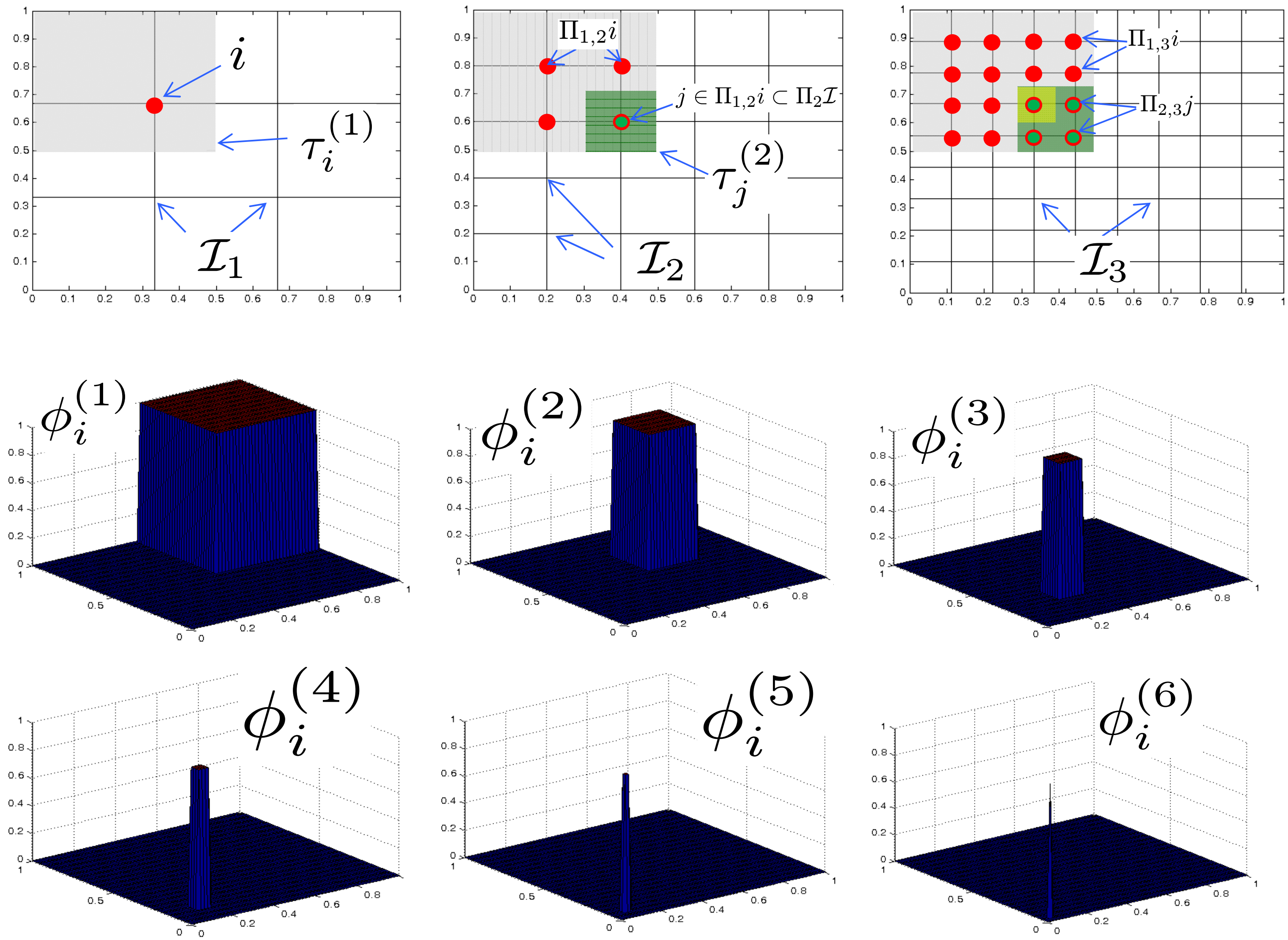
Example

$\phi^{(k)}_i$: Indicator functions of a hierarchical nested partition of Ω of resolution $H_k = 2^{-k}$



$$\phi^{(1)}_2 = 1_{\tau^{(1)}_2} \qquad \phi^{(2)}_{2,3} = 1_{\tau^{(2)}_{2,3}} \qquad \phi^{(3)}_{2,3,1} = 1_{\tau^{(3)}_{2,3,1}}$$

In the discrete setting simply aggregate elements (as in algebraic multigrid)



Formulation of the hierarchy of games

Player I

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases}$$

Player II

Chooses

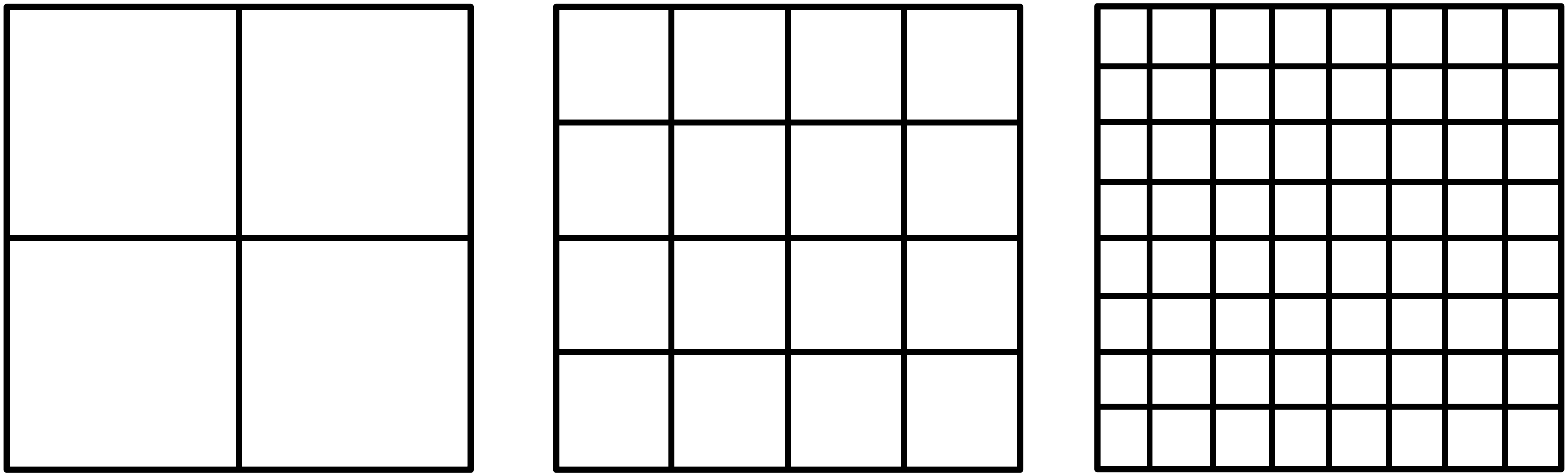
$g \in L^2(\Omega)$

$\|g\|_{L^2(\Omega)} \leq 1$

Sees $\{\int_\Omega u\phi_i^{(k)},\ i \in \mathcal{I}_k\}$

Must predict

u and $\{\int_\Omega u\phi_j^{(k+1)},\ j \in \mathcal{I}_{k+1}\}$



Player II's best strategy

$$\xi \sim \mathcal{N}(0, \mathcal{L})$$

$$\boxed{\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ \qquad\qquad u = 0 \text{ on } \partial\Omega, \end{cases}} \Longleftrightarrow \boxed{\begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ \qquad\qquad v = 0 \text{ on } \partial\Omega, \end{cases}}$$

Player II's bets

$$\boxed{u^{(k)}(x) := \mathbb{E}\Big[v(x)\Big| \int_\Omega v(y)\phi_i^{(k)}(y)\,dy = \int_\Omega u(y)\phi_i^{(k)}(y)\,dy,\ i \in \mathcal{I}_k\Big]}$$

The sequence of approximations forms a martingale under the mixed strategy emerging from the game

$$\mathcal{F}_k = \sigma\big(\int_\Omega v\phi_i^{(k)},\ i \in \mathcal{I}_k\big) \qquad \boxed{v^{(k)}(x) := \mathbb{E}\big[v(x)\big|\mathcal{F}_k\big]}$$

Theorem

$$\boxed{\mathcal{F}_k \subset \mathcal{F}_{k+1}}$$

$$\boxed{v^{(k)}(x) := \mathbb{E}\big[v^{(k+1)}(x)\big|\mathcal{F}_k\big]}$$

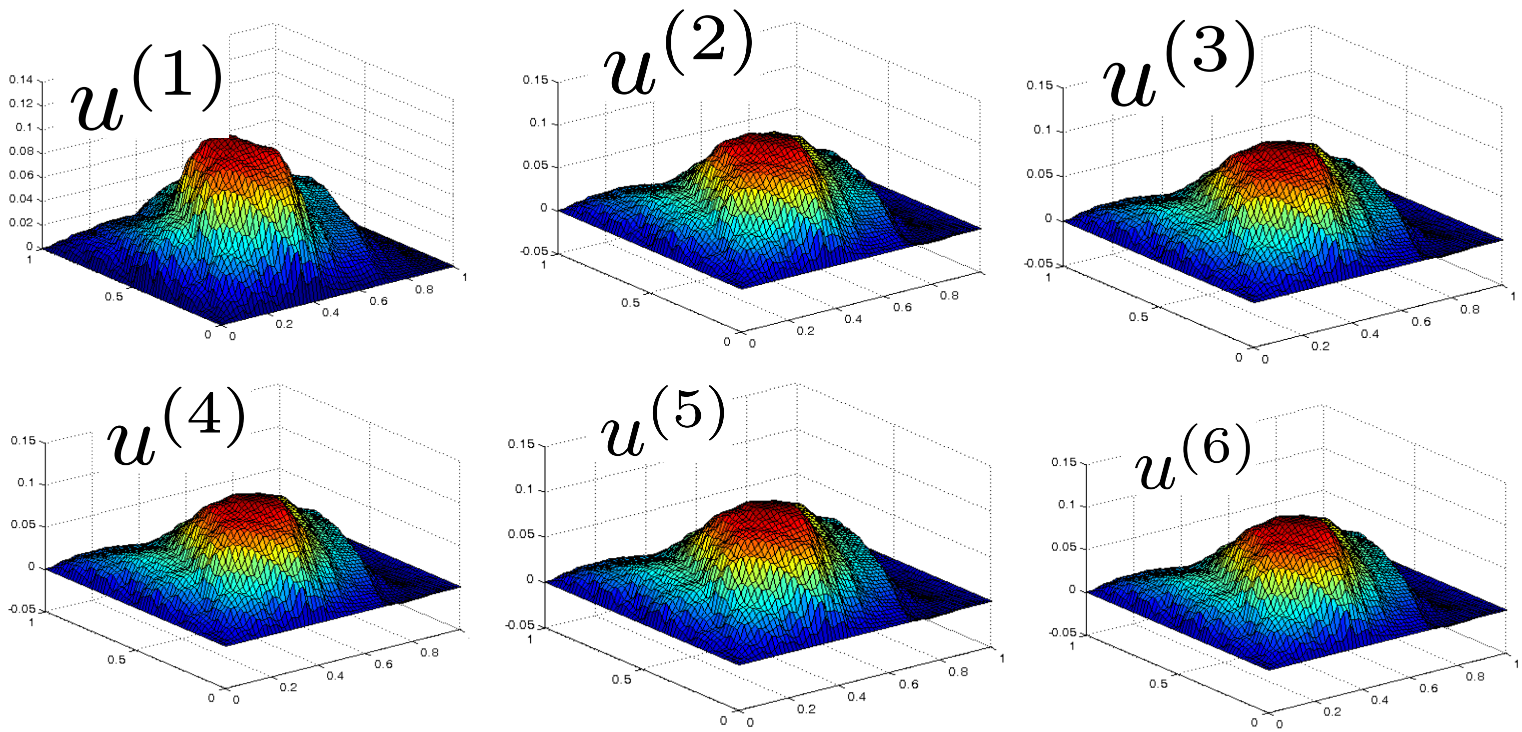
Player II's best strategy

$$\xi \sim \mathcal{N}(0, \mathcal{L})$$

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ \qquad\qquad u = 0 \text{ on } \partial\Omega, \end{cases} \quad \Longleftrightarrow \quad \begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ \qquad\qquad v = 0 \text{ on } \partial\Omega, \end{cases}$$

Player II's bets

$$\boxed{u^{(k)}(x) := \mathbb{E}\Big[v(x) \Big| \int_\Omega v(y)\phi_i^{(k)}(y)\,dy = \int_\Omega u(y)\phi_i^{(k)}(y)\,dy,\ i \in \mathcal{I}_k\Big]}$$



