



Data-Driven Mechanics: Constitutive Model-Free Approach

$$\inf_{y \in D} \inf_{z \in E} \|y - z\| = \inf_{z \in E} \inf_{y \in D} \|y - z\|$$

Michael Ortiz – Lecture 5

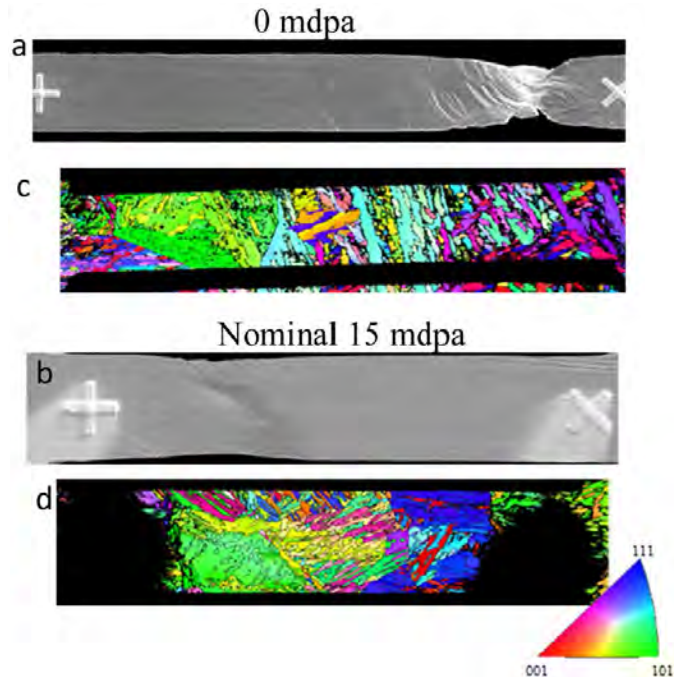
California Institute of Technology and
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Centre International des Sciences Mécaniques (CSIM)
Udine (Italy), October 10-14, 2022

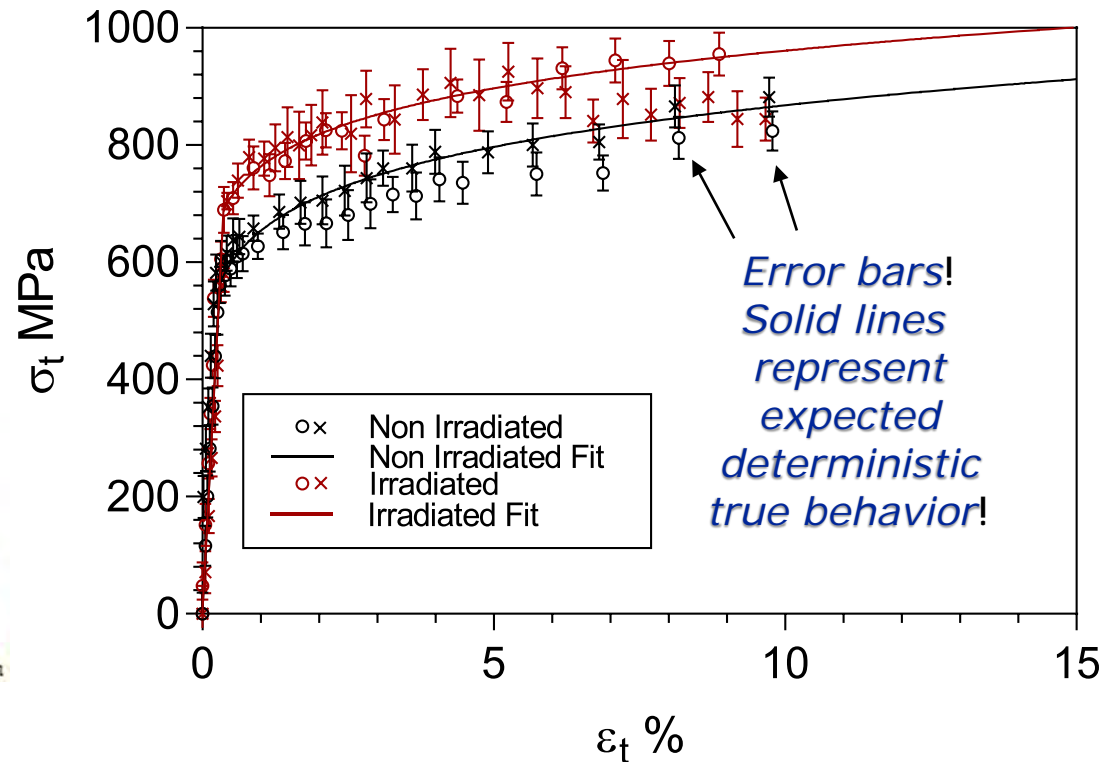
Model-Free Data-Driven inference – Motivation

- Recall: *Deterministic Data-Driven problems* are defined by:
 - A *phase space* Z of dimension $2N$
 - A *material data set* D in the form of a graph (manifold) of dimension N
 - An *admissible set* E in the form of an affine subspace of dimension N
- The set of *classical solutions* of the Data-Driven problem is $D \cap E$ (possibly \emptyset)
- But: *Problems can be stochastic* in nature due to:
 - *Observational error* (scatter) but *deterministic* true material law

Model-Free Data-Driven inference – Motivation

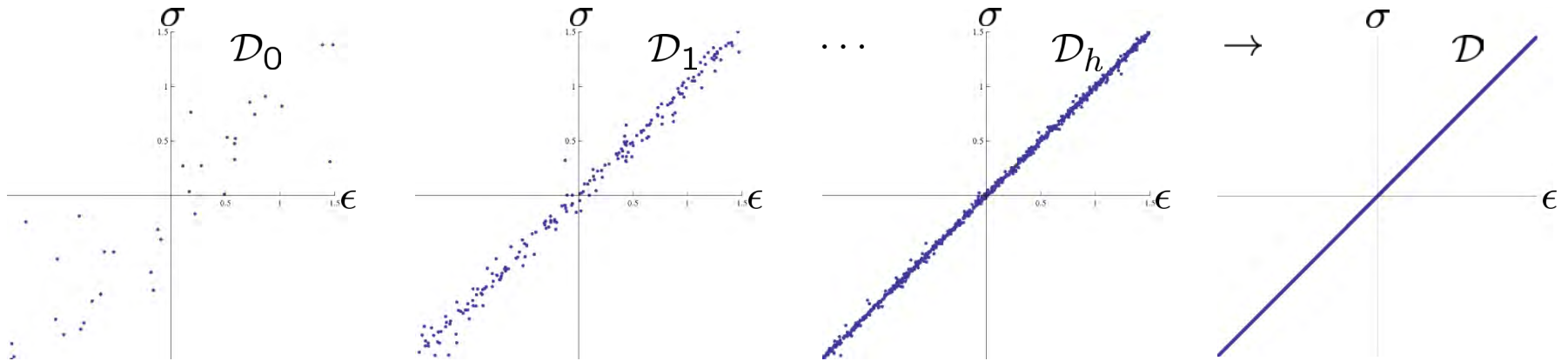


Post necking behavior of non-irradiated and irradiated *micro-tensile specimens*. (a,b) Secondary electron images. (c,d) Electron backscattered diffraction (EBSD) orientation maps



True stress–true strain curves generated by XRD/DIC technique for irradiated and non-irradiated SA-508-4N ferritic steel specimens. Solid lines depict fitted curves assuming *power-law hardening*.

Model-Free Data-Driven inference – Motivation

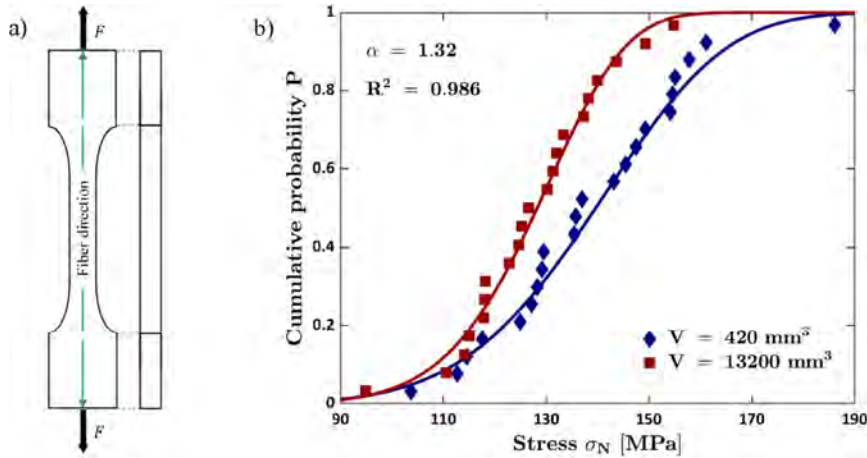


Sequence of material data sets *converging uniformly* (increasing number of points, decreasing scatter) to a limiting *deterministic* material law.

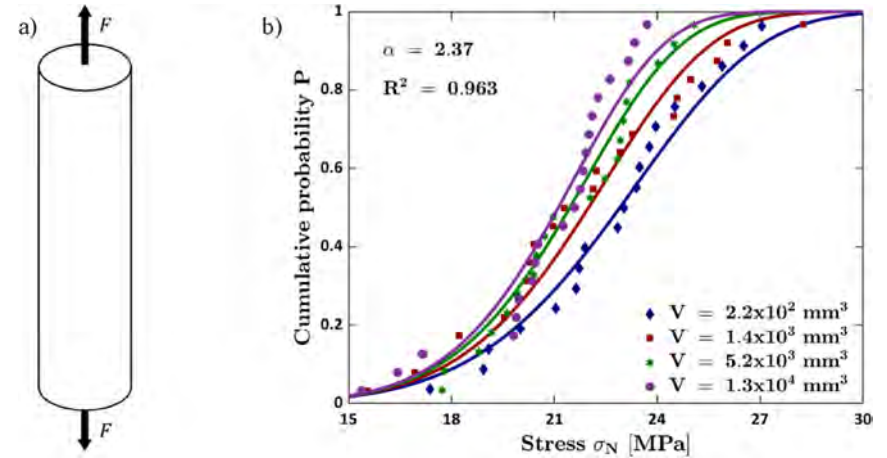
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 - *Intrinsic randomness* of the material behavior (e.g., *strength*)

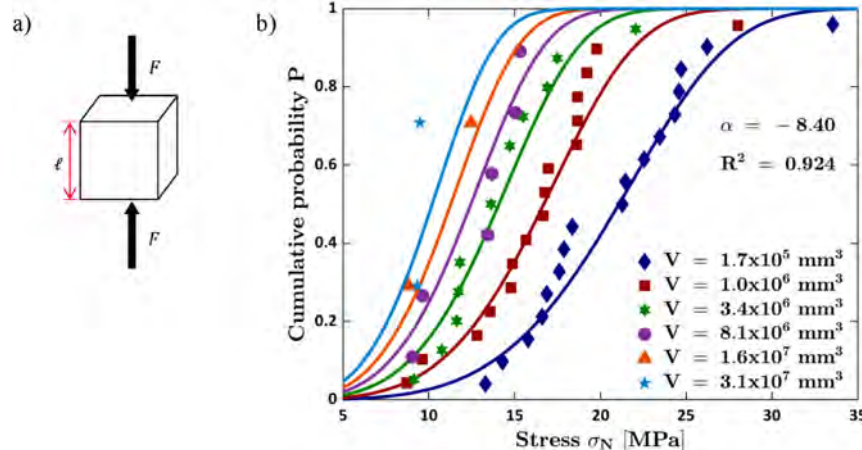
Model-Free Data-Driven inference – Motivation



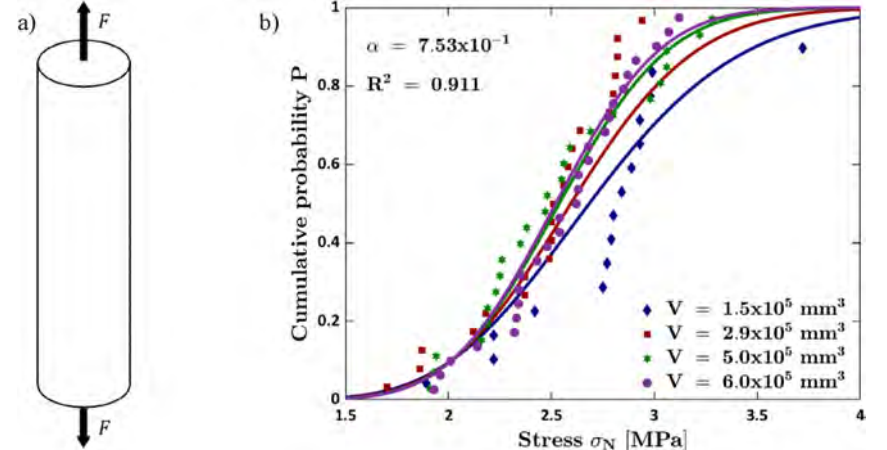
Spruce (*Picea abies*) tensile strength



Graphite tensile strength



Coal seam compressive strength



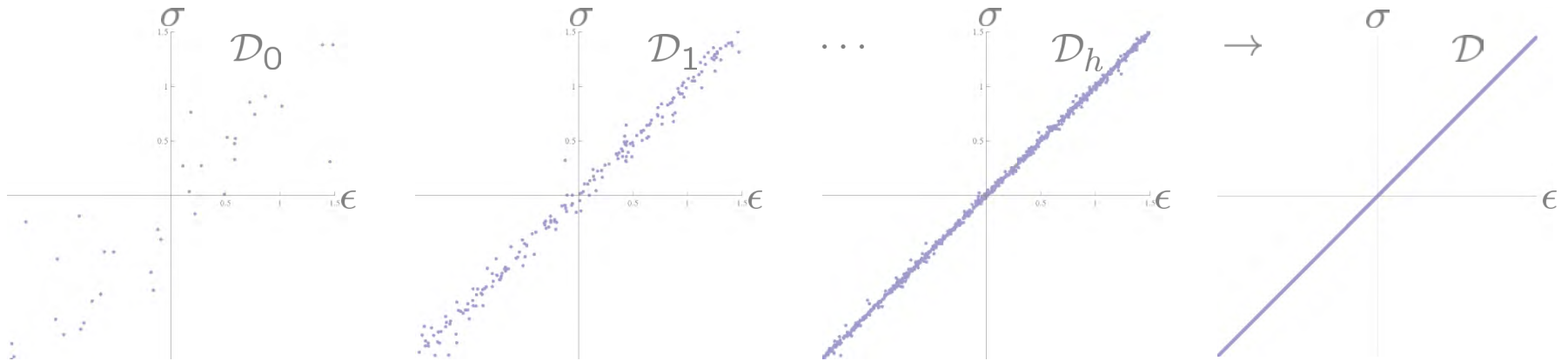
Aluminum foam tensile strength

Experimental strength data and Largest Extreme Value Distribution (LEVD) fit.

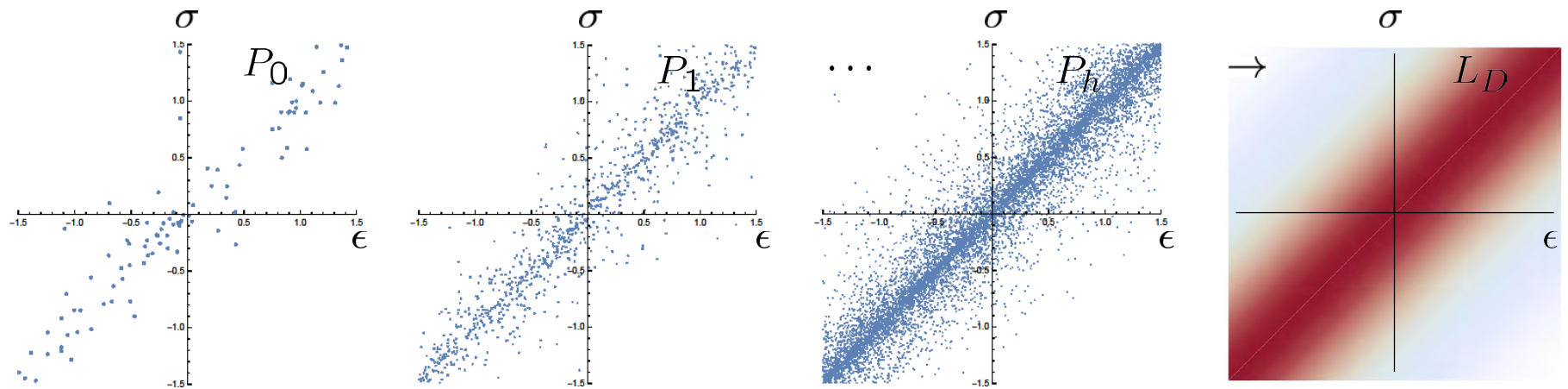
E. Gumbel, *Statistics of Extremes*, Columbia University Press, New York, 1958.

A.P. Pagnoncelli, A. Tridello and D.S. Paolino, *Mater. Des.*, **195** (2020) 109052.

Model-Free Data-Driven inference – Motivation



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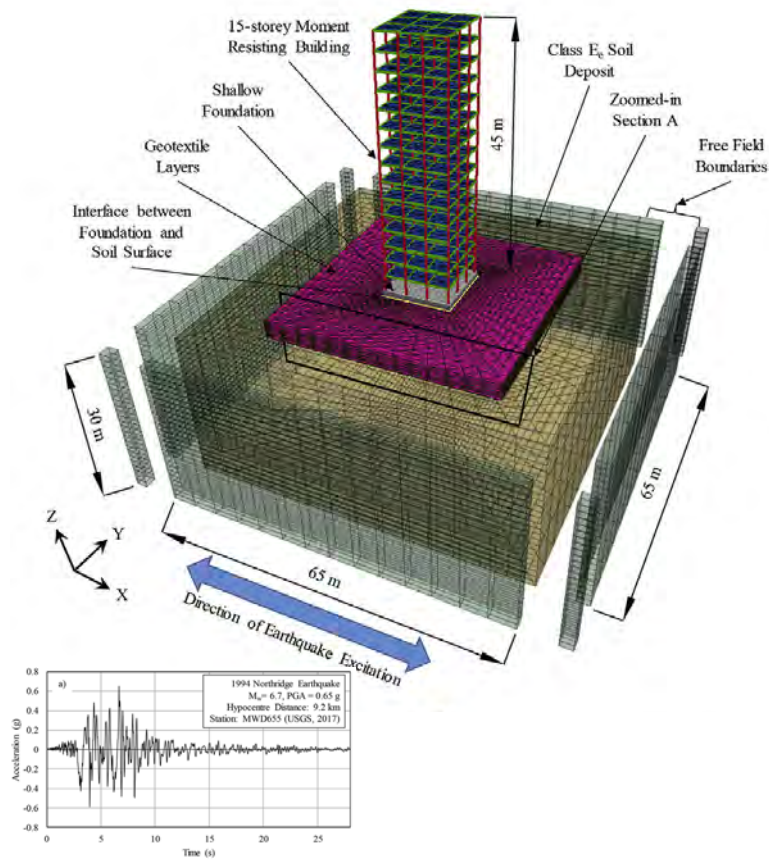


Sequence of discrete point-data sets *converging weakly* (in the sense of 'local averages') to a limiting *material likelihood density*.

Model-Free Data-Driven inference – Motivation

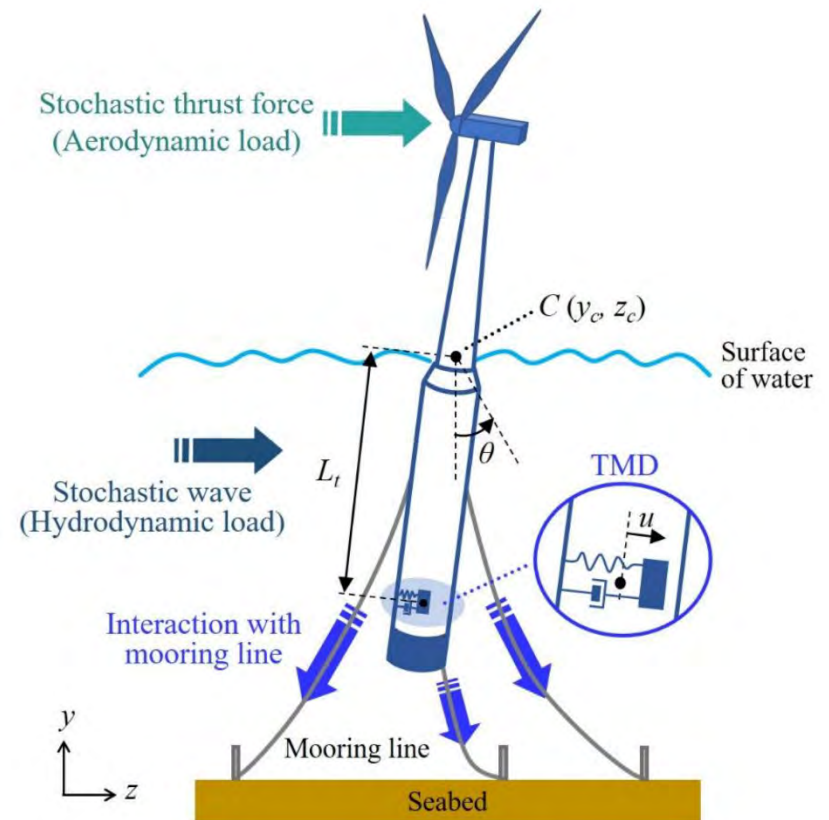
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 - *Stochastic loading*, fabrication errors (misfit strains, residual stresses...)

Model-Free Data-Driven inference – Motivation



Schematic of high-rise building subjected to strong ground motion

R. Xu and B. Fatahi,
Geotext. Geomembr., **46** (2018) 511–528.



Schematic of floating offshore wind turbine subjected to stochastic wave and wind loading

G. Park, K.Y. Oh and W. Nam,
J. Mar. Sci. Eng., **8** (2020) 876.

Model-Free Data-Driven inference – Motivation

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 - *Intrinsic randomness* of the material behavior (e.g., *strength*)
 - *Stochastic loading*, fabrication errors (misfit strains, residual stresses...)
- Conventional treatment: Stipulate a material law of the form:

$$\sigma = f(\epsilon) + \delta \quad \left\{ \begin{array}{l} f(\epsilon) \equiv \text{'forward' material model} \\ \delta \equiv \text{stochastic stress} \end{array} \right.$$

- Need to *model*:
 - Forward function $f(\epsilon)$, e.g., neural networks + regression
 - Prior distribution $P(\delta)$, e.g., Gaussian distribution
- Instead: Draw inferences directly from the data, without recourse to modeling (*Model-Free Data-Driven inference!*). *How?*

Modeling galore!

Example: Elastic bar

- Phase space, $Z = \{(\epsilon, \sigma)\} = \mathbb{R}^2$.
- Deterministic admissible space,

$$E(u_0) = \{(\epsilon, \sigma) : \sigma A = k(u_0 - \epsilon L)\}.$$

Definition (Physical likelihood)

With $z = (\epsilon, \sigma)$, $L_E(z) \equiv$ **likelihood** that z be **physically admissible**, in the sense of compatibility and equilibrium with random loads. Then, $d\mu_E(z) = L_E(z) dz$ is the corresponding **likelihood measure**.