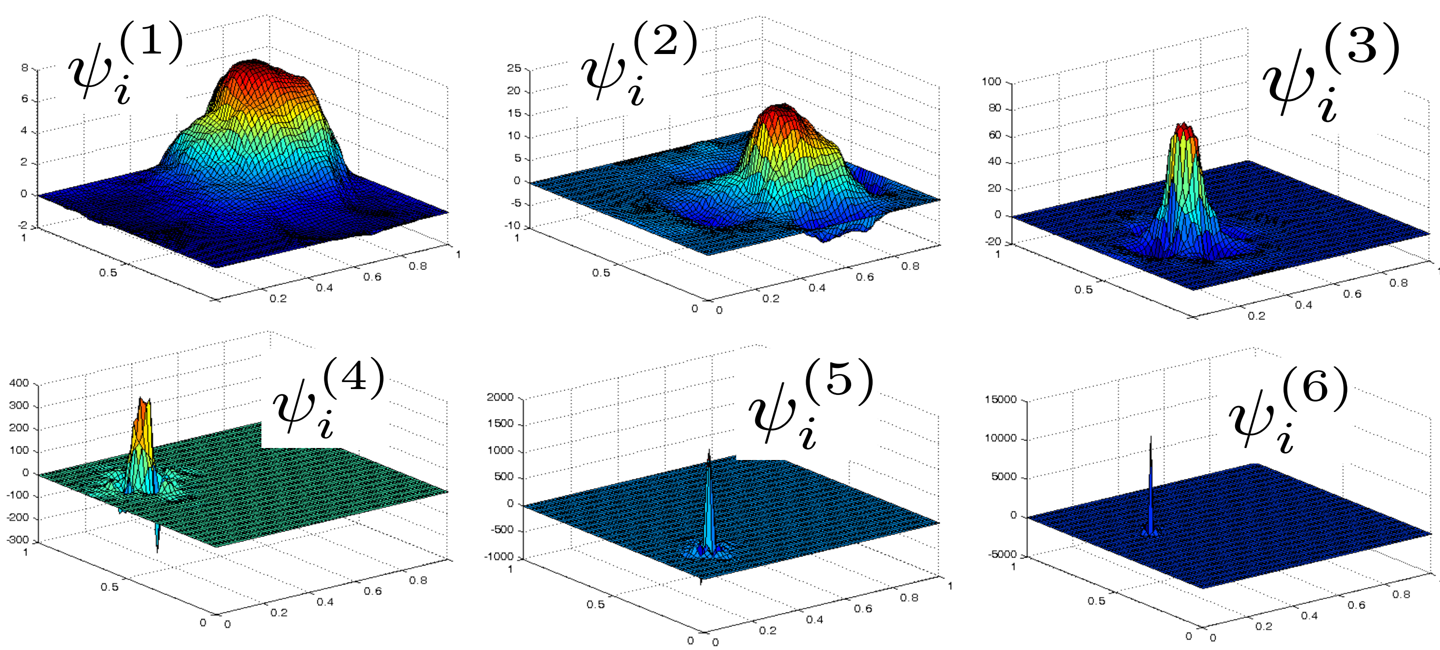
Gamblets **Elementary gambles form a hierarchy of deterministic basis functions for player II's hierarchy of bets**

Theorem

$$u^{(k)}(x) = \sum_i \psi_i^{(k)}(x) \int_\Omega u(y)\phi_i^{(k)}(y)\, dy$$

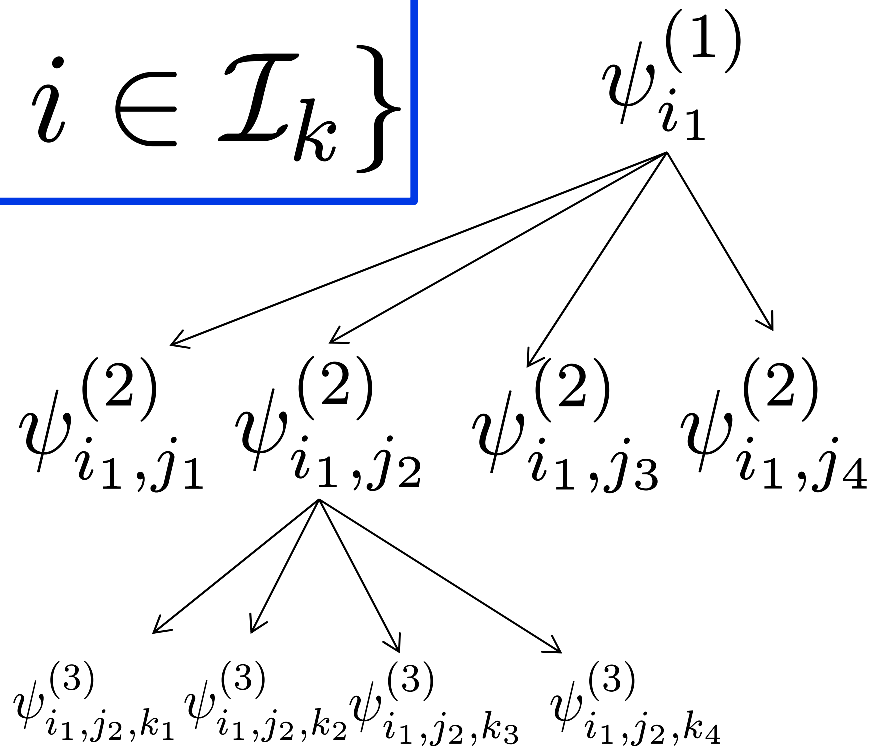
$\psi_i^{(k)}$: Elementary gambles/bets at resolution $H_k = 2^{-k}$

$$\psi_i^{(k)}(x) := \mathbb{E}\Big[v(x)\Big| \int_\Omega v(y)\phi_j^{(k)}(y)\, dy = \delta_{i,j},\, j \in \mathcal{I}_k\Big]$$



Gamblets are nested

$$\boxed{\mathfrak{V}^{(k)} := \operatorname{span}\{\psi_i^{(k)}, i \in \mathcal{I}_k\}}$$



Theorem

$$\boxed{\mathfrak{V}^{(k)} \subset \mathfrak{V}^{(k+1)}}$$

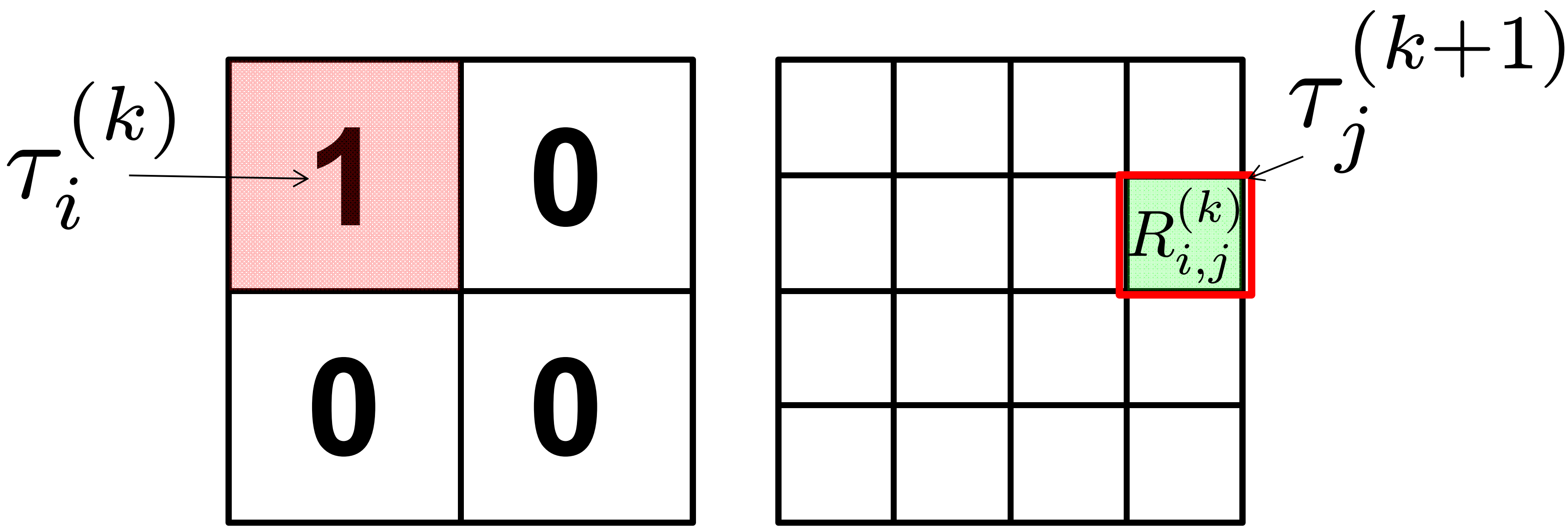
$$\boxed{\psi_i^{(k)}(x) = \sum_{j \in \mathcal{I}_{k+1}} R_{i,j}^{(k)} \psi_j^{(k+1)}(x)}$$

Interpolation/Prolongation operator

$$R^{(k)}_{i,j} = \mathbb{E}\big[\int_\Omega v(y)\phi^{(k+1)}_j(y)\,dy \big| \int_\Omega v(y)\phi^{(k)}_l(y)\,dy = \delta_{i,l},\, l\in\mathcal{I}_k\big]$$

$\boxed{R^{(k)}_{i,j}}$ Your best bet on the value of $\int_{\tau^{(k+1)}_j} u$ given the information that

$\int_{\tau^{(k)}_i} u = 1$ and $\int_{\tau_l} u = 0$ for $l \neq i$



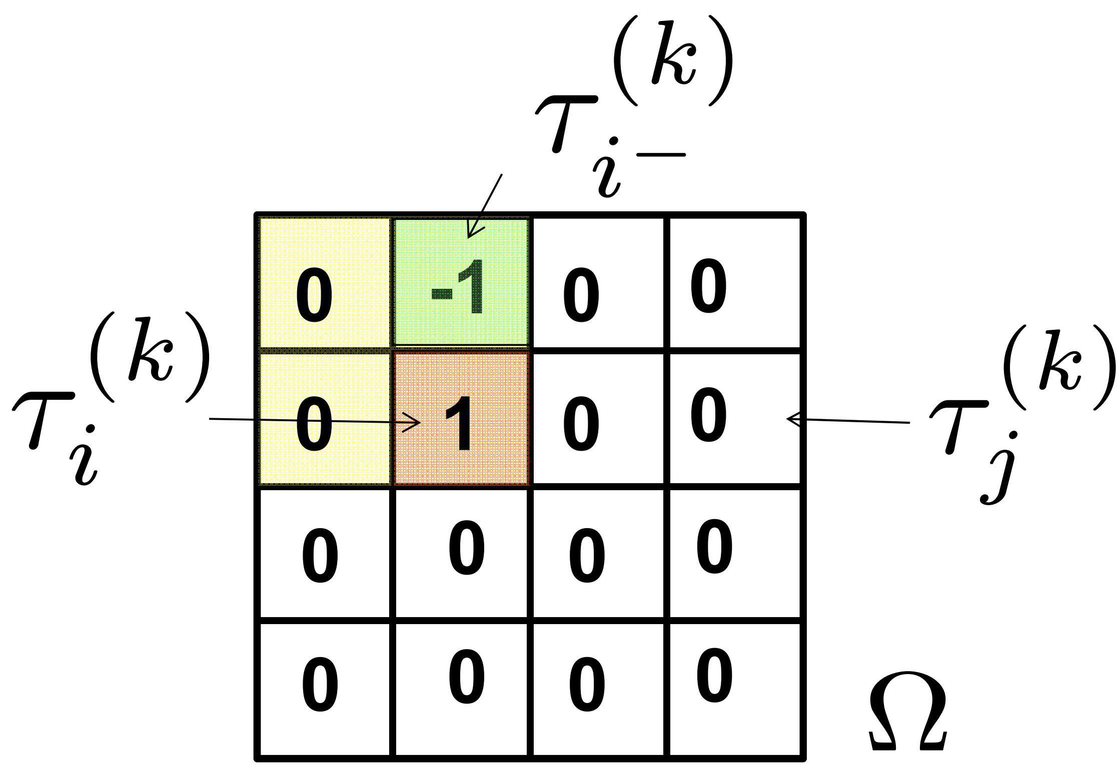
At this stage you can finish with classical multigrid

But we want multiresolution decomposition

Elementary gamble

$\boxed{\chi_i^{(k)}}$ Your best bet on the value of u given the information that

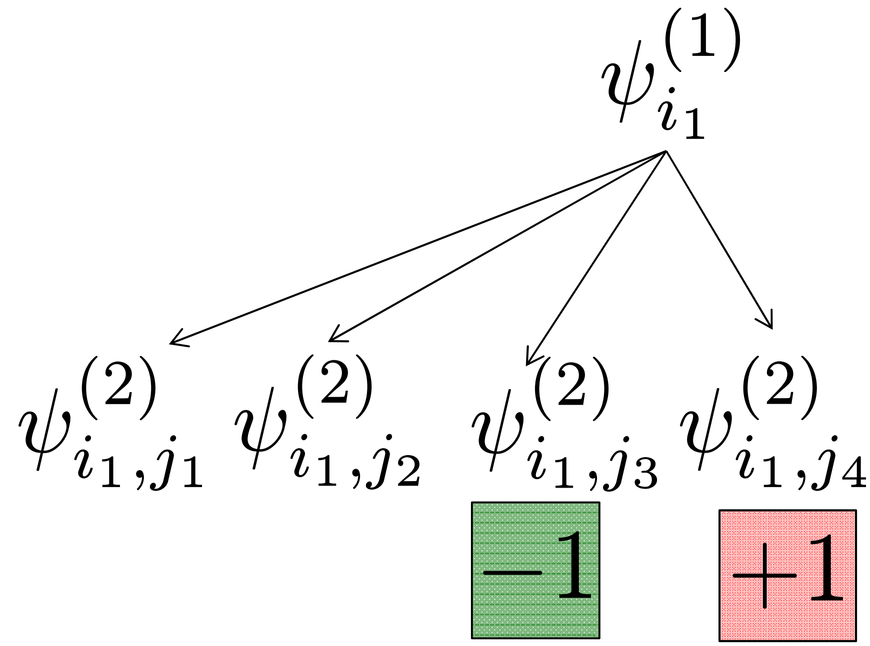
$$\int_{\tau_i^{(k)}} u = 1,\ \int_{\tau_{i-}^{(k)}} u = -1 \text{ and } \int_{\tau_j^{(k)}} u = 0 \text{ for } j \neq i$$

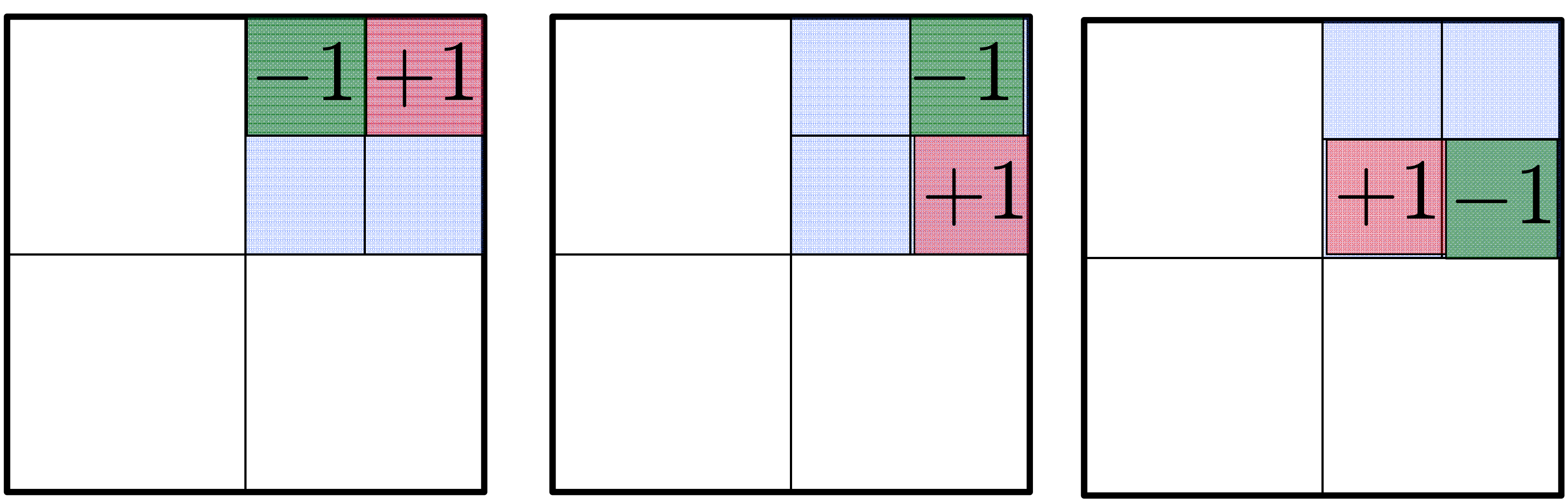


$$\boxed{\chi_i^{(k)} = \psi_i^{(k)} - \psi_{i^-}^{(k)}}$$

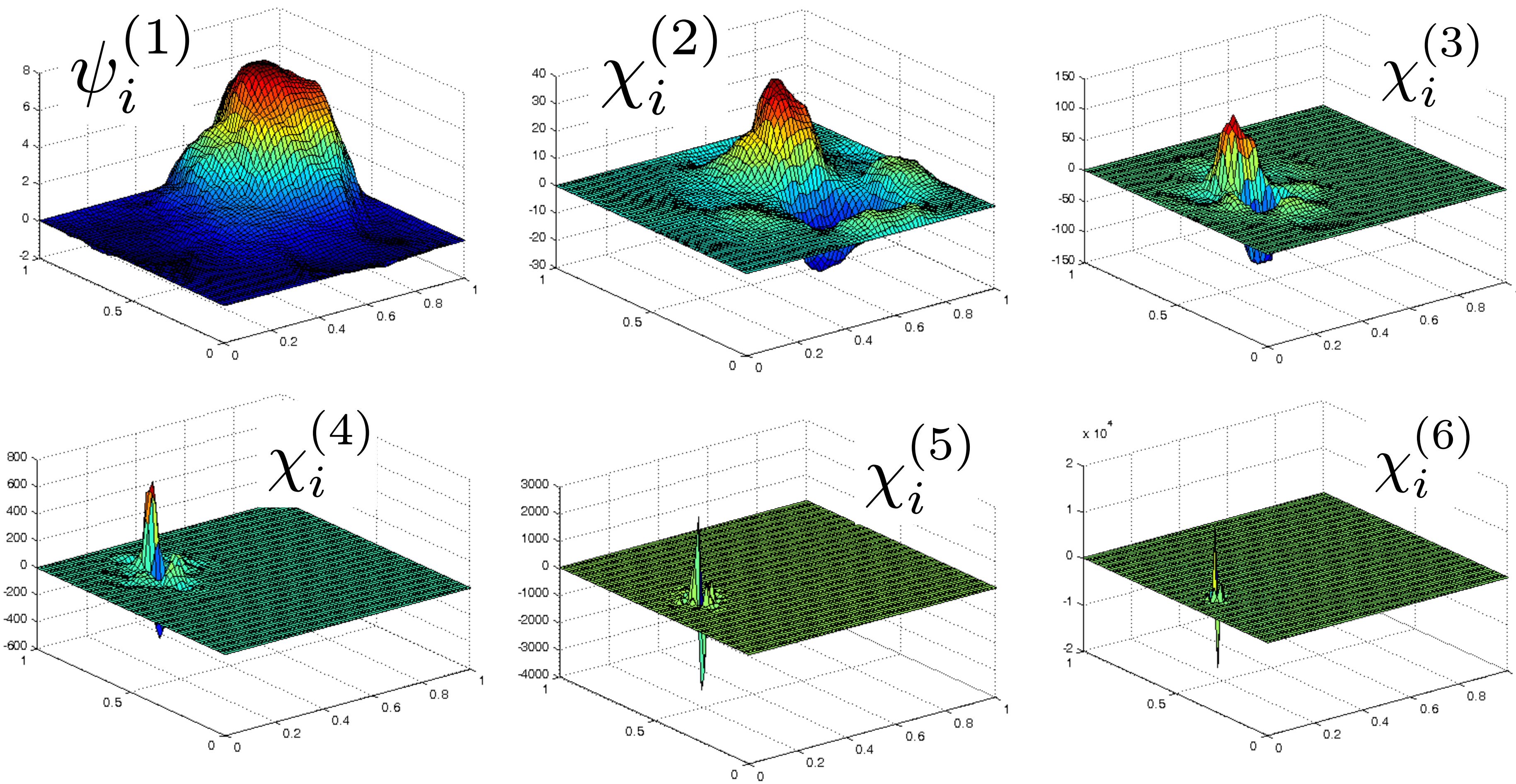
$$i = (i_1, \ldots, i_{k-1}, i_k)$$

$$i^- = (i_1, \ldots, i_{k-1}, i_k - 1)$$





$$\boxed{\chi_i^{(k)} = \psi_i^{(k)} - \psi_{i^-}^{(k)}}$$



Multiresolution decomposition of the solution space

$$\boxed{\mathfrak{V}^{(k)} := \text{span}\{\psi_i^{(k)}, i \in \mathcal{I}_k\}}$$

$$\boxed{\mathfrak{W}^{(k)} := \text{span}\{\chi_i^{(k)}, i\}}$$

$\mathfrak{W}^{(k+1)}$: Orthogonal complement of $\mathfrak{V}^{(k)}$ in $\mathfrak{V}^{(k+1)}$ with respect to $< \psi, \chi >_a := \int_\Omega (\nabla \psi)^T a \nabla \chi$

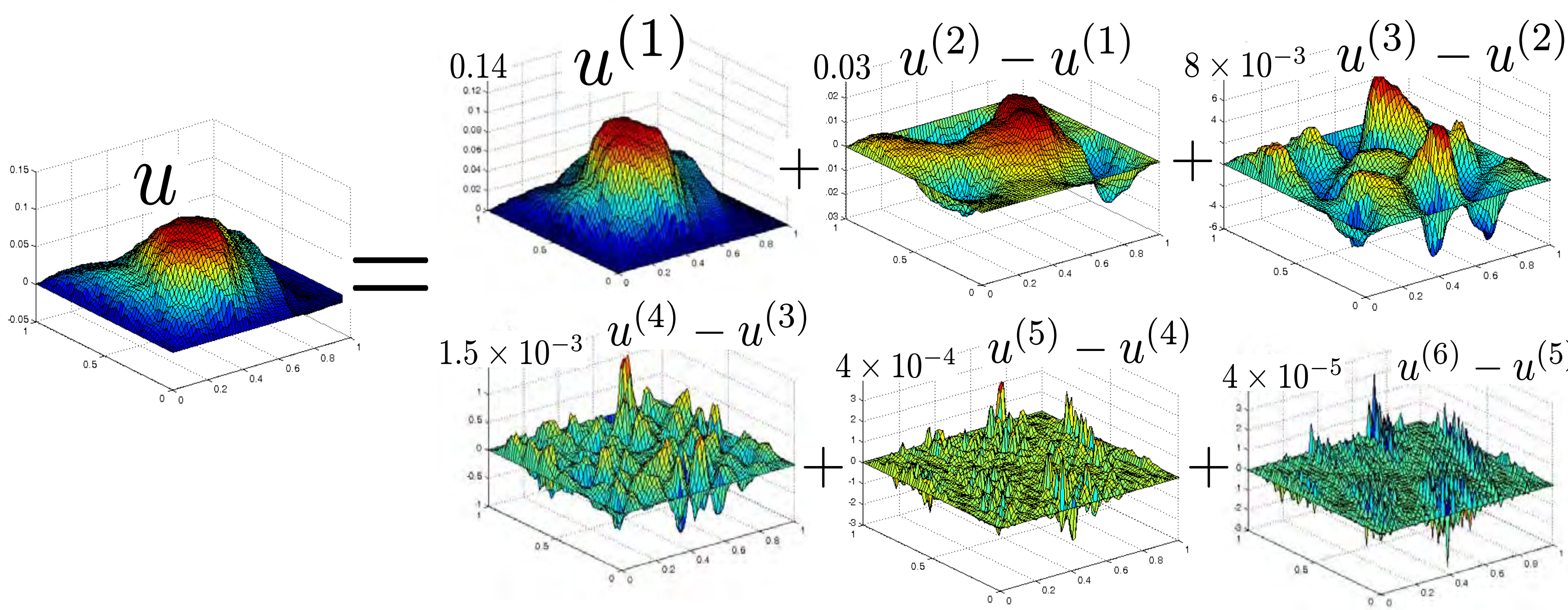
Theorem

$$\boxed{H_0^1(\Omega) = \mathfrak{V}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots}$$

Multiresolution decomposition of the solution

Theorem

$$u^{(k+1)} - u^{(k)} = \text{F.E. sol. of PDE in } \mathfrak{W}^{(k+1)}$$



Subband solutions $u^{(k+1)} - u^{(k)}$
can be computed independently

Uniformly bounded condition numbers

$$A_{i,j}^{(k)} := \langle \psi_i^{(k)}, \psi_j^{(k)} \rangle_a$$

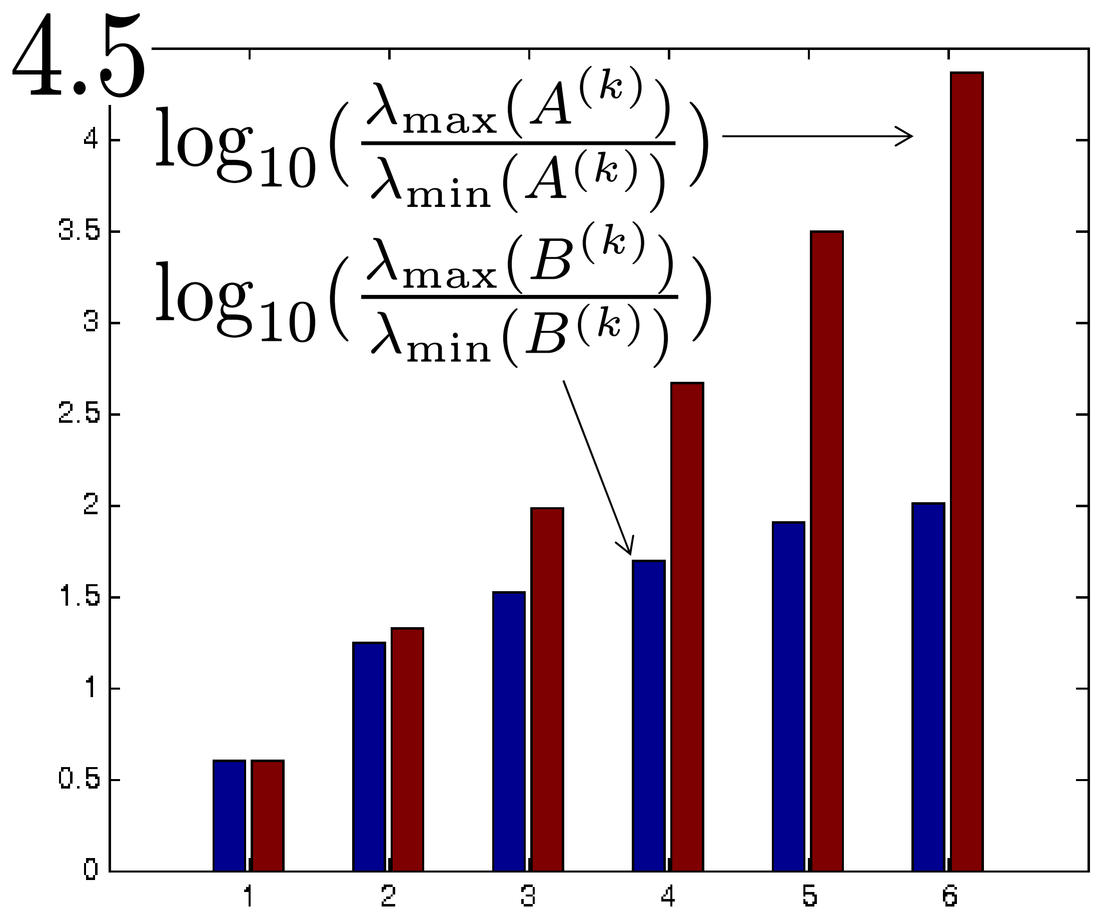
$$B_{i,j}^{(k)} := \langle \chi_i^{(k)}, \chi_j^{(k)} \rangle_a$$