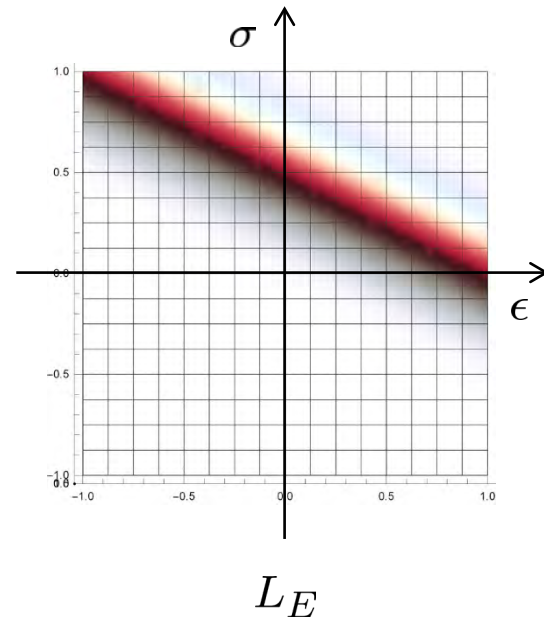
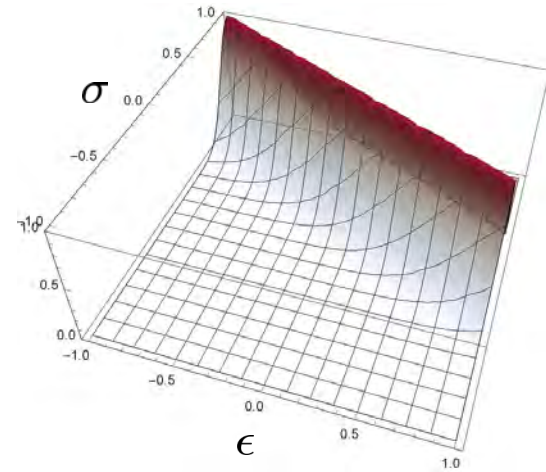
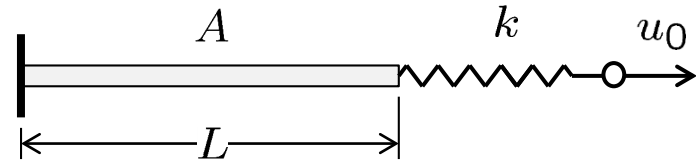
- Likelihood of a continuous function $f \in C_c(Z)$ (quantity of interest): $\mu_E(f) =$

$$\int_Z f(z) L_E(z) dz \equiv \int_Z f(z) d\mu_E(z).$$

Example (Random actuation)

Assume u_0 random: $\mu_E(f) =$

$$\int_{\mathbb{R}} \left(\int_{E(u_0)} f(z) d\mathcal{H}^1(z) \right) L_0(u_0) du_0,$$



Example: Elastic bar

- Phase space, $Z = \{(\epsilon, \sigma)\} = \mathbb{R}^2$.

Definition (Material likelihood)

With $y = (\epsilon, \sigma)$, $L_D(y) \equiv$ **likelihood** that y be **material**, i. e., that it be observed in the laboratory. Then, $d\mu_D(y) = L_D(y) dy$ is the corresponding **material measure**.

- Likelihood of a continuous function $f \in C_c(Z)$ (quantity of interest): $\mu_D(f) =$

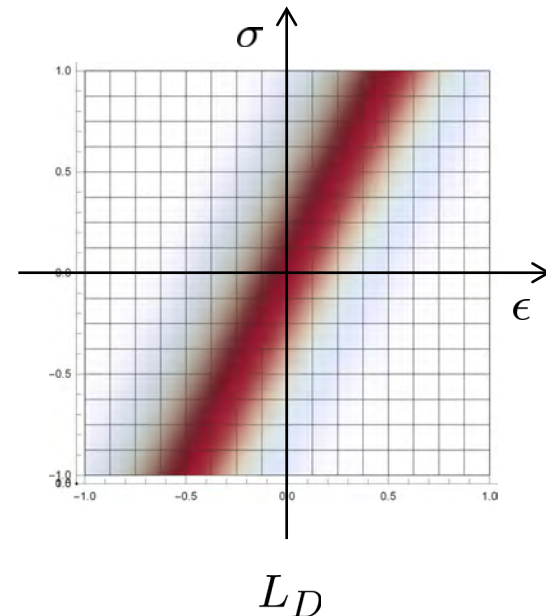
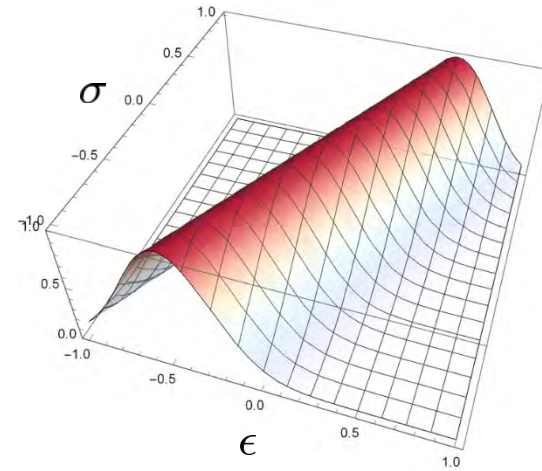
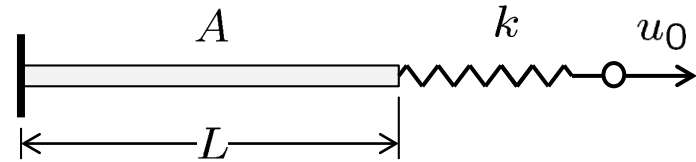
$$\int_Z f(y) L_D(y) dy \equiv \int_Z f(y) d\mu_D(y).$$

Example (Sliding Gaussian)

With $y = (\epsilon, \sigma)$, stipulate

$$L_D(y) = \exp\left(-\frac{AL}{2s^2} \mathbb{C}^{-1}(\sigma - \mathbb{C}\epsilon)^2\right),$$

where $s \equiv$ transversal standard deviation.



Example: Elastic bar

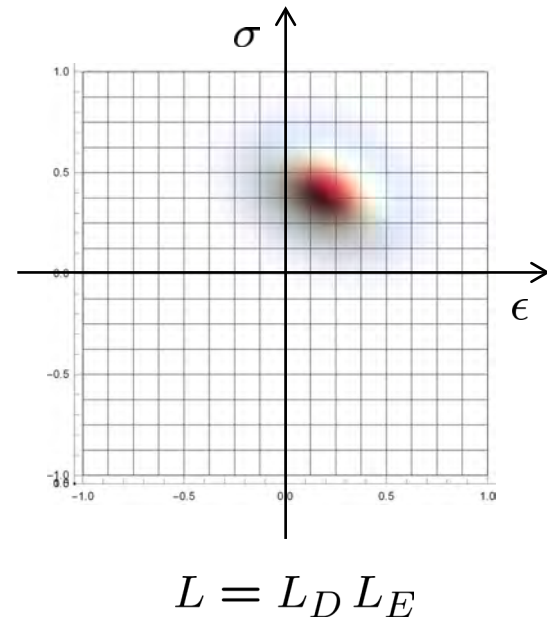
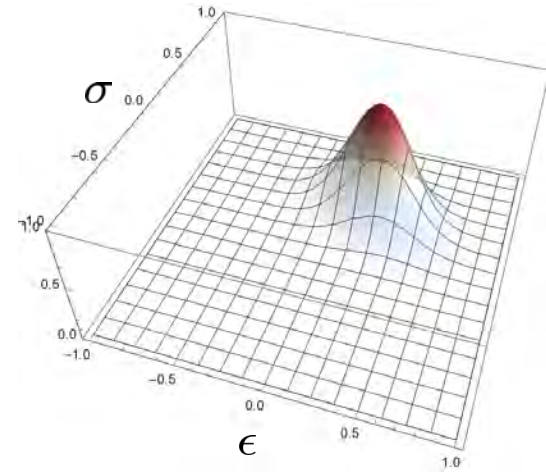
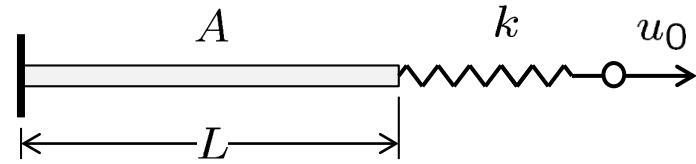
- Phase space, $Z = \{(\epsilon, \sigma)\} = \mathbb{R}^2$.
- Suppose that we know the priors:
 - $L_D(y) \equiv$ material likelihood function.
 - $L_E(z) \equiv$ physical likelihood function.

Definition (Classical inference)

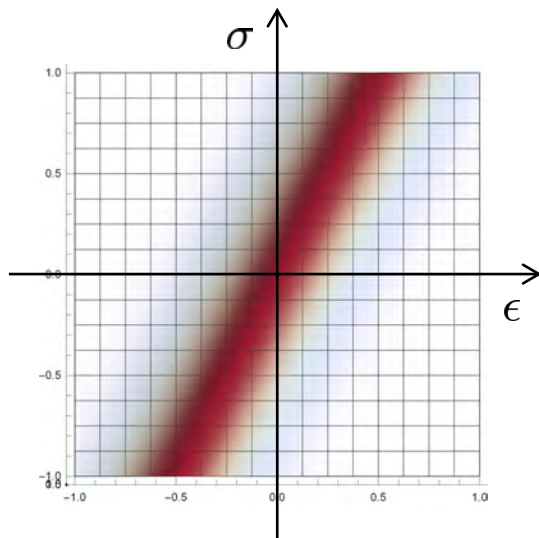
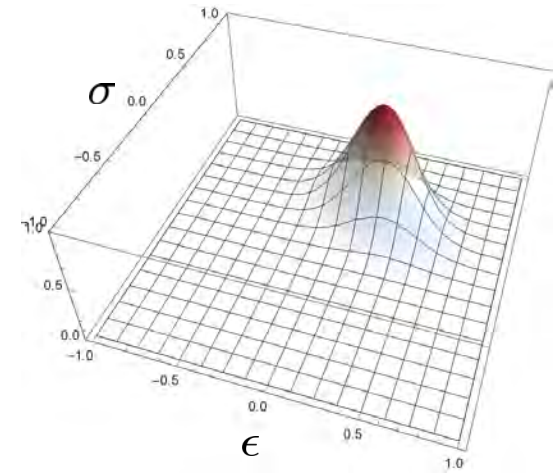
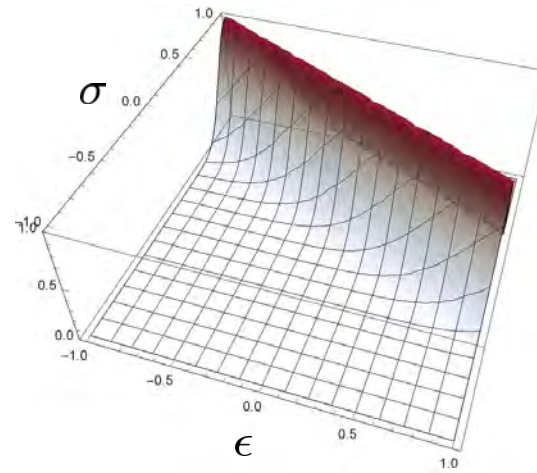
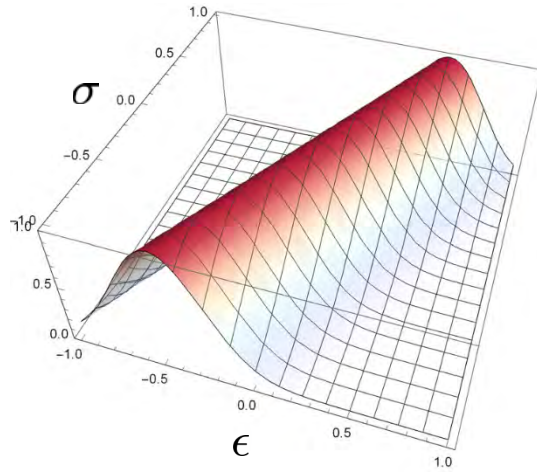
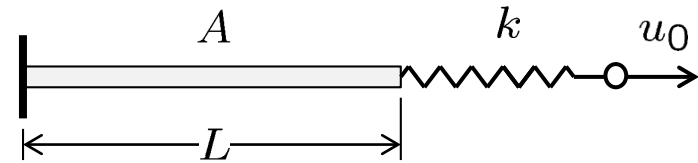
The classical **posterior likelihood function** $L(x) = L_D(x)L_E(x)$ is the likelihood of y being material and z being physical **conditioned** to $x = y = z$. Then, $d\mu(x) = L(x) dx$ is the corresponding **posterior likelihood measure**.