Theorem

$$\frac{\lambda_{\max}(B^{(k)})}{\lambda_{\min}(B^{(k)})} \leq C$$

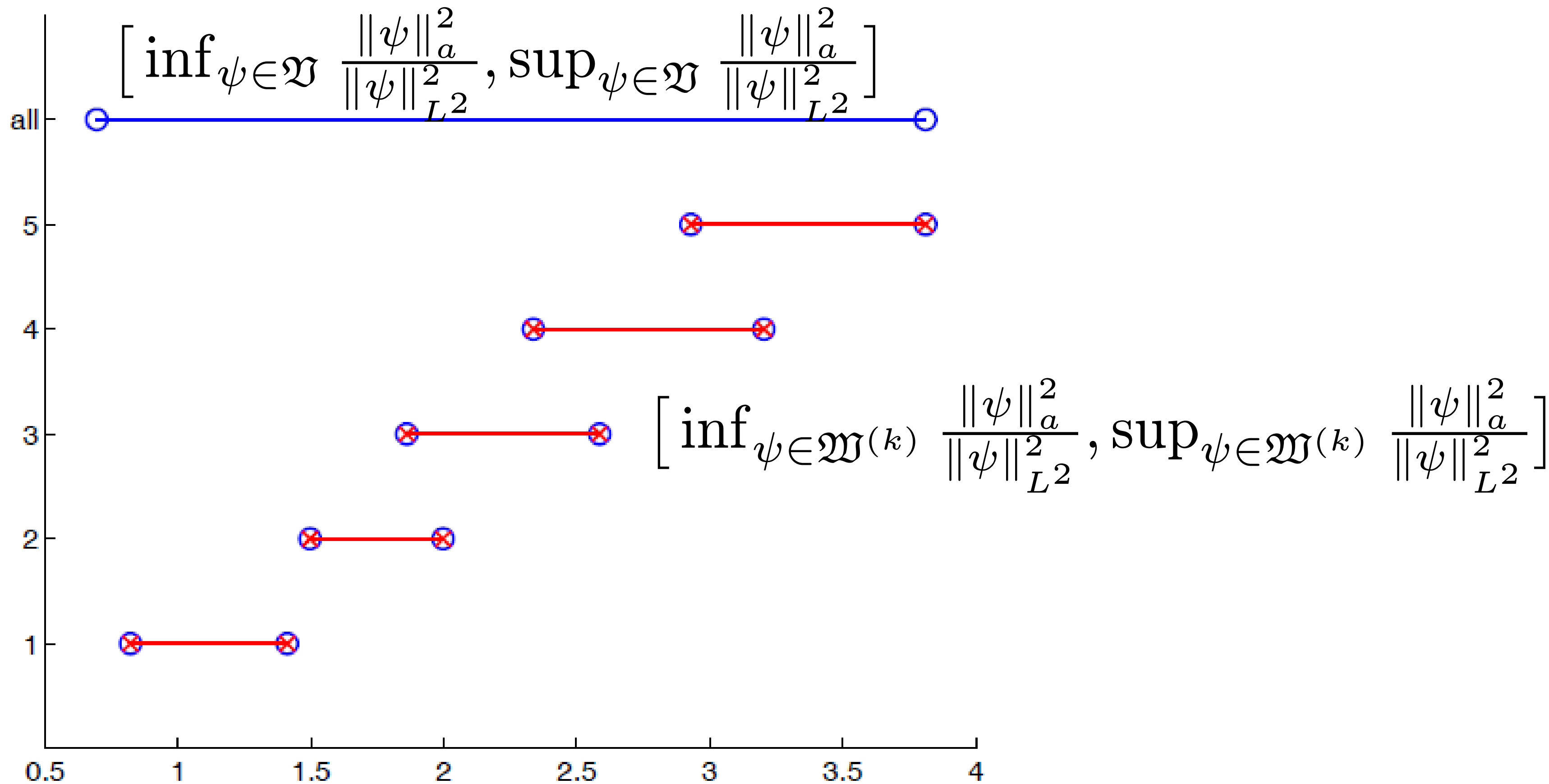
Just relax!

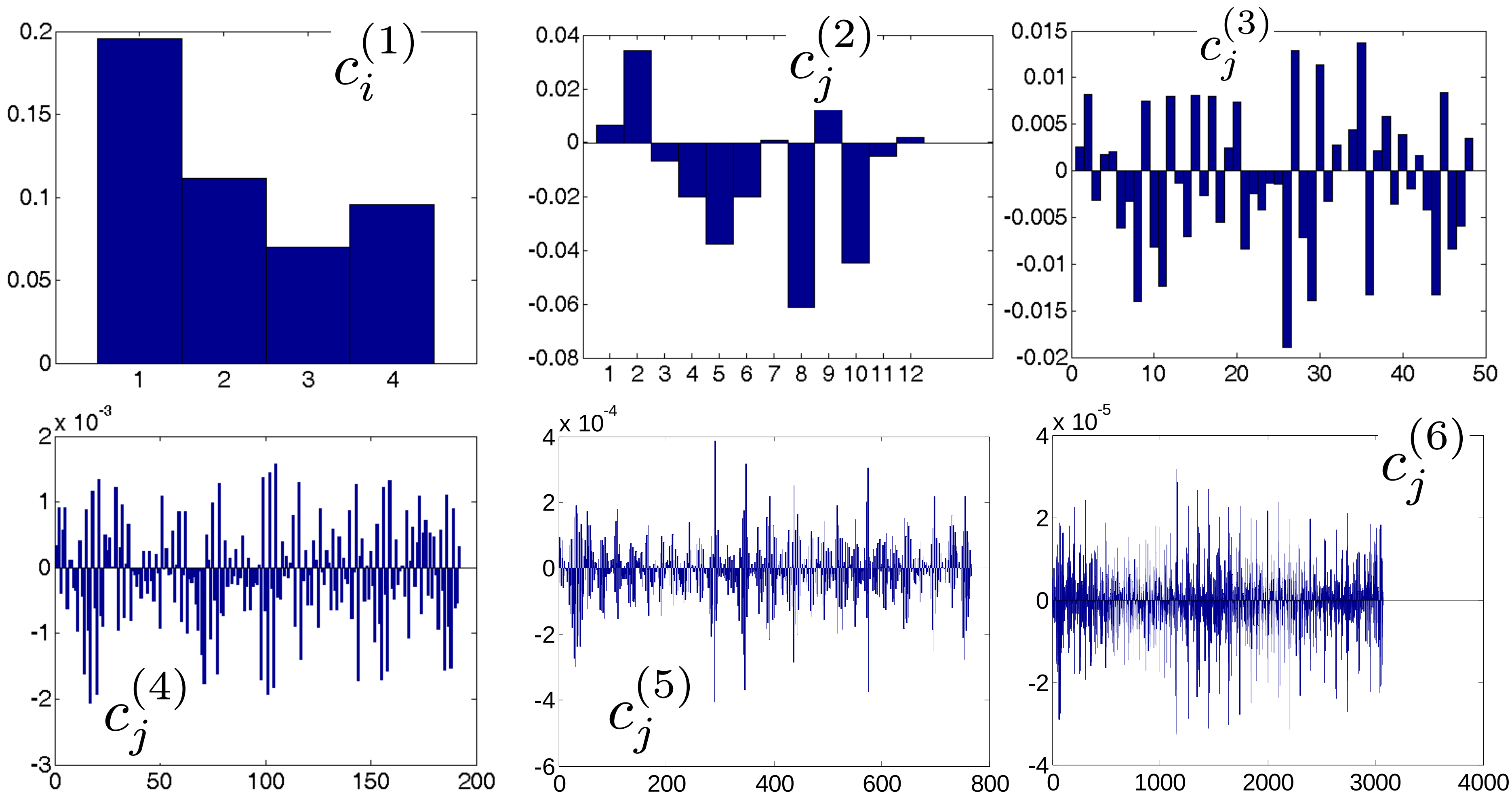
In $v \in \mathfrak{W}^{(k)}$
to get
$u^{(k)} - u^{(k-1)}$



$$\boxed{\mathfrak{V} = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)}}$$

Ranges of eigenvalues in $\mathfrak{V}$ and $\mathfrak{W}^{(k)}$ $(k = 1, \dots, 5)$ in log scale



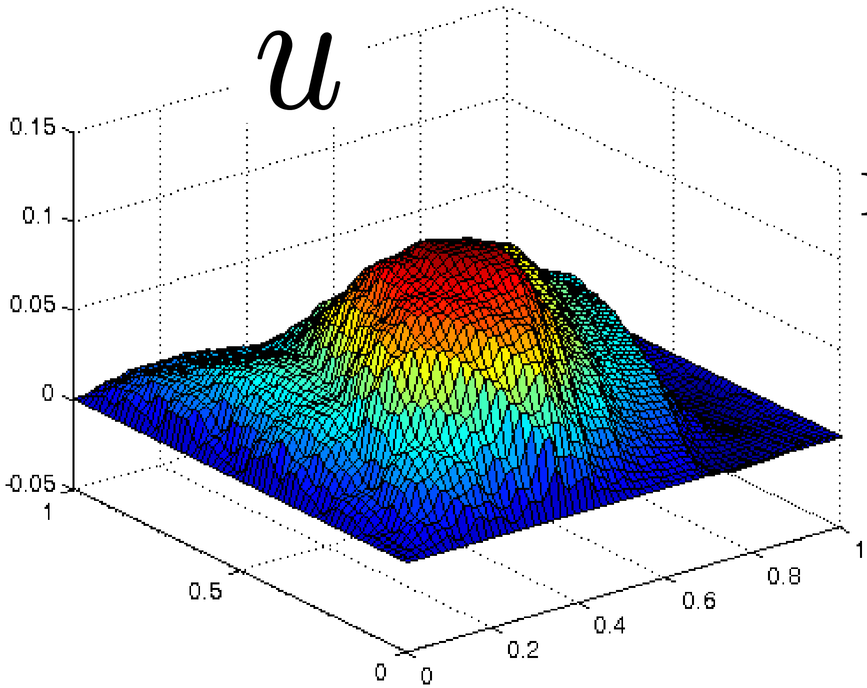


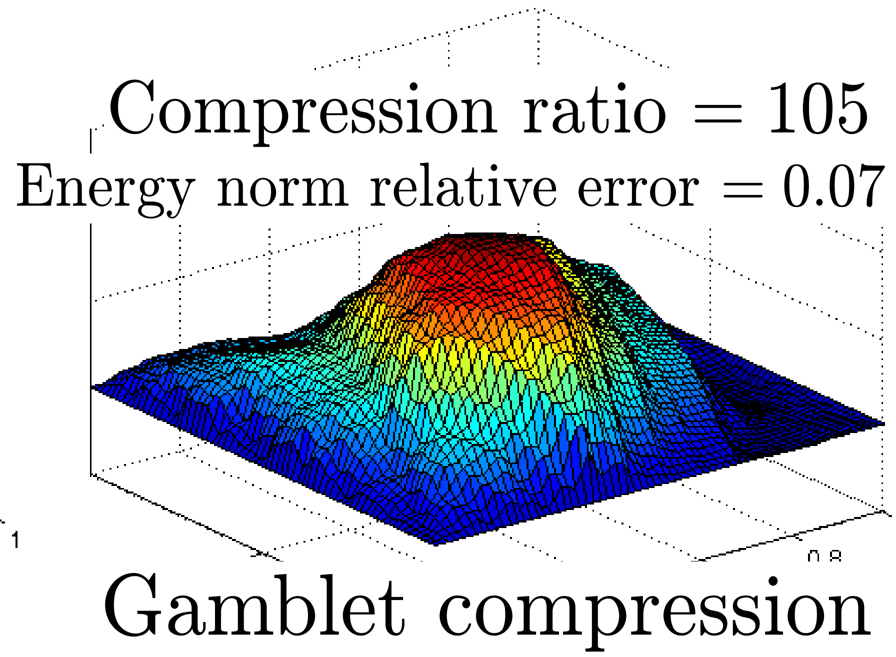
$$u = \sum_i c_i^{(1)} \frac{\psi_i^{(1)}}{\|\psi_i^{(1)}\|_a} + \sum_{k=2}^{q} \sum_j c_j^{(k)} \frac{\chi_j^{(k)}}{\|\chi_j^{(k)}\|_a}$$

Coefficients of the solution in the gamblet basis

Operator Compression

Gamblets behave like wavelets but they are adapted to the PDE and can compress its solution space





Throw 99% of the coefficients

Fast gamblet transform $\boxed{\mathcal{O}(N \ln^{3d} N) \text{ complexity}}$

Nesting $\boxed{A^{(k)} = (R^{(k,k+1)})^T A^{(k+1)} R^{(k,k+1)}}$

Level(k) gamblets and stiffness matrices can be computed from level(k+1) gamblets and stiffness matrices

Well conditioned linear systems

Underlying linear systems have uniformly bounded condition numbers

$$\boxed{\psi_i^{(k)} = \psi_{(i,1)}^{(k+1)} + \sum_j C_{i,j}^{(k+1),\chi} \chi_j^{(k+1)}} \qquad \boxed{C^{(k+1),\chi} = (B^{(k+1)})^{-1} Z^{(k+1)}}$$

$$Z_{j,i}^{(k+1)} := -(e_j^{(k+1)} - e_{j^-}^{(k+1)})^T A^{(k+1)} e_{(i,1)}^{(k+1)}$$

Localization

The nested computation can be localized without compromising accuracy or condition numbers

Theorem

Localizing $(\psi_i^{(k)})_{i\in\mathcal{I}_k}$ and $(\chi_i^{(k)})_i$ to subdomains of size

$\geq C H_k \ln \frac{1}{H_k}$ ⇒ $\boxed{\text{Cond. No } (B^{(k),\text{loc}}) \leq C}$

$\geq C H_k (\ln \frac{1}{H_k} + \ln \frac{1}{\epsilon})$ ⇒

$$\boxed{\left\| u - u^{(1),\text{loc}} - \sum_{k=1}^{q-1} (u^{(k+1),\text{loc}} - u^{(k),\text{loc}}) \right\|_a \leq \epsilon}$$

Theorem

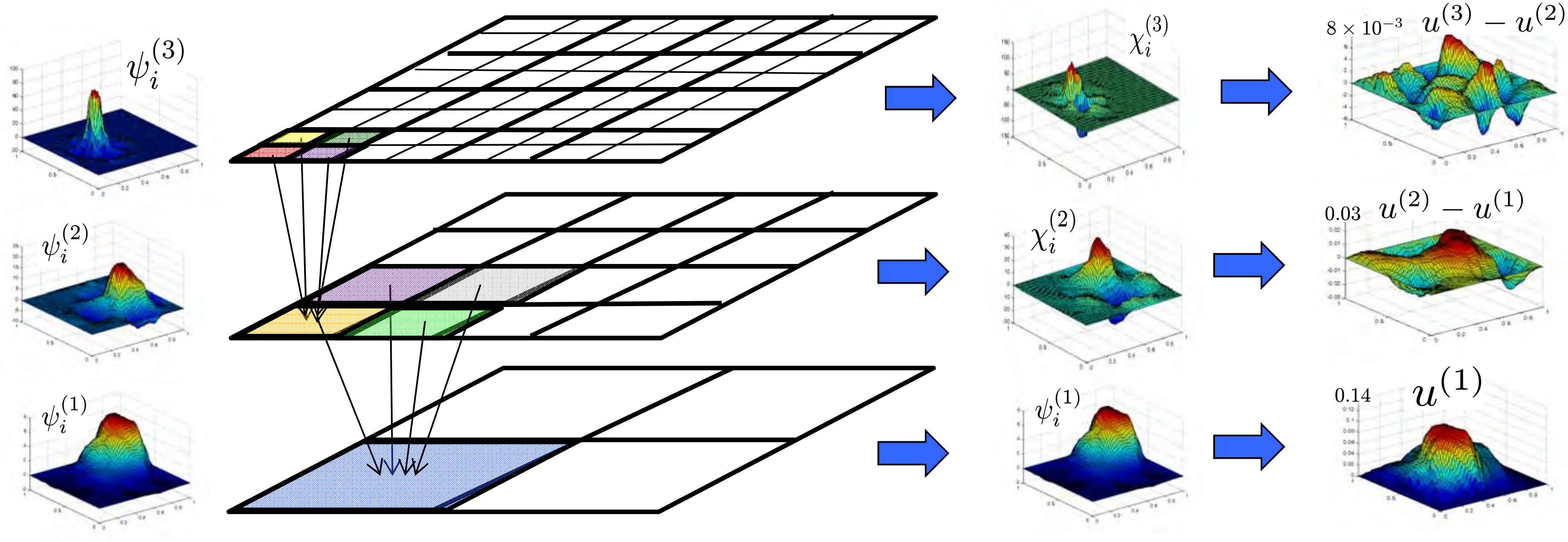
The number of operations to compute gamblets and achieve accuracy ϵ is $\mathcal{O}\big(N \ln^{3d}\big(\max(\frac{1}{\epsilon}, N^{1/d})\big)\big)$ (and $\mathcal{O}\big(N \ln^{d}(N^{1/d}) \ln \frac{1}{\epsilon}\big)$ for subsequent solves)

Complexity

Gamblet Transform $\boxed{\mathcal{O}(N \ln^{3d} N)}$ Linear Solve $\boxed{\mathcal{O}(N \ln^{d+1} N)}$

$$
\begin{tikzcd}
\varphi_i, A^h, M^h \arrow[r] & \psi_i^{(q)},\ A^{(q)} \arrow[r] \arrow[d] & \chi_i^{(q)}, B^{(q)} \arrow[r] \arrow[dl] & u^{(q)} - u^{(q-1)} \\
& \psi_i^{(q-1)},\ A^{(q-1)} \arrow[r] & \chi_i^{(q-1)}, B^{(q-1)} \arrow[r] & u^{(q-1)} - u^{(q-2)} \\
& \vdots & \vdots & \vdots \\
& \psi_i^{(3)},\ A^{(3)} \arrow[r] \arrow[d] & \chi_i^{(3)}, B^{(3)} \arrow[r] \arrow[dl] & u^{(3)} - u^{(2)} \\
& \psi_i^{(2)},\ A^{(2)} \arrow[r] \arrow[d] & \chi_i^{(2)}, B^{(2)} \arrow[r] \arrow[dl] & u^{(2)} - u^{(1)} \\
& \psi_i^{(1)},\ A^{(1)} \arrow[rr] & & u^{(1)}
\end{tikzcd}
$$

Parallel operating diagram both in space and in frequency



Numerical Homogenization

Harmonic Coordinates Babuska, Caloz, Osborn, 1994

Kozlov, 1979 Allaire Brizzi 2005; Owhadi, Zhang 2005

MsFEM [Hou, Wu: 1997]; [Efendiev, Hou, Wu: 1999]

[Fish - Wagiman, 1993] [Gloria 2010] Arbogast, 2011: Mixed MsFEM

Projection based method Nolen, Papanicolaou, Pironneau, 2008

HMM Engquist, E, Abdulle, Runborg, Schwab, et Al. 2003-...

Flux norm Berlyand, Owhadi 2010; Symes 2012

Localization [Chu-Graham-Hou-2010] (limited inclusions)

[Efendiev-Galvis-Wu-2010] (limited inclusions or mask)

[Babuska-Lipton 2010] (local boundary eigenvectors)

[Owhadi-Zhang 2011] (localized transfer property)

[Malqvist-Peterseim 2012] Volume averaged interpolation

[Owhadi-Zhang-Berlyand 2013] (Rough Polyharmonic Splines)

[Owhadi, SIAM MMS, 2015]
Bayesian Numerical Homogenization

[Hou and Liu,DCDS-A, 2016]

Statistical approach to numerical approximation

[Henri Poincaré. Calcul des probabilités. 1896.]

[A. V. Sul'din, Wiener measure and its applications to approximation methods. Matematika 1959]

[A. Sard. Linear approximation. 1963.]

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[E. W. Packel. The algorithm designer versus nature: a game-theoretic approach to information-based complexity. J. Complexity, 1987]

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Statistical approach to numerical approximation

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Some high level remarks

What is the worst?

$u^\dagger$: Unknown element of $\mathcal{A}$

$\mathcal{A}$

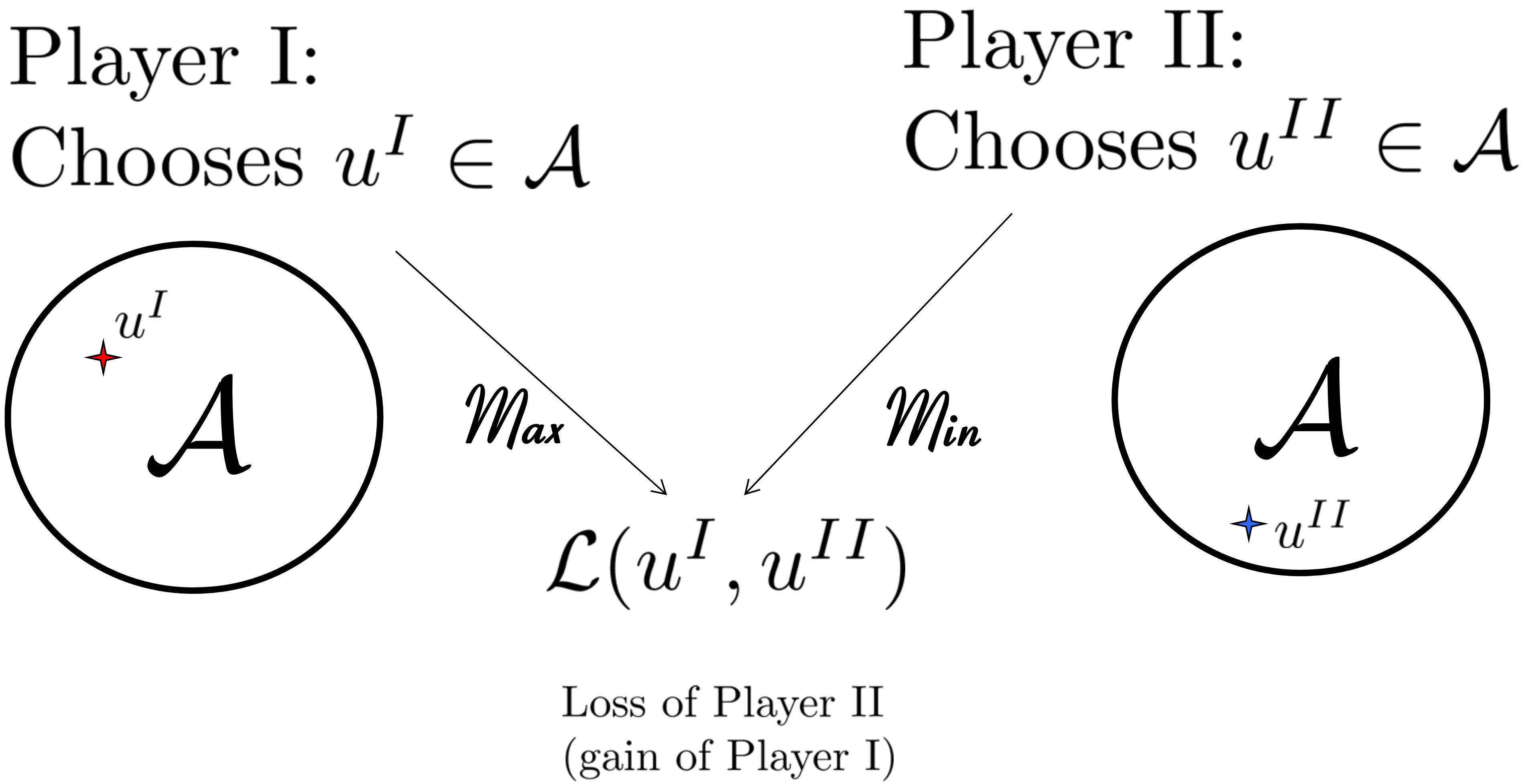
$$\Phi : \mathcal{A} \longrightarrow \mathbb{R}$$

$$u \longrightarrow \Phi(u) \quad \text{Quantity of Interest}$$

What is $\Phi(u^\dagger)$?

$$\inf_{u\in\mathcal{A}} \Phi(u) \leq \Phi(u^\dagger) \leq \sup_{u\in\mathcal{A}} \Phi(u)$$

Robust Optimization worst case



Game theoretic worst case

Robust Optimization worst case

Failure is not an option.
You want to always be right.

Game theoretic worst case

Interpretation depends on the choice of loss function.