- $L(x)$ expresses the likelihood of x being **both** material **and** physical.
- Likelihood of a continuous function $f \in C_b(Z)$ (quantity of interest): $\mu(f) =$

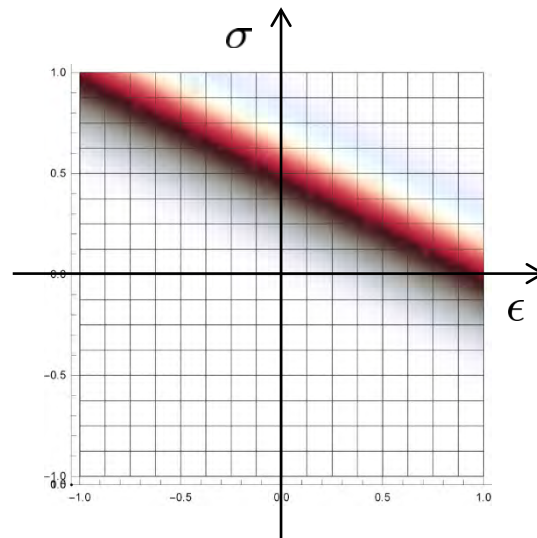
$$\int_Z f(x) L(x) dx \equiv \int_Z f(x) d\mu(x).$$



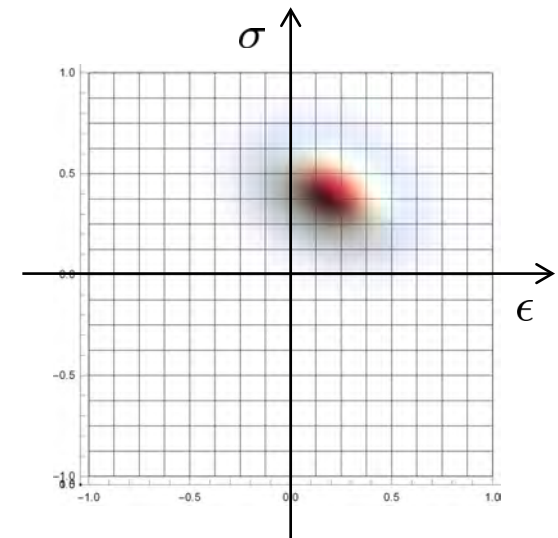
Example: Elastic bar



L_D



L_E



$L = L_D L_E$

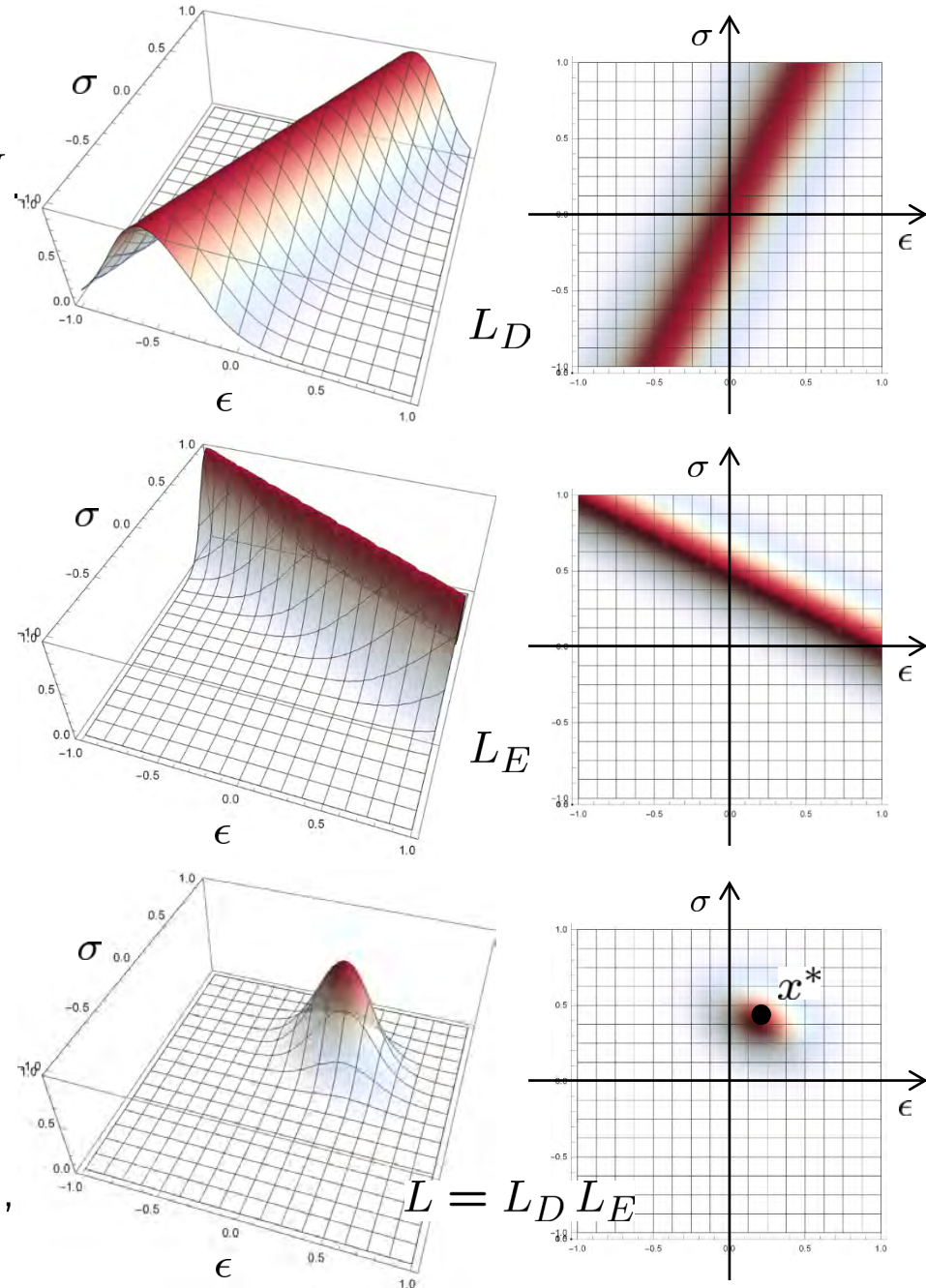
The classical inference paradigm

- *Phase space*, $Z = \{(\epsilon, \sigma)\} = \mathbb{R}^N \times \mathbb{R}^N$
- **Prior** and **posterior** likelihoods:
 - $L_D(y) \equiv$ material likelihood.
 - $L_E(z) \equiv$ physical likelihood.
 - $L(x) = L_D(x)L_E(x) \equiv$ posterior.
- **Maximum-likelihood solution**,

$$x^* \in \operatorname{argmax} L(\cdot).$$
- **Prior** and **posterior** measures:
 - $d\mu_D(y) = L_D(y) dy \equiv$ material.
 - $d\mu_E(z) = L_E(z) dz \equiv$ physical.
 - $d\mu(x) = L(x) dx \equiv$ posterior.

Definition (Intersection of measures)

Given $\mu_D, \mu_E \in \mathcal{M}(Z)$, we denote by $\mu = \mu_D \cap \mu_E$ the corresponding posterior measure, i. e., the likelihood of y material, z physical, conditioned to $y = z$.



The classical inference paradigm

- Phase space, $Z = \{(\epsilon, \sigma)\} = \mathbb{R}^N \times \mathbb{R}^N$.
- Extension to **deterministic loading**:
 - $E = \{z = (\epsilon, \sigma) \in Z, \text{ admissible}\}$.
 - $\mu_E = \mathcal{H}^N \llcorner E \equiv$ Hausdorff measure.

- Likelihood of $f \in C_c(Z)$ admissible:

$$\mu_E(f) = \int_E f(z) d\mathcal{H}^N(z).$$

- Posterior likelihood of $f \in C_b(Z)$:

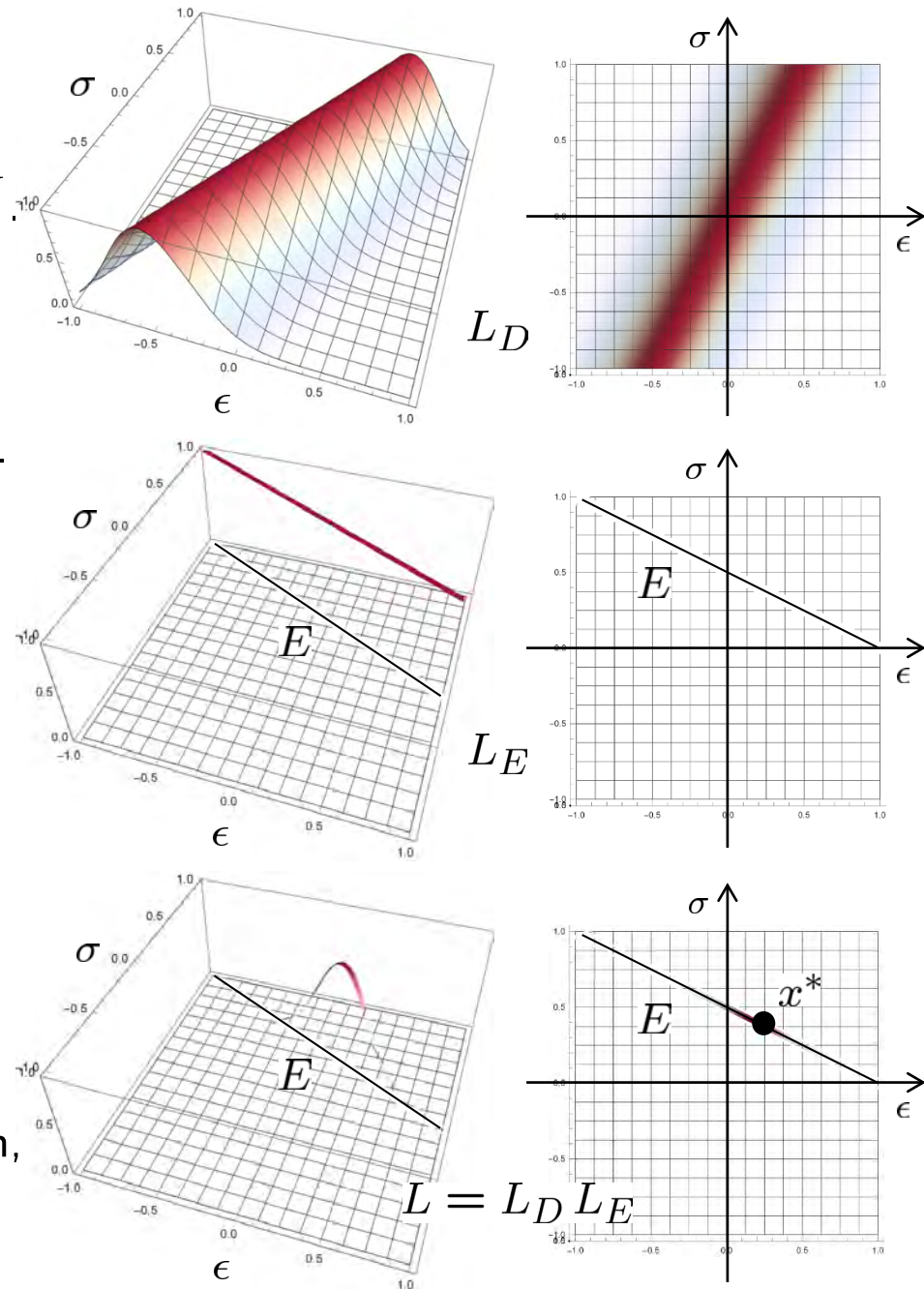
$$\mu(f) = \int_E f(x) L_D(x) d\mathcal{H}^N(x).$$

- **Maximum-likelihood solution**,

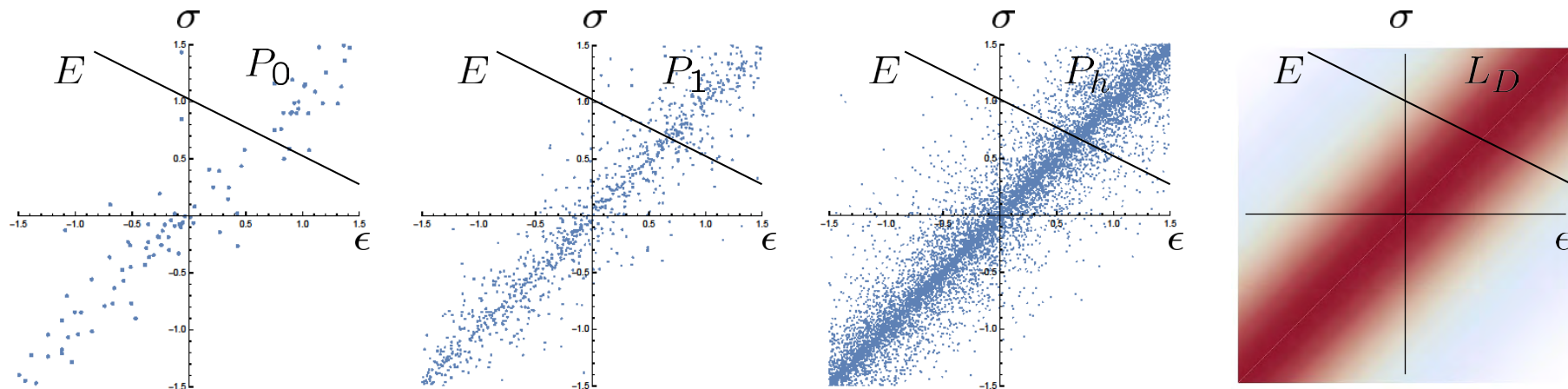
$$x^* \in \operatorname{argmax} \{L_D(x) : x \in E\}$$

- Potential: $\Psi_D(x) = -\log L_D(x)$. Then,

$$x^* \in \operatorname{argmin} \{\Psi_D(x) : x \in E\}.$$



The Data-Driven inference paradigm



Sequence of discrete point-data sets converging weakly to a limiting material likelihood density + deterministic loading.