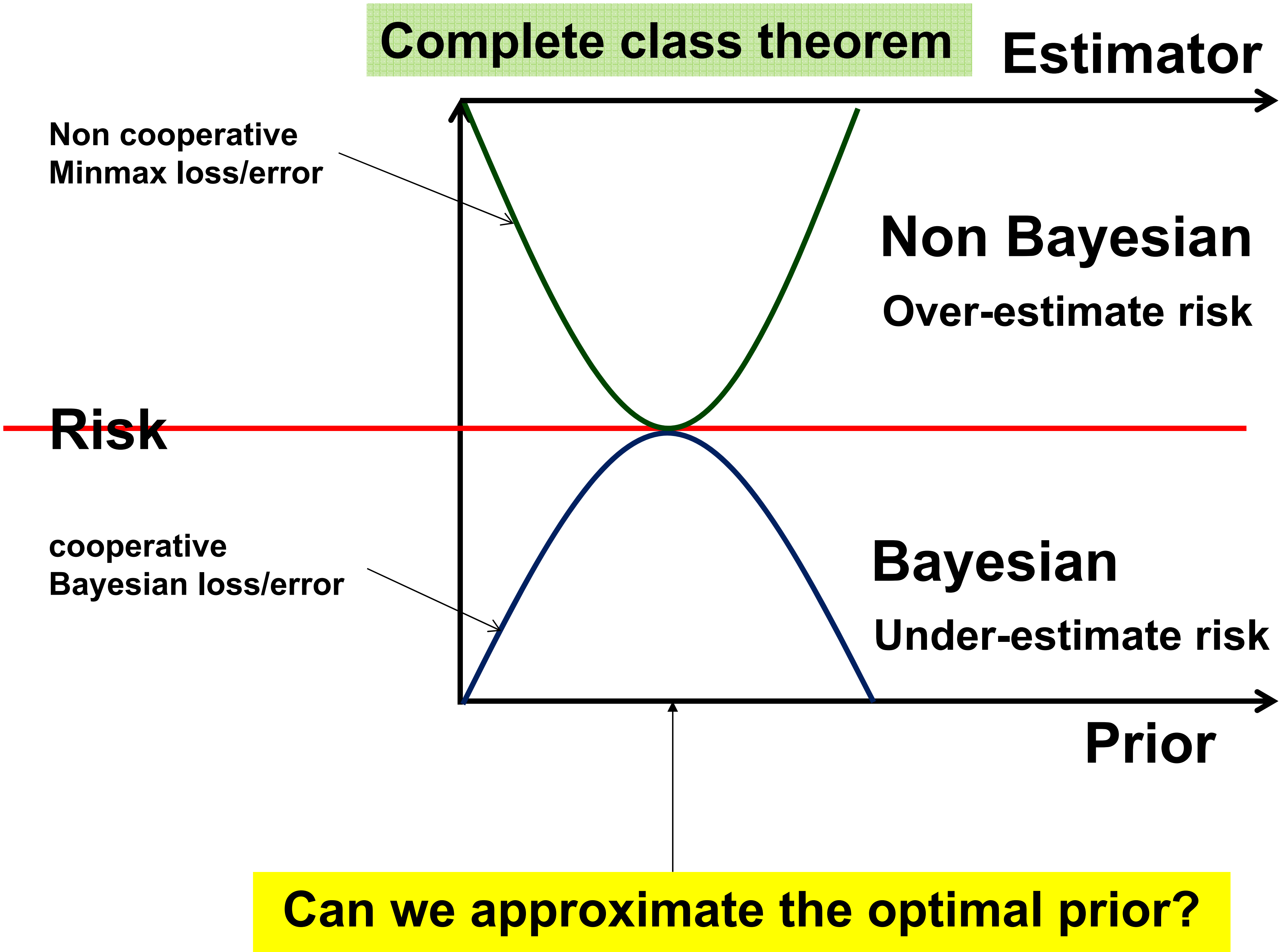
Confidence error

You want to be right with high probability.

Quadratic error

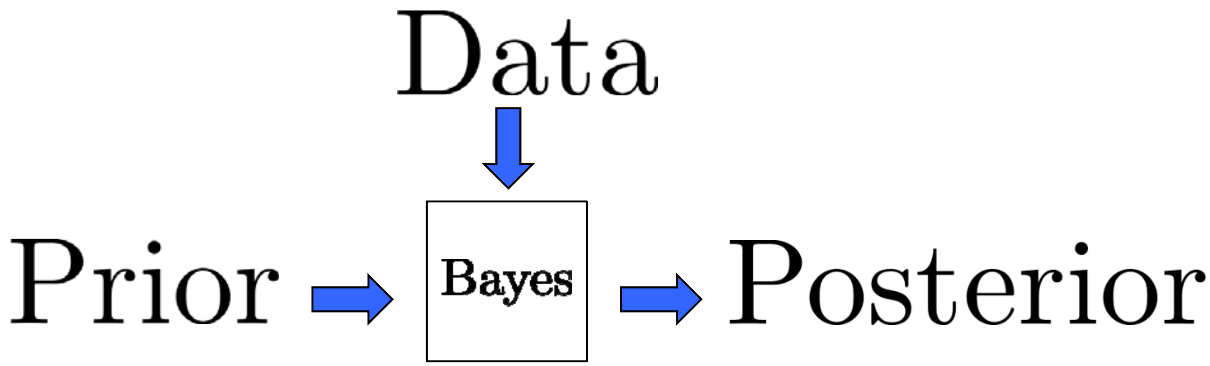
You want to be right on average.

Well suited for numerical computation where you need to keep computing with partial information (e.g. invert a 1,000,000 by 1,000,000 matrix)


Complete class theorem
Estimator
Non cooperative
Minmax loss/error
Non Bayesian
Over-estimate risk
Risk
cooperative
Bayesian loss/error
Bayesian
Under-estimate risk
Prior
Can we approximate the optimal prior?

Numerical robustness of Bayesian inference

$$\theta_\pi(d) = \mathbb{E}_{\mu\sim\pi,\, d\sim\mu^n}\left[\Phi(\mu)\middle|d\right]$$



Can we numerically approximate the prior when closed form expressions are not available for posterior values?

Prior → Numerical approximation → Prokhorov approximated prior

Densities → Numerical approximation → KL approximated prior

Curse of dimensionality

Prokhorov → TV → KL

TV ↕ Hellinger

Perturbed data → Prior → Bayes → Hellinger perturbed posterior

Data → TV perturbed prior → Bayes → Brittle posterior

Data → Prior → MC MC → TV approximated posterior

Data → KL perturbed prior → Bayes → KL perturbed posterior

Robustness of Bayesian conditioning in continuous spaces

- Brittleness of Bayesian Inference under Finite Information in a Continuous World. H. Owhadi, C. Scovel and T. Sullivan. Electronic Journal of Statistics, vol 9, pp 1-79, 2015. arXiv:1304.6772
- Brittleness of Bayesian inference and new Selberg formulas. H. Owhadi and C. Scovel. Communications in Mathematical Sciences (2015). arXiv:1304.7046
- On the Brittleness of Bayesian Inference. H. Owhadi, C. Scovel and T. Sullivan. SIAM Review, 57(4), 566-582, 2015, arXiv:1308.6306
- Qualitative Robustness in Bayesian Inference (2015). H. Owhadi and C. Scovel. arXiv:1411.3984

Positive

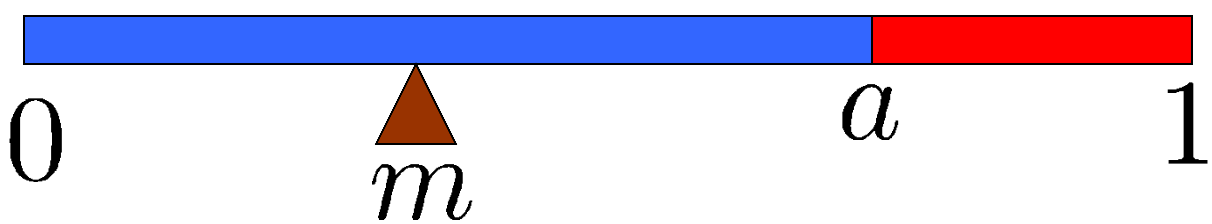
- Classical Bernstein Von Mises
- Wasserman, Lavine, Wolpert (1993)
- P Gustafson & L Wasserman (1995)
- Castillo and Rousseau (2013)
- Castillo and Nickl (2013)
- Stuart & Al (2010+).
- ....

Negative

- Freedman (1963, 1965)
- P Gustafson & L Wasserman (1995)
- Diaconis & Freedman 1998
- Johnstone 2010
- Leahu 2011
- Belot 2013

Brittleness of Bayesian Inference under Finite Information in a Continuous World. H. Owhadi, C. Scovel and T. Sullivan. Electronic Journal of Statistics, vol 9, pp 1-79, 2015. arXiv:1304.6772

10.000 children are given one pound of play-doh. On average, how much mass can they put above <u>a</u> while, on average, keeping the seesaw balanced around <u>m</u>?



Paul is given one pound of play-doh. What can you say about how much mass he is putting above a if all you have is the belief that he is keeping the seesaw balanced around m?

What is the least upper bound on

$$\mathbb{E}_{\mu\sim\pi}\left[\mu[X \geq a]\right]$$

If all you know is $\mathbb{E}_{\mu\sim\pi}\left[\mathbb{E}_{\mu}[X]\right] = m$ **?**

$$\mu \in \mathcal{A} := \mathcal{M}\big([0,1]\big)$$

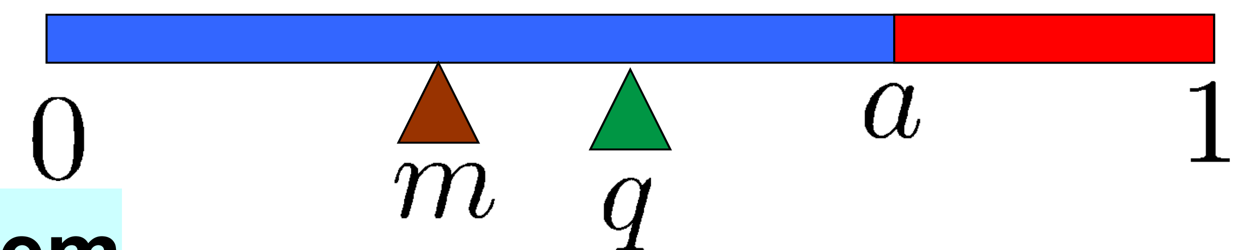
Answer

$$\boxed{\sup_{\pi\in\Pi} \mathbb{E}_{\mu\sim\pi}\left[\mu[X \geq a]\right]}$$

$$\boxed{\Pi := \left\{\pi \in \mathcal{M}(\mathcal{A}) \,:\, \mathbb{E}_{\mu\sim\pi}\left[\mathbb{E}_{\mu}[X]\right] = m\right\}}$$

$$\boxed{\sup_{\pi\in\Pi} \mathbb{E}_{\mu\sim\pi}\left[\mu[X\geq a]\right]}$$

$$\boxed{\Pi := \left\{\pi \in \mathcal{M}\big(\mathcal{M}([0,1])\big) \;:\; \mathbb{E}_{\mu\sim\pi}\left[\mathbb{E}_\mu[X]\right] = m\right\}}$$

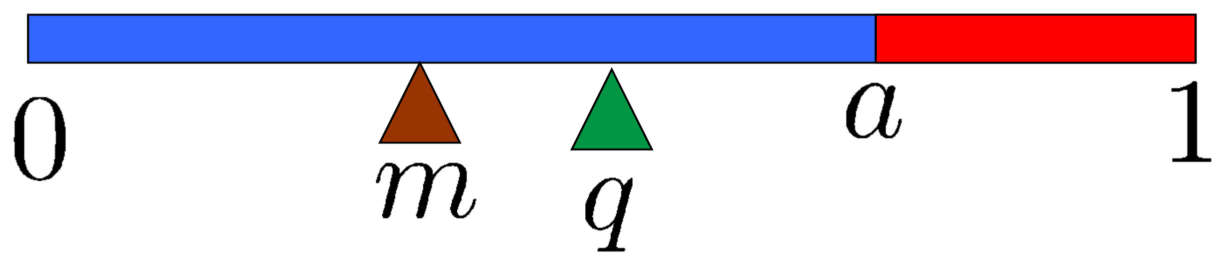


Theorem

$$\boxed{\begin{aligned}\sup_{\pi\in\Pi} \mathbb{E}_{\mu\sim\pi}\left[\mu[X\geq a]\right] = &\sup_{\mathbb{Q}\in\mathcal{M}([0,1])\,:\,\mathbb{E}_{\mathbb{Q}}[q]=m} \\ &\mathbb{E}_{q\sim\mathbb{Q}}\left[\sup_{\mu\in\mathcal{M}([0,1])\,:\,\mathbb{E}_\mu[X]=q} \mu[X\geq a]\right]\end{aligned}}$$

$$\sup_{\pi \in \Pi} \mathbb{E}_{\mu \sim \pi} \left[\mu[X \geq a] \right]$$

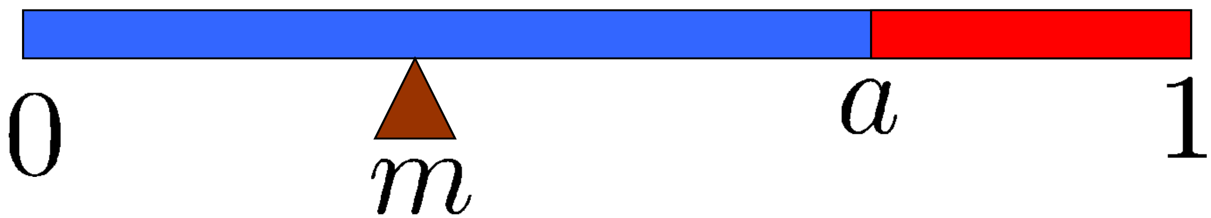
$$\Pi := \left\{ \pi \in \mathcal{M}\big(\mathcal{M}([0,1])\big) \;:\; \mathbb{E}_{\mu \sim \pi} \left[\mathbb{E}_{\mu}[X] \right] = m \right\}$$



$$\sup_{\pi \in \Pi} \mathbb{E}_{\mu \sim \pi} \left[\mu[X \geq a] \right] = \sup_{\mathbb{Q} \in \mathcal{M}([0,1]) \,:\, \mathbb{E}_{\mathbb{Q}}[q] = m} \mathbb{E}_{q \sim \mathbb{Q}} \left[\min\left(\frac{q}{a}, 1\right) \right]$$

$$\boxed{\sup_{\pi \in \Pi} \mathbb{E}_{\mu \sim \pi}\left[\mu[X \geq a]\right]}$$

$$\boxed{\Pi := \left\{\pi \in \mathcal{M}(\mathcal{M}([0,1])) \,:\, \mathbb{E}_{\mu \sim \pi}\left[\mathbb{E}_{\mu}[X]\right] = m\right\}}$$



$$\boxed{\sup_{\pi \in \Pi} \mathbb{E}_{\mu \sim \pi}\left[\mu[X \geq a]\right] = \frac{m}{a}}$$