- Suppose that L_D is **not known exactly**, only **sampled** on point-set sequence (P_h) .
- Approximate μ_D by **empirical measures**

$$\mu_{D,h} = \sum_{\xi \in P_h} c_\xi \delta_\xi, \quad c_\xi \geq 0.$$

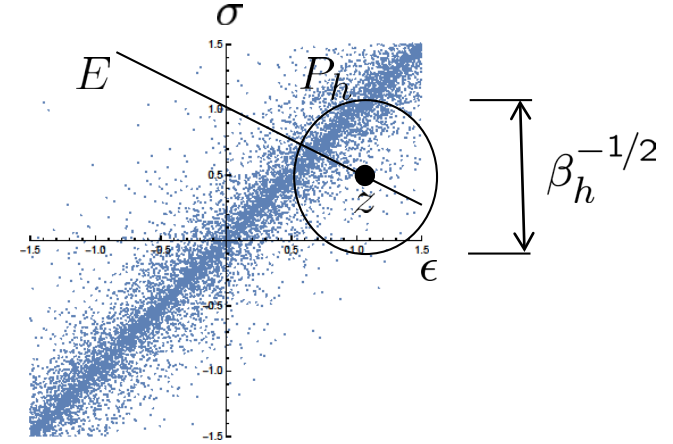
- Suppose **deter. loads**: $\mu_E = \mathcal{H}^N \llcorner E$.

- Posteriors $\mu_h = \mu_{D,h} \cap \mu_E = \emptyset!$
- **Classical inference breaks down** along the sequence, (μ_h) does not approximate the exact posterior $\mu = \mu_D \cap \mu_E$.
- Must extend the concept of inference, classical inference is too rigid! **How?**

The Data-Driven inference paradigm

- L_D sampled on point-set sequence (P_h) .
- Deterministic loads: $\mu_E = \mathcal{H}^N \llcorner E$.
- Approximate μ_D by empirical measures

$$\mu_{D,h} = \sum_{\xi \in P_h} c_\xi \delta_\xi, \quad c_\xi \geq 0.$$



- **Decorrelation**: Allow for non-zero likelihood of $y \neq z$ but require likelihood to be rapidly decreasing with $\|y - z\|$ on an intermediate scale $1/\sqrt{\beta_h}$.
- **Variational characterization**: Consider trial relaxed posteriors of the form

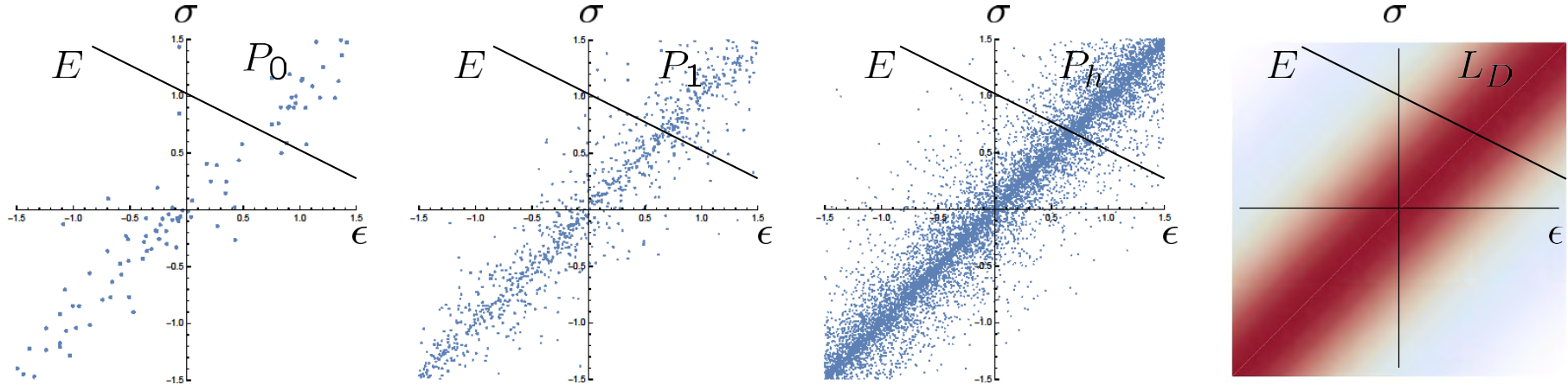
$$d\nu_h(y, z) = \sum_{\xi \in P_h} p_\xi(z) d\delta_\xi(y) d\mathcal{H}^N(z) \quad \left(\Leftrightarrow \nu_h \ll \mu_{D,h} \times \mu_E \right).$$

- Stipulate that posterior minimizes the **regularized Kullback-Leibler divergence**:

$$G_{\beta_h}(\nu_h) = \sum_{\xi \in P_h} \int_E \underbrace{\left(\beta_h \|\xi - z\|^2 \right)}_{\text{decorrelation cost}} + \underbrace{\log \frac{p_\xi(z)}{c_\xi}}_{\text{relative entropy}} p_\xi(z) dz \rightarrow \min!$$

- Minimizer: $p_\xi(z) = c_\xi e^{-\beta_h \|\xi - z\|^2} \equiv \text{'relevance' of } \xi \text{ to } z.$

The Data-Driven inference paradigm



- **Model-Free Data-Driven inference:** Expectation of QOI $f \in C_b(Z \times Z)$,

$$\mathbb{E}_h[f] = \frac{\sum_{\xi \in P_h} c_\xi \int_E f(\xi, z) e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}{\sum_{\xi \in P_h} c_\xi \int_E e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}$$

*Explicit in the data!
No modeling of priors!
No modeling of material!*

- Questions:
 - Convergence of $\mathbb{E}_h[f] \rightarrow \mathbb{E}[f]$ (weak convergence of posteriors) as:
 - a) $\mu_{D,h} \rightharpoonup \mu_D$ (**material sampling**);
 - b) $\beta_h \rightarrow +\infty$? (**annealing**).
 - Error bounds? Convergence rate? Optimal annealing rate (β_h)?
 - Practical implementation? Scope? Numerical performance?

The Data-Driven inference paradigm



The term 'annealing' refers to a heat treatment in metallurgy (Steel sword from Toledo, Spain)

Theorem (Annealing convergence)

Assume:

- i) *Regular material likelihood*: $d\mu_D(y) = e^{-\Phi(y)} dy$, Φ Borel, quadratic growth.
- ii) *Deterministic loading*: $\mu_E(z) = \mathcal{H}^N \llcorner E$, E N -dimensional affine subspace Z .
- iii) *Transversality*: There exist $\beta_0 > 0$, $c > 0$ and $b \geq 0$ such that

$$\beta_0 \|y - z\|^2 + \Phi(y) \geq c(\|y\|^2 + \|z\|^2) - b \quad \text{for all } y \in Z, z \in E.$$

Then:

- i) *Inference*: The posterior measure μ is such that, for every $f \in C_b(Z \times Z)$,

$$\mu(f) = \int_{Z \times Z} f(y, z) d\mu(y, z) = \int_E f(\xi, \xi) e^{-\Phi(\xi)} d\mathcal{H}^N(\xi). \quad \text{Explicit!}$$

- ii) *Error bound for annealing*: There is $C > 0$ such that $\underbrace{\|\mu_\beta - \mu\|_{\text{FN}}}_{\text{Annealing error reduces to zero as } \beta^{-1/2}} \leq C\beta^{-\frac{1}{2}}.$

Annealing error reduces
to zero as $\beta^{-1/2}$

Annealing error
(in flat norm)

The Data-Driven inference paradigm

Theorem (Sampling convergence)

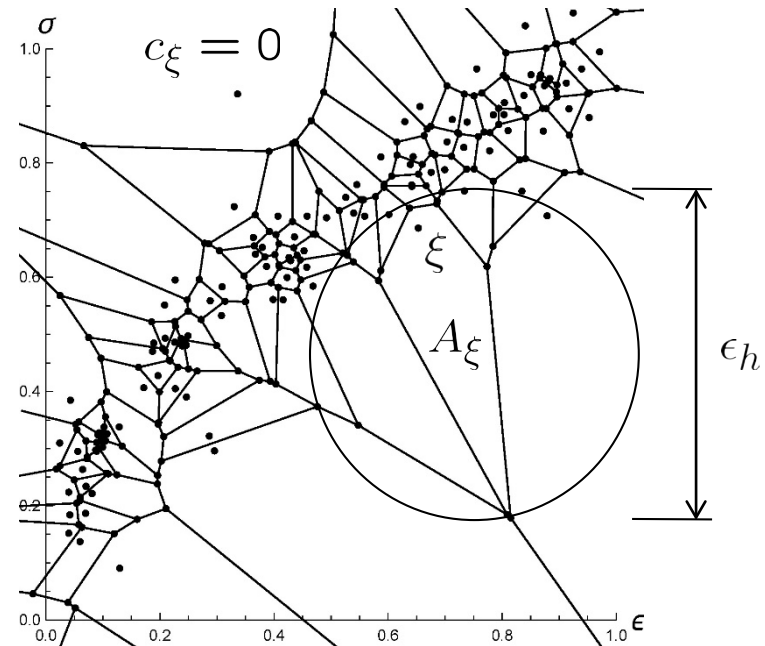
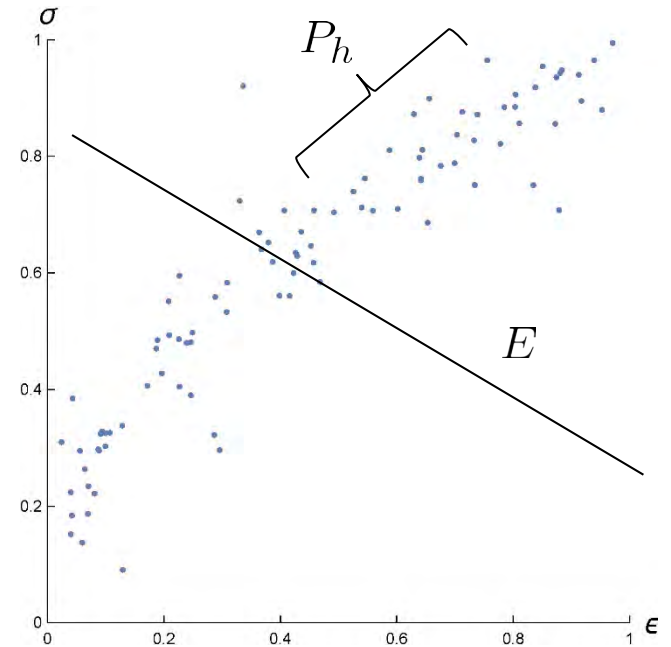
Assume annealing convergence, approximation by point-set samples, deterministic loading. Assume further that, for every h , there is a partition $\mathcal{A}_h = \{A_\xi : \xi \in P_h\}$ of Z , with $\xi \in A_\xi$ and $\mu_D(A_\xi) < \infty$ for every $\xi \in P_h$ and every h , and sequences $\delta_h \downarrow 0$, $\epsilon_h \downarrow 0$, s. t. (possibly after tail clipping):

- i) **Cell mass:** $|c_\xi - \mu_D(A_\xi)| \leq \delta_h \mu_D(A_\xi)$.
- ii) **Cell size:** If $c_\xi > 0$, then $\text{diam}(A_\xi) \leq \epsilon_h$.
- iii) **Annealing:** Sequence $(\beta_h \epsilon_h^2)$ is bounded.