Reduction calculus with measures over measures

$$\mathcal{M}(\mathcal{X}) \supset \mathcal{A} \xrightarrow{\Psi} \mathcal{Q}$$

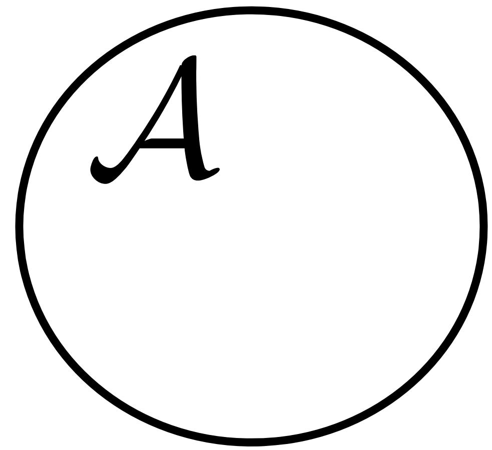
Polish space

$$\mathcal{M}(\mathcal{A}) \supset \Pi \xleftarrow{\Psi^{-1}} \mathfrak{Q} \subset \mathcal{M}(\mathcal{Q})$$

Theorem Brittleness of Bayesian Inference under Finite Information in a Continuous World. H. Owhadi, C. Scovel and T. Sullivan. Electronic Journal of Statistics, vol 9, pp 1-79, 2015. arXiv:1304.6772

$$\boxed{\begin{gathered}\sup_{\pi \in \Psi^{-1}\mathfrak{Q}} \mathbb{E}_{\mu\sim\pi}\big[\Phi(\mu)\big] \\ \| \\ \sup_{\mathbb{Q}\in\mathfrak{Q}} \Big[\mathbb{E}_{q\sim\mathbb{Q}}\big[\sup_{\mu\in\Psi^{-1}(q)} \Phi(\mu)\big]\Big]\end{gathered}}$$

What is the worst with random data?

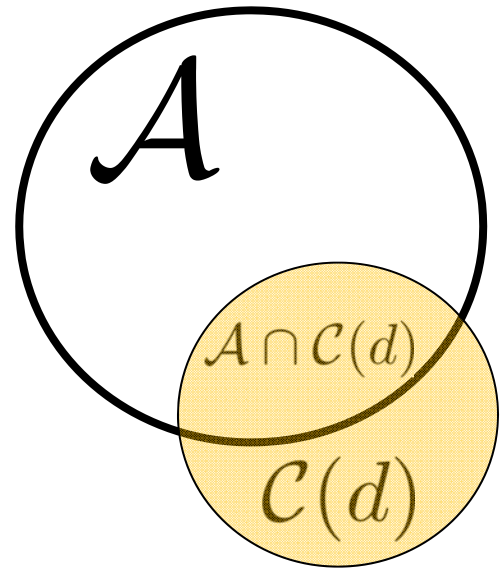


$\mu^\dagger$: Unknown element of $\mathcal{A}$

$$\begin{aligned}\Phi \ : \ \mathcal{A} &\longrightarrow \mathbb{R} \\ \mu &\longrightarrow \Phi(\mu) \quad \text{Quantity of Interest}\end{aligned}$$

You observe data $d \sim (\mu^\dagger)^n$

What is $\Phi(\mu^\dagger)$?



Find a (confidence) set $\mathcal{C}(d)$ such that with probability $1-\epsilon$

$$\mu^\dagger \in \mathcal{C}(d)$$

With probability $1-\epsilon$

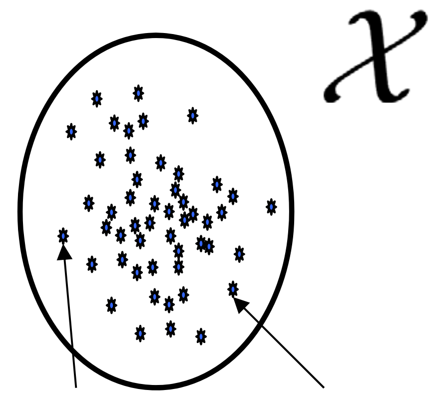
$$\inf_{\mu\in\mathcal{A}\cap\mathcal{C}(d)} \Phi(\mu) \leq \Phi(\mu^\dagger) \leq \sup_{\mu\in\mathcal{A}\cap\mathcal{C}(d)} \Phi(\mu)$$

Notion of worst/sharpest depends on the particular choice of $\mathcal{C}(d)$

Frequentist/Concentration of measure worst case

$$\mu \in \mathcal{M}(\mathcal{X})$$

$$\mu_n := \frac{1}{n}\sum_{i=1}^n \delta_{X_i} \in \mathcal{M}(\mathcal{X})$$

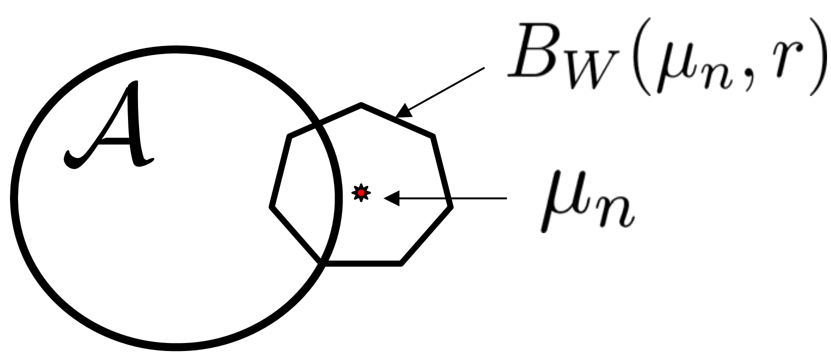


$$d = (X_1, \ldots, X_n)$$

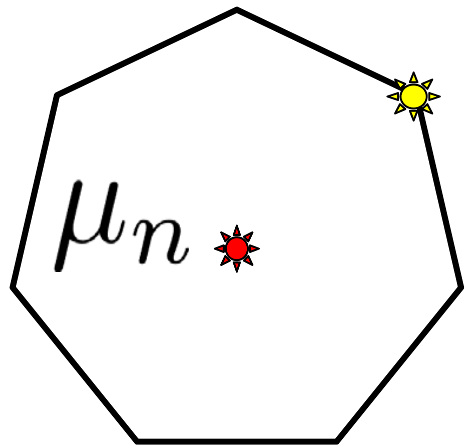
Theorem $d_{\text{Wasserstein}}(\mu,\mu_n) = \sup_{f\in \text{Lip}_1}\left(\mathbb{E}_\mu[f] - \mathbb{E}_{\mu_n}[f]\right)$ $\quad \mathbb{E}_{X\sim\mu}\left[e^{\|X\|^a}\right] < \infty$

$$\mu^n\left[d_{\text{W}}(\mu,\mu_n) \geq r\right] \leq C\left(e^{-cnr^m}1_{r\leq 1} + e^{-cnr^a}1_{r>1}\right)$$

N. Fournier and A. Guillin, On the rate of convergence in Wasserstein distance of the empirical measure, Probability Theory and Related Fields, (2014), pp. 1-32.



Reduction calculus of the ball about the empirical distribution



- D. Wozabal. A framework for optimization under ambiguity. Annals of Operations Research, 193(1):21–47, 2012.
- P. M. Esfahani and D. Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: performance guarantees and tractable reformulations. arXiv:1505.05116, 2015.
- Extreme points of a ball about a measure with finite support (2015). H. Owhadi and Clint Scovel. arXiv:1504.06745

The extreme points of the Prokhorov, Monge-Wasserstein and Kantorovich metric balls about a measure whose support has at most n points, consist of measures whose supports have at most n+2 points.

Question

Game/Decision Theory + Information Based Complexity

⬇

Turn the process of discovery of scalable numerical solvers into an algorithm

Worst case calculus

⬇

?

The truncated moment problem

$$\mathcal{M}[0,1] \xrightarrow{\quad\Psi\quad} \mathbb{R}^k$$

$$\mu \longrightarrow \left(\mathbb{E}_{X\sim\mu}[X], \mathbb{E}_{X\sim\mu}[X^2], \ldots, \mathbb{E}_{X\sim\mu}[X^k]\right)$$

$$\boxed{\text{Study of the geometry of } M_k := \Psi\big(\mathcal{M}([0,1])\big)}$$