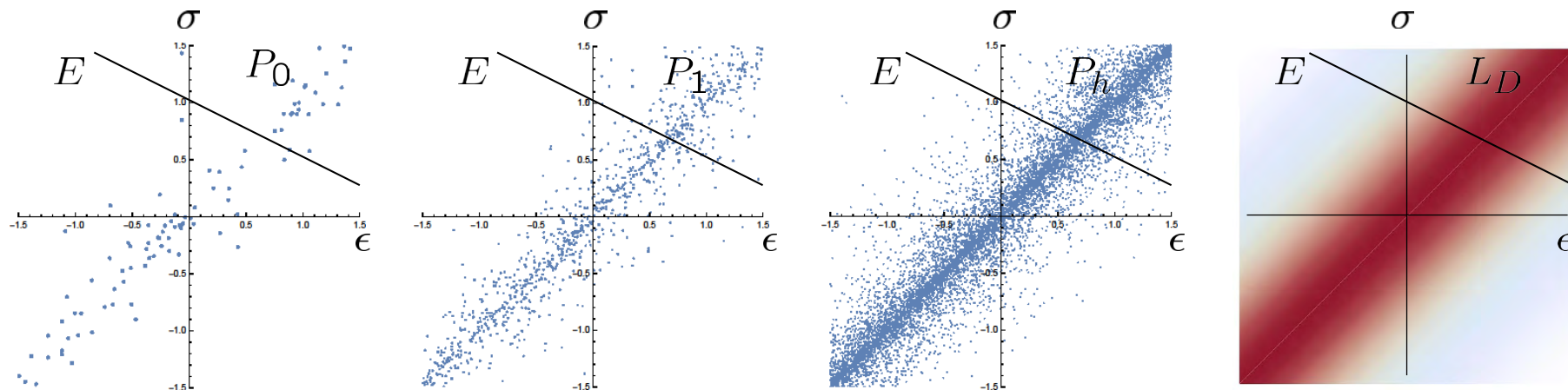
Then: $\underbrace{\|\mu_{h,\beta_h} - \mu_{\beta_h}\|_{\text{FN}}}_{\text{Sampling error (in flat norm)}} \leq C \beta_h^{1/2} \epsilon_h.$

*Sampling error
(in flat norm)*

Conti, S., F. Hoffmann and M. Ortiz,
arXiv:4503091 (2022).



The Data-Driven inference paradigm



• **Data-Driven inference:**
$$\mathbb{E}_h[f] = \frac{\sum_{\xi \in P_h} c_\xi \int_E f(\xi, z) e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}{\sum_{\xi \in P_h} c_\xi \int_E e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}$$

Corollary Assume annealing convergence and sampling convergence. Then:

- i) **Total posterior error:** $\|\mu_{h,\beta_h} - \mu\|_{\text{FN}} \leq C(\beta_0^{1/2} \beta_h^{-1/2} + \beta_h^{1/2} \epsilon_h).$
 - ii) **Optimal annealing rate:** $\beta_h = \beta_0^{1/2} \epsilon_h^{-1} \Leftrightarrow \beta_h^{-1/2} = \beta_0^{-1/4} \epsilon_h^{1/2}.$
 - iii) **Optimal convergence rate:** $\|\mu_{h,\beta_h} - \mu\|_{\text{FN}} \leq 2C \beta_0^{1/4} \epsilon_h^{1/2}.$
 - iv) **Convergence of likelihood:** $\mathbb{E}_h[f] \rightarrow \mathbb{E}[f],$ for all $f \in C_b(Z \times Z),$
- } **Optimal annealing averages data on intermediate scale!**

- Remaining questions: Practical implementation? Scope? Numerical performance?

Maximum-likelihood Data-Driven solution

- Data-Driven **posterior likelihood**: For $z \in E$,

$$L_h(z) = \sum_{\xi \in P_h} p_\xi(z) \rightarrow \max!$$

- Equivalently, **posterior potential**: For $z \in E$,

$$F_h(z) = -\frac{1}{\beta_h} \log L_h(z) \rightarrow \min!$$

- Optimality condition: With $z \in E$,

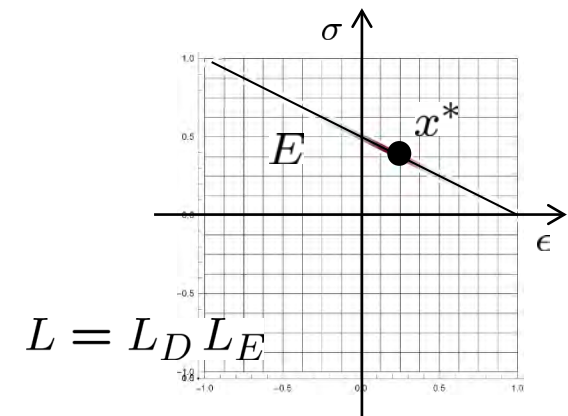
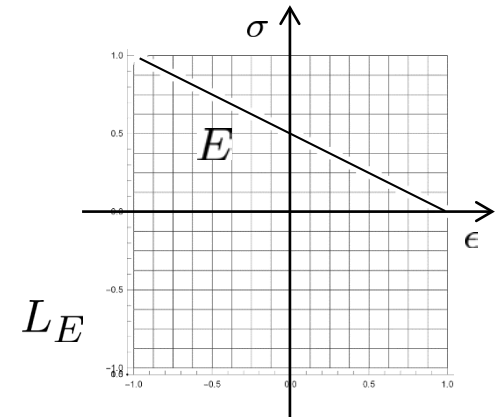
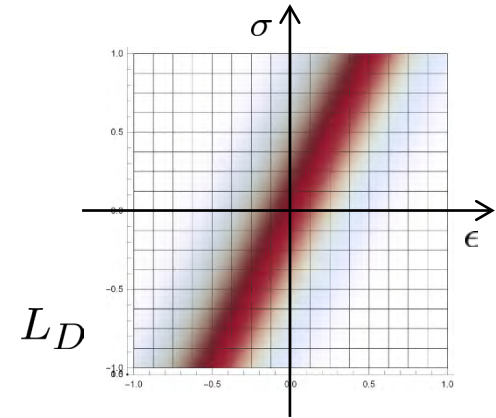
$$DF_h(z) = z - \sum_{\xi \in P_h} p_\xi(z) \xi \perp E. \quad (\text{EL})$$

- With $P_E \equiv$ orthogonal projection onto E ,

$$(\text{EL}) \Leftrightarrow z = P_E \left(\sum_{\xi \in P_h} p_\xi(z) \xi \right).$$

- **Fixed-point solver**: Iteration step,

$$z^{(k+1)} = P_E \left(\sum_{\xi \in P_h} p_\xi(z^{(k)}) \xi \right) \equiv g_h(z^{(k)}).$$



Maximum-likelihood Data-Driven solution

Theorem (Fixed-point solver)

Suppose that, for all $z \in E$,

$$\frac{1}{\beta_h} > \sum_{\xi \in P_h} p_\xi(z) \|\xi - \bar{z}_h\|^2, \quad (\text{AC})$$

with $\bar{z}_h = \sum_{\xi \in P_h} p_\xi(z) \xi$. Then,

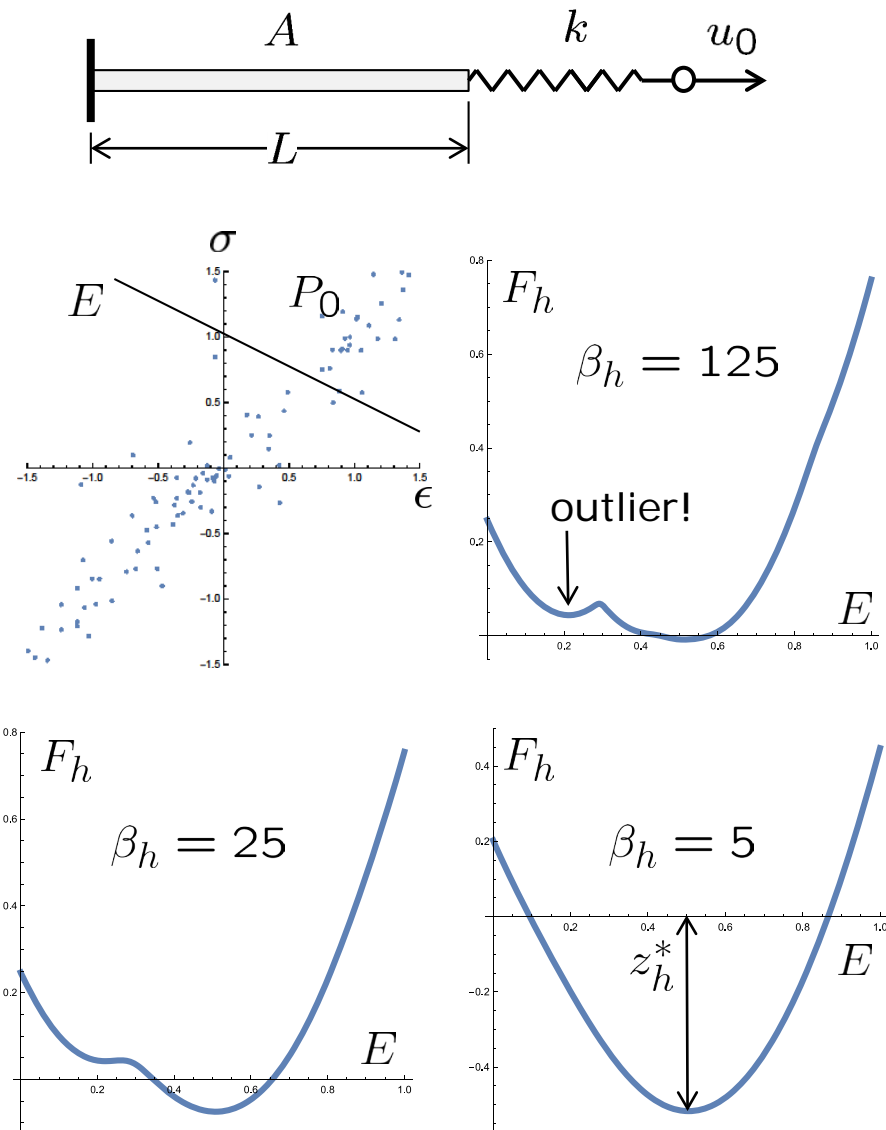
- i) $F_h(z)$ is **convex** over E .
- ii) $g_h(z)$ is **contractive**.

Proof.

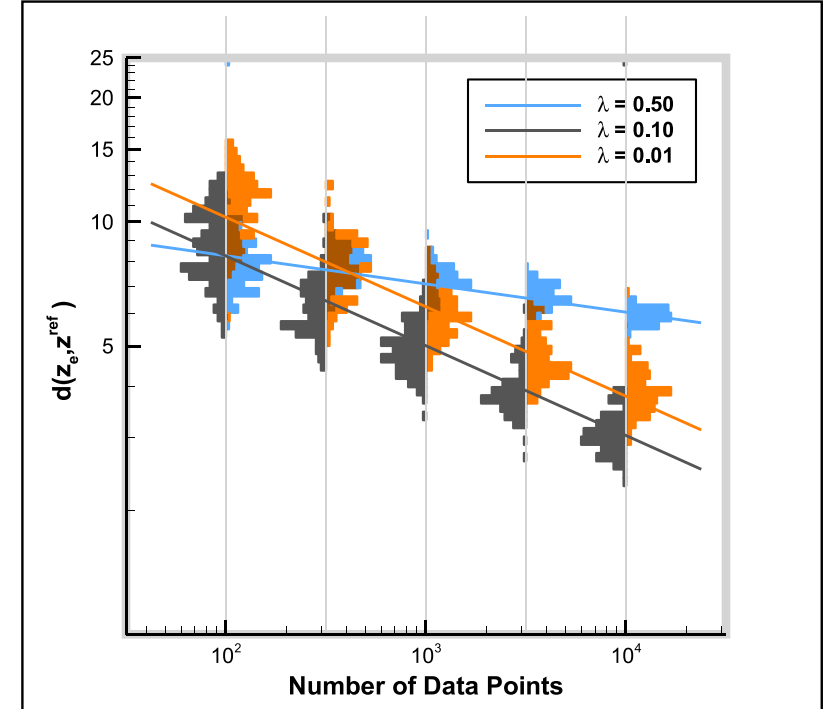
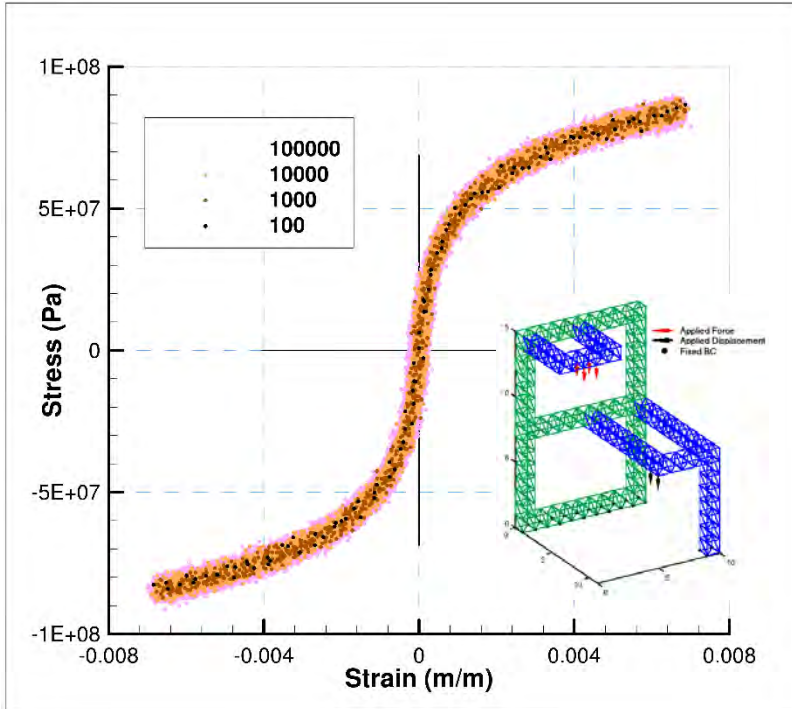
(Main idea). By direct calculation, verify that the annealing condition (AC) implies $D^2 F_h(z) > 0$, hence $F_h(z)$ convex. Contractivity of g_h follows directly from the convexity of $F_h(z)$. \square

Corollary

Assume (AC). Then, g_h has a fixed point $z_h^* = \text{maximum-likelihood solution}$.



Maximum-likelihood Data-Driven solution

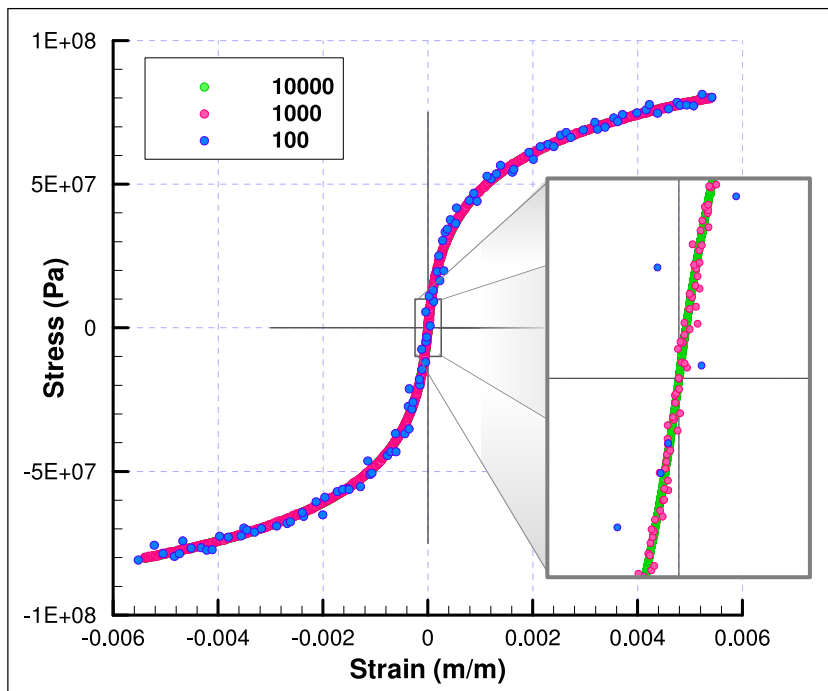


3D truss test case. Data sets of different sizes sampled assuming Gaussian noise superposed on linear+cubic material law.

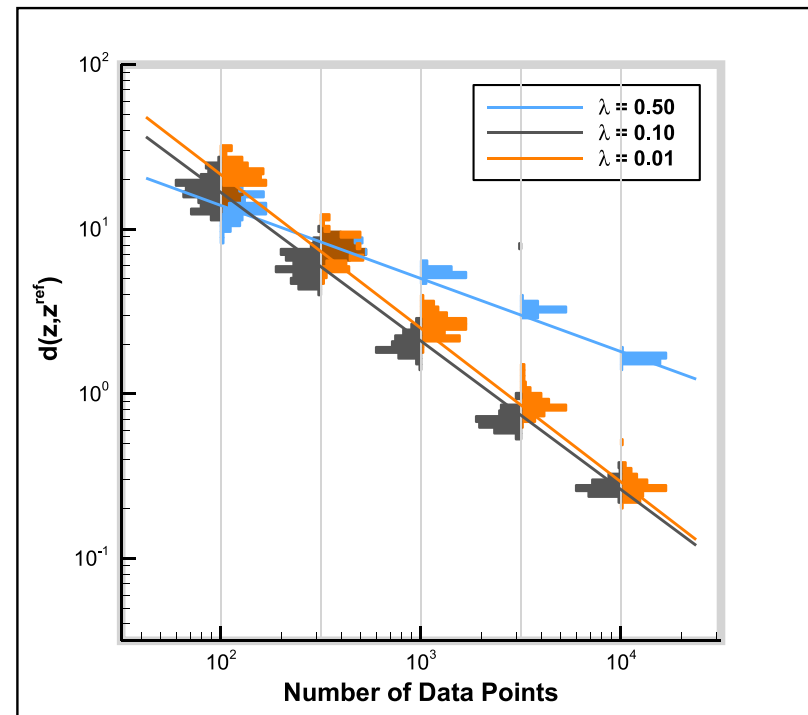
Convergence with respect to dataset size and annealing rate. Over-relaxed annealing schedule:

$$\beta_h^{(k+1)} = (1-\lambda) \left(\sum_{\xi \in P_h} p_{\xi}(z^{(k)}, \beta_h^{(k)}) \xi \right)^{-1} + \lambda \beta_h^{(k)}$$

Maximum-likelihood Data-Driven solution



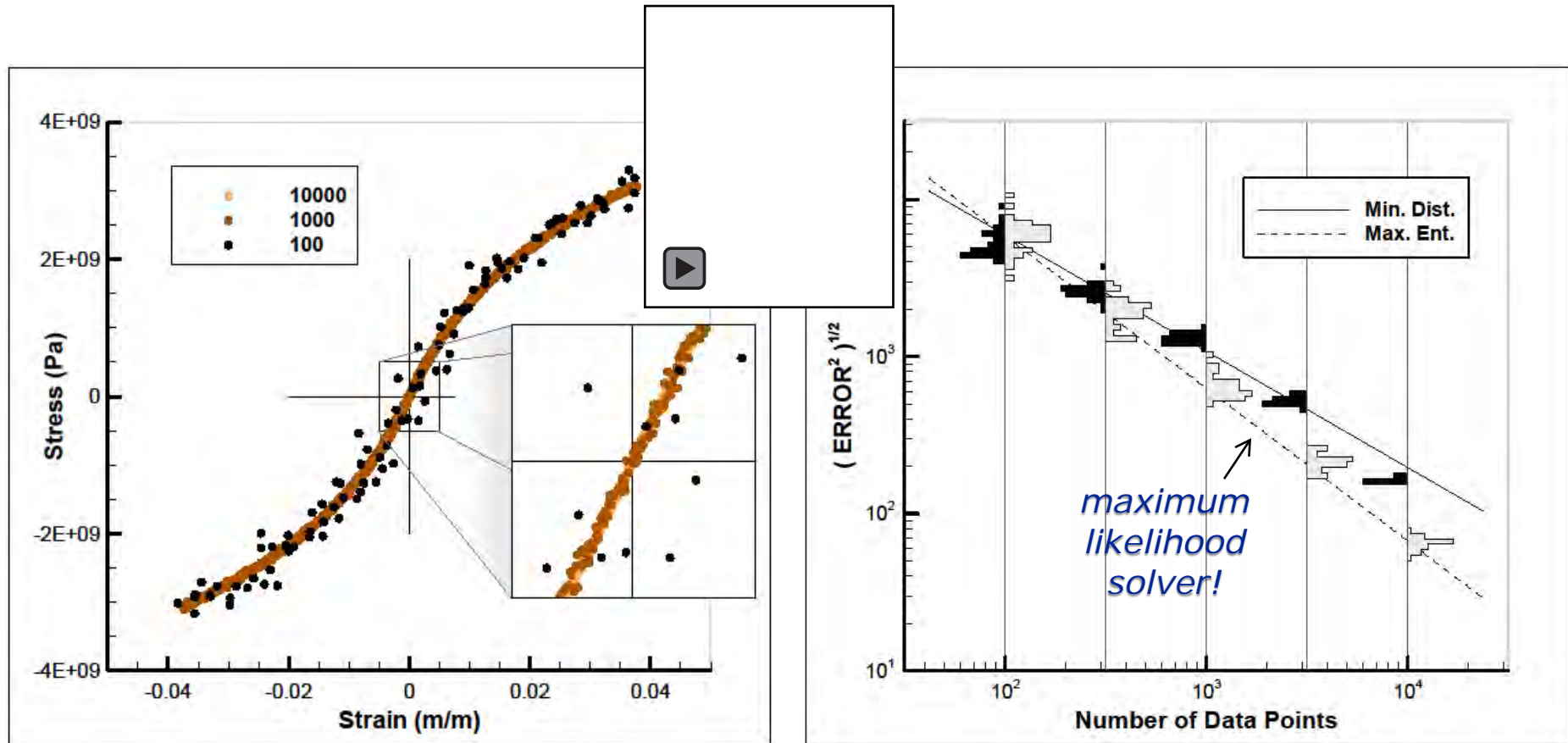
3D truss test case. Data sets of different sizes converging uniformly to a linear+cubic material law.