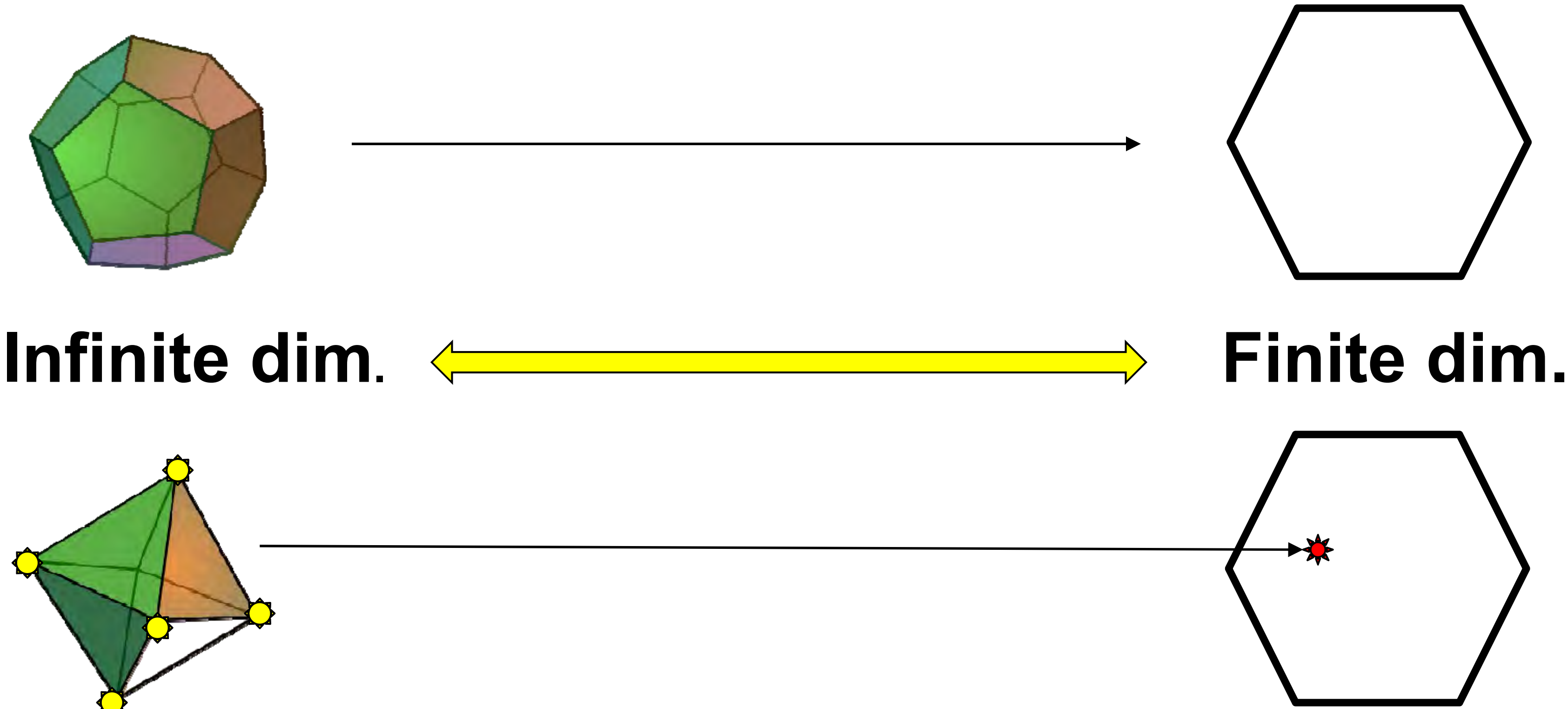
P. L. Chebyshev
1821-1894

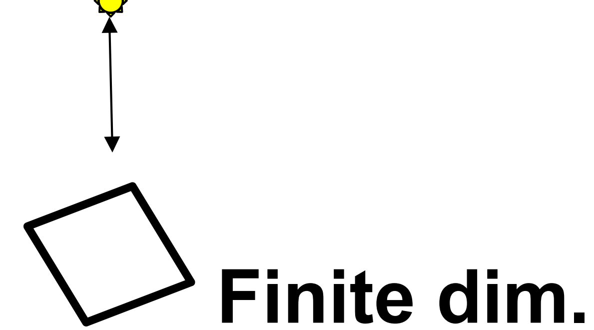
A. A. Markov
1856-1922

M. G. Krein
1907-1989

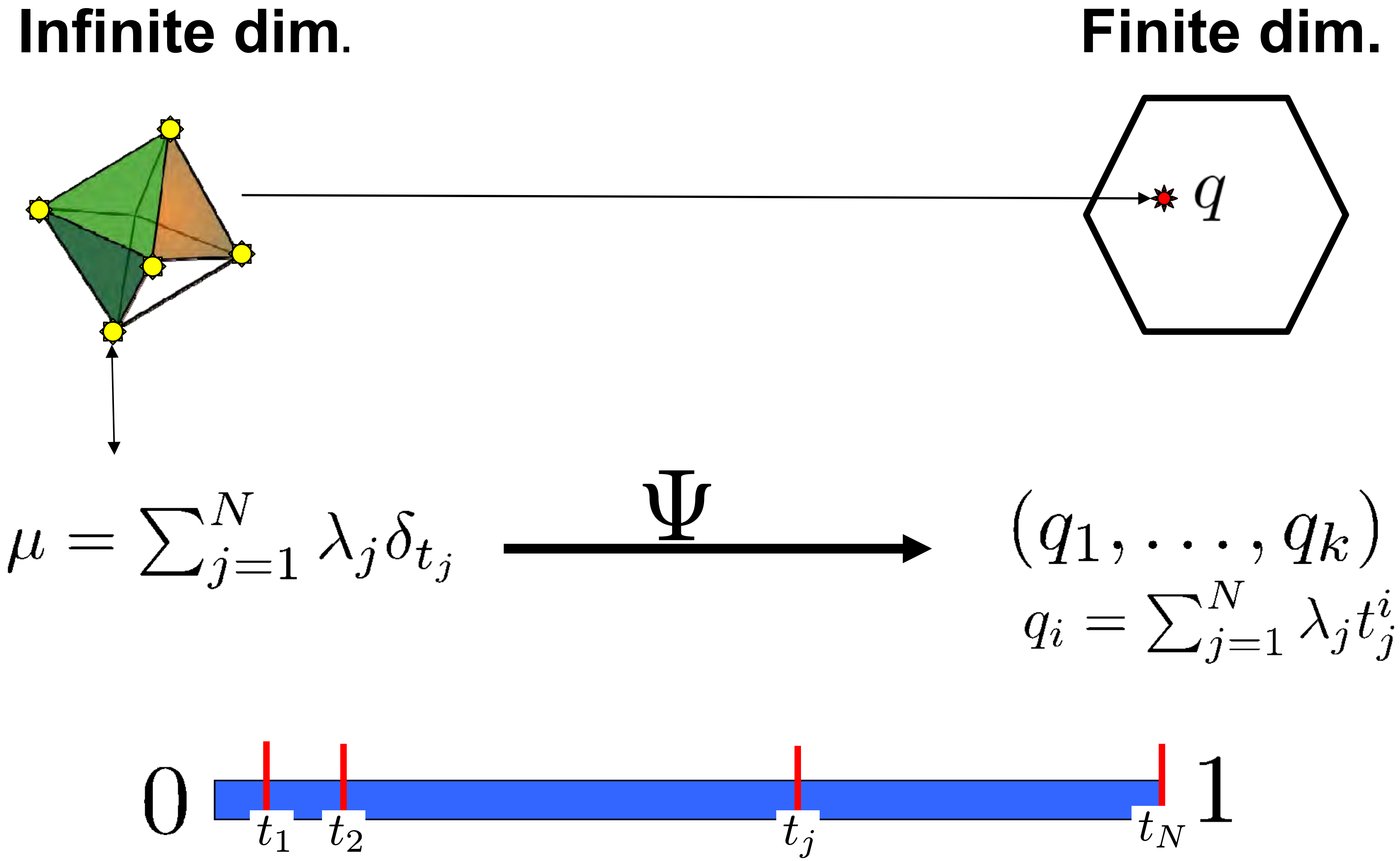
$$\mathcal{M}[0,1] \xrightarrow{\quad\Psi\quad} \mathbb{R}^k \qquad \boxed{M_k := \Psi(\mathcal{M}([0,1]))}$$

$$\mu \longrightarrow \left(\mathbb{E}_{X\sim\mu}[X], \mathbb{E}_{X\sim\mu}[X^2], \ldots, \mathbb{E}_{X\sim\mu}[X^k]\right)$$





Let us compute $\mathrm{Vol}(M_k)$ using different extreme points representations.


Infinite dim.
Finite dim.
q
$\mu = \sum_{j=1}^{N} \lambda_j \delta_{t_j}$
Ψ
$(q_1, \ldots, q_k)$
$q_i = \sum_{j=1}^{N} \lambda_j t_j^i$
0
1
t_1
t_2
t_j
t_N

$$\boxed{\mu = \sum_{j=1}^{N} \lambda_j \delta_{t_j}}$$

Index $i(\mu)$: Number of support points of μ

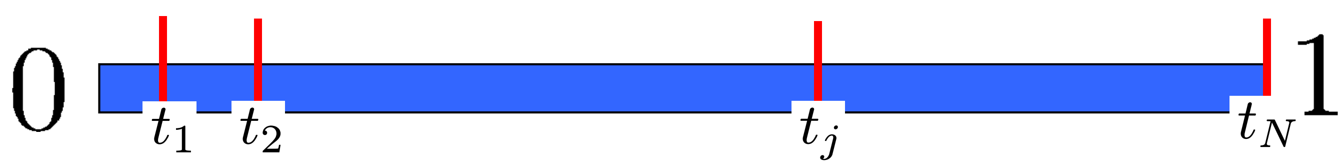
Counting interior points with weight 1 and boundary points with weight $\frac{1}{2}$

μ is called
- principal if $i(\mu) = \frac{k+1}{2}$
- canonical if $i(\mu) = \frac{k+2}{2}$
- upper if support points include 1
- lower if support points do not include 1

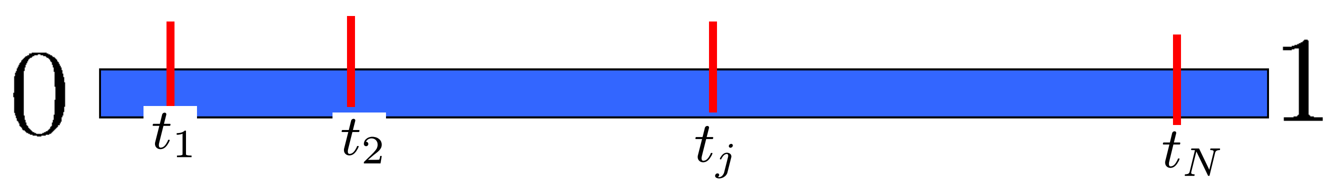
Theorem

Every point $q \in \mathrm{Int}(M_k)$ has a unique upper and lower principal representation.

Upper



Lower



$\mathrm{Vol}(M_{2m-1})$ using Upper Rep. $=$ $\mathrm{Vol}(M_{2m-1})$ using Lower Rep.

$$\boxed{\frac{1}{(m-1)!} S_{m-1}(3,3,2) = \frac{1}{m!} S_m(1,1,2)}$$

$\mathrm{Vol}(M_{2m})$ using Upper Rep. $=$ $\mathrm{Vol}(M_{2m})$ using Lower Rep.

$$\boxed{S_m(1,3,2) = S_m(3,1,2)}$$

Selberg Identities

$$S_n(\alpha,\beta,\gamma) = \prod_{j=0}^{n-1} \frac{\Gamma(\alpha+j\gamma)\Gamma(\beta+j\gamma)\Gamma(1+(j+1)\gamma)}{\Gamma(\alpha+\beta+(n+j-1)\gamma)\Gamma(1+\gamma)}$$

$$S_n(\alpha,\beta,\gamma) := \int_{[0,1]^n} \prod_{j=1}^{n} t_j^{\alpha-1}(1-t_j)^{\beta-1}|\Delta(t)|^{2\gamma} dt\,.$$

$$\Delta(t) := \prod_{j<k} (t_k - t_j)$$

Brittleness of Bayesian inference and new Selberg formulas. H. Owhadi and C. Scovel. Communications in Mathematical Sciences (2015). arXiv:1304.7046

Forrester and Warnaar 2008

The importance of the Selberg integral

Used to prove outstanding conjectures in Random matrix theory and cases of the Macdonald conjectures

Central role in random matrix theory, Calogero-Sutherland quantum many-body systems, Knizhnik-Zamolodchikov equations, and multivariable orthogonal polynomial theory

$$\boxed{\mu = \sum_{j=1}^{N} \lambda_j \delta_{t_j}}$$

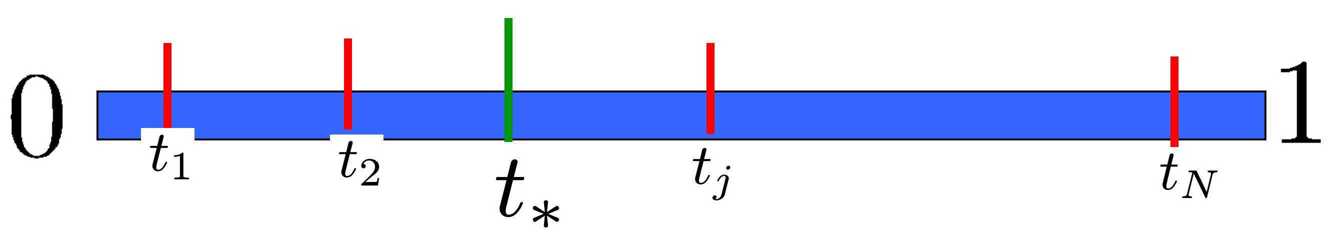
Index $i(\mu)$: Number of support points of μ

Counting interior points with weight 1 and boundary points with weight $\frac{1}{2}$

μ is called
- principal if $i(\mu) = \frac{k+1}{2}$
- canonical if $i(\mu) = \frac{k+2}{2}$
- upper if support points include 1
- lower if support points do not include 1

Theorem

For $t_* \in (0,1)$, every point $q \in \mathrm{Int}(M_k)$ has a unique canonical representation whose support contains t_*. When $t_* = 0$ or 1, there exists a unique principal representation whose support contains t_*.



New Reproducing Kernel Hilbert Spaces and Selberg Integral formulas related to the Markov-Krein representations of moment spaces.

$$\mathcal{M}[0,1] \xrightarrow{\quad\Psi\quad} [0,1]^k$$

$$\mu \longrightarrow \left(\mathbb{E}_{X\sim\mu}[X], \mathbb{E}_{X\sim\mu}[X^2], \ldots, \mathbb{E}_{X\sim\mu}[X^k]\right)$$

$$\boxed{\int_{I^m} \Sigma t^{-1} \cdot \prod_{j=1}^m t_j^2 (1-t_j)^2 \Delta_m^4(t) dt = \frac{S_m(5,1,2) - S_m(3,3,2)}{2}}$$

$$\boxed{\int_{I^m} \Sigma t^{-1} \cdot \prod_{j=1}^m t_j^2 \cdot \Delta_m^4(t) dt = \frac{m}{2} S_{m-1}(5,3,2)}$$

$$\Delta_m(t) := \prod_{j<k} (t_k - t_j) \quad I := [0,1]$$

$$\left(\Sigma\phi\right)(t) := \sum_{j=1}^m \phi(t_j), \quad t \in I^m$$

$$S_n(\alpha,\beta,\gamma) = \prod_{j=0}^{n-1} \frac{\Gamma(\alpha+j\gamma)\Gamma(\beta+j\gamma)\Gamma(1+(j+1)\gamma)}{\Gamma(\alpha+\beta+(n+j-1)\gamma)\Gamma(1+\gamma)}$$

$$e_j(t) := \sum_{i_1<\cdots<i_j} t_{i_1}\cdots t_{i_j}$$

Π_0^n: n-th degree polynomials which vanish on the boundary of $[0,1]$

$M_n \subset \mathbb{R}^n$: set of $q = (q_1, \ldots, q_n) \in \mathbb{R}^n$ such that there exists a probability measure μ on $[0,1]$ with $\mathbb{E}_\mu[X^i] = q_i$ with $i \in \{1, \ldots, n\}$.

Theorem

Bi-orthogonal systems of Selberg Integral formulas

Consider the basis of Π_0^{2m-1} consisting of the associated Legendre polynomials $Q_j, j = 2,..,2m-1$ of order 2 translated to the unit interval I. For $k = 2,..,2m-1$ define

$$a_{jk} := \frac{(j+k+k^2)\Gamma(j+2)\Gamma(j)}{\Gamma(j+k+2)\Gamma(j-k+1)}, \quad k \le j \le 2m-1$$

$$\tilde{h}_k(t) := \sum_{j=k}^{2m-1} (-1)^{j+1} a_{jk} e_{2m-1-j}(t,t)\,.$$

Then for $j = k \bmod 2$, $j, k = 2,..,2m-1$, we have

$$\boxed{\int_{I^{m-1}} \tilde{h}_k(t)\Sigma Q_j(t) \prod_{j'=1}^{m-1} t_{j'}^2 \cdot \Delta_{m-1}^4(t)dt = Vol(M_{2m-1})(2m-1)!(m-1)!\frac{(k+2)!}{(8k+4)(k-2)!}\delta_{jk}\,.}$$

Collaborators

Clint Scovel (Caltech), Tim Sullivan (Warwick), Mike McKerns (Caltech), Michael Ortiz (Caltech), Lei Zhang (Jiaotong), Leonid Berlyand (PSU), Lan Huong Nguyen, Paul Herve Tamogoue Kamga.

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National Nuclear Security Administration