Convergence with respect to data-set size and annealing rate. Over-relaxed annealing schedule:

$$\beta_h^{(k+1)} = (1-\lambda) \left(\sum_{\xi \in P_h} p_{\xi}(z^{(k)}, \beta_h^{(k)}) \xi \right)^{-1} + \lambda \beta_h^{(k)}$$

Maximum-likelihood Data-Driven solution – Dynamics



3D truss structure shaking under ground motion.
 Random data sets generated according to capped normal distribution
 centered on the true material curve with standard deviation
 in inverse proportion to the square root of the data set size

Full Data-Driven inference

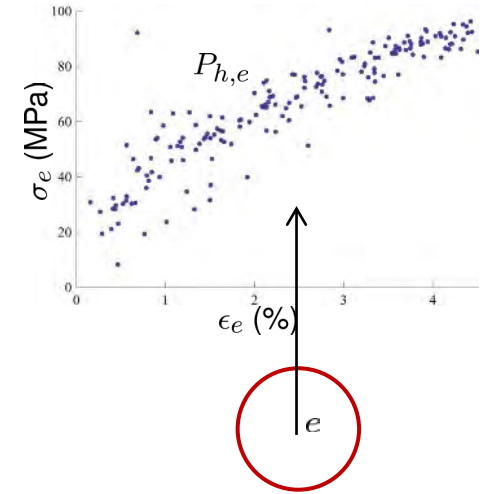
- Wish to compute likelihoods of general QOI $f \in C_b(Z)$,

$$\mathbb{E}_h[f] = \frac{\sum_{\xi \in P_h} c_\xi \int_E f(z) e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}{\sum_{\xi \in P_h} c_\xi \int_E e^{-\beta_h \|\xi - z\|^2} d\mathcal{H}^N(z)}.$$

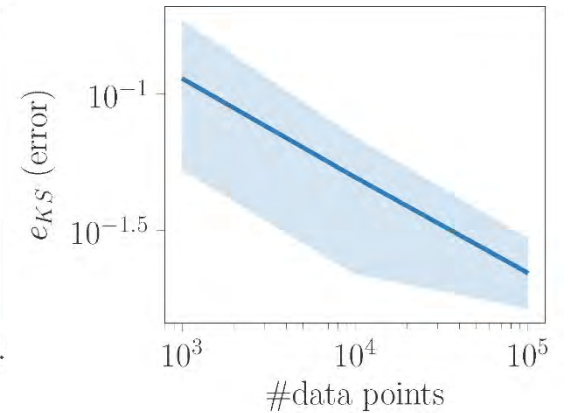
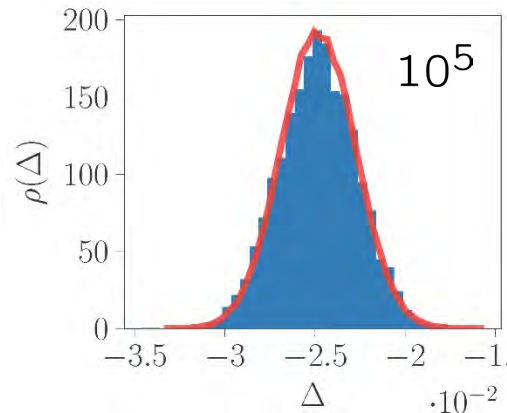
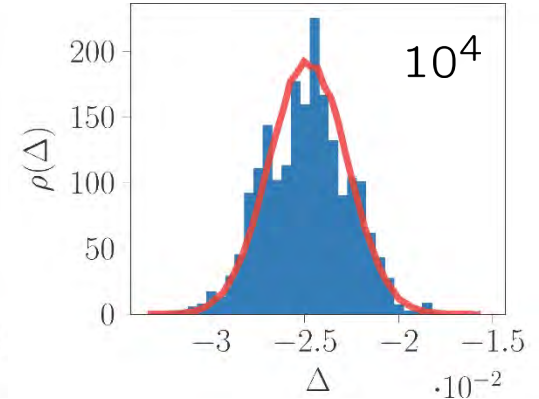
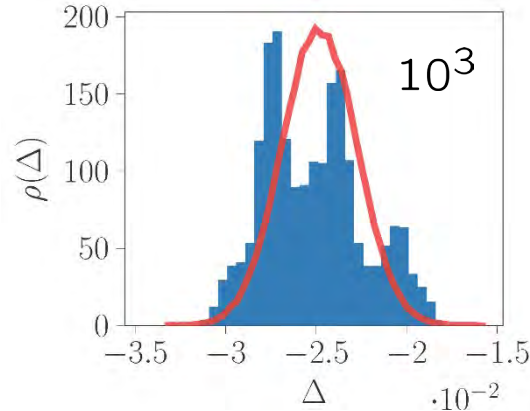
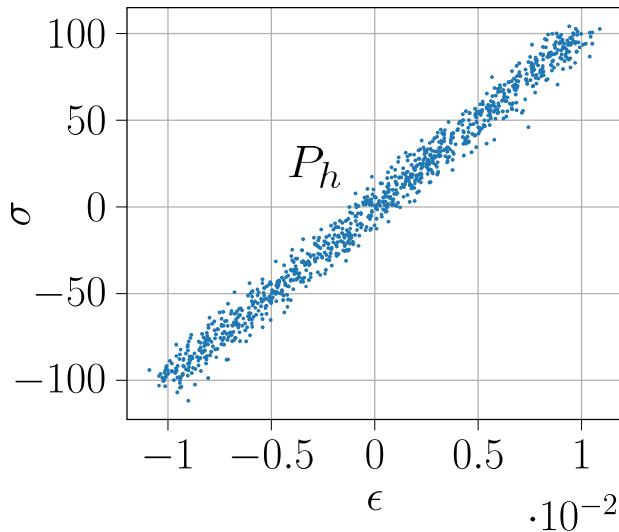
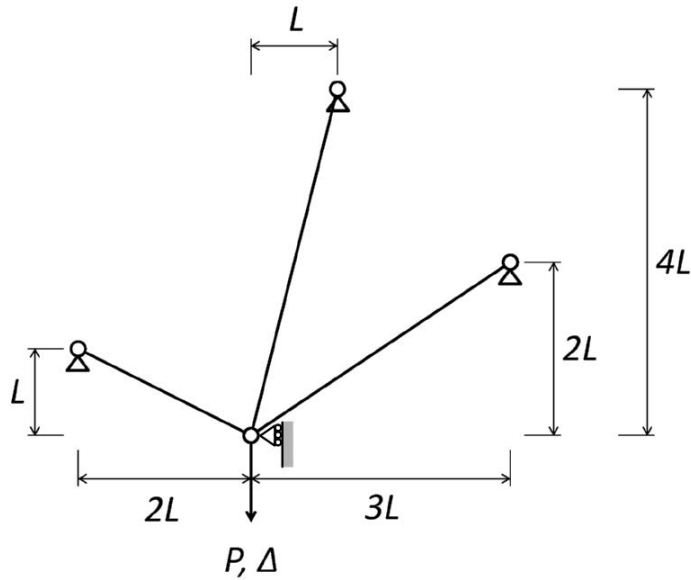
- **Uncorrelated** material points: $L_D(z) = \prod_{e=1}^m L_{D,e}(z_e)$.
- **Independent** material point-data sets: $P_h = \prod_{e=1}^m P_{h,e}$.
- Then: Likelihood **factorizes** into local material-point computations,

$$\mathbb{E}_h[f] = \frac{\int_E f(z) \prod_{e=1}^m \left(\sum_{\xi_e \in P_{h,e}} c_{\xi_e} e^{-\beta_{e,h} \|\xi_e - z_e\|^2} \right) d\mathcal{H}^N(z)}{\int_E \prod_{e=1}^m \left(\sum_{\xi_e \in P_{h,e}} c_{\xi_e} e^{-\beta_{e,h} \|\xi_e - z_e\|^2} \right) d\mathcal{H}^N(z)}.$$

- **Polynomial complexity** $O(m \#P_{h,loc})$ vs. combinatorial complexity $O((\#P_{h,loc})^m)$.
- Remaining implementational challenges:
 - Computation of \int_E : **Stochastic quadrature**, Monte Carlo + population annealing.
 - Evaluation of $\sum_{\xi_e \in P_{h,e}}$: **Importance sampling**, restricted sums, k -means trees.

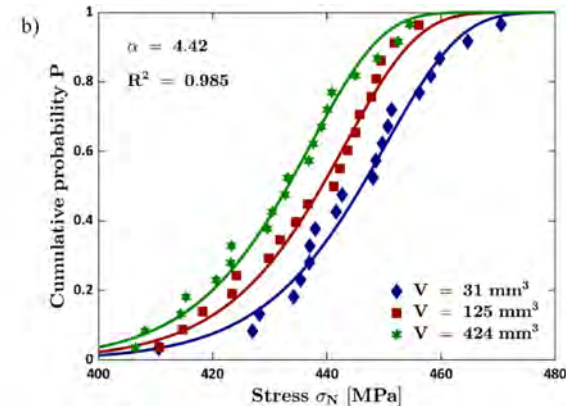
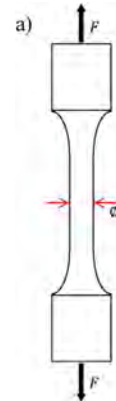
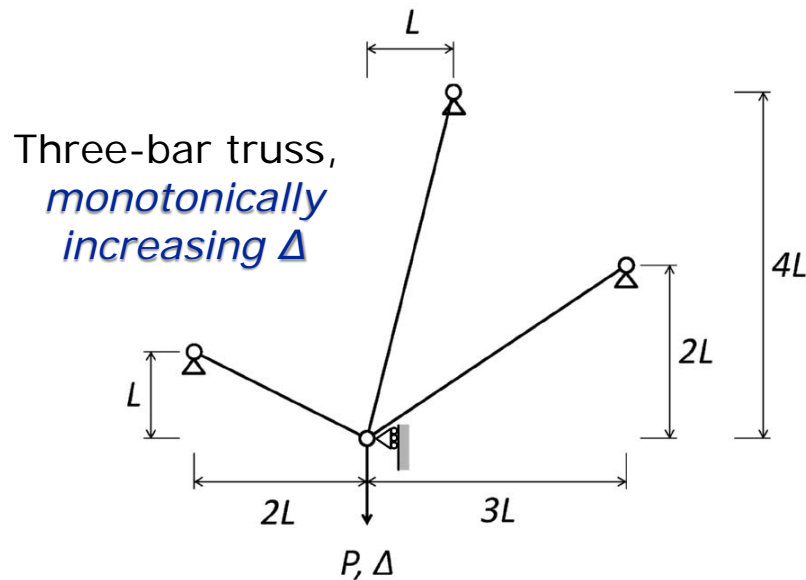


Full Data-Driven inference – Convergence



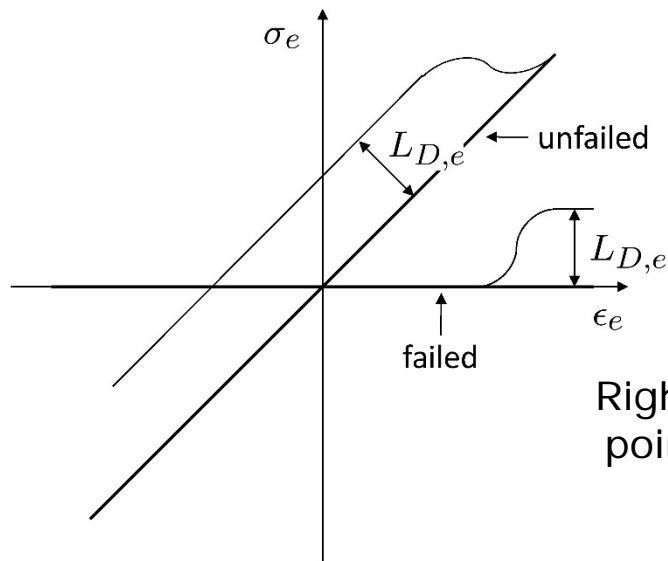
Three-bar truss with sliding-Gaussian material data. Computed histograms vs. exact distribution (red) of Δ for material data-sets of sizes: a) 10^3 ; b) 10^4 ; c) 10^5 . d) Kolmogorov-Smirnov error vs. material data-set size.

Full Data-Driven inference – Convergence

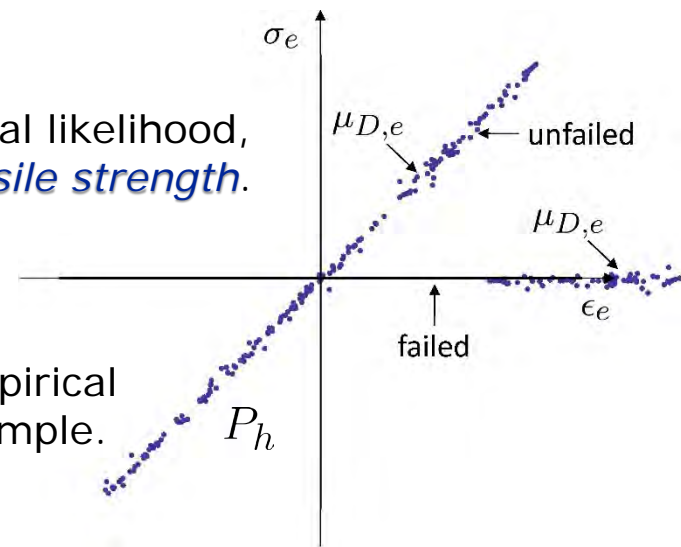


γ -titanium aluminide alloy, Ti-48Al-2Cr-2Nb,
cumulative probability of tensile strength.

C. Dresbach *et al.*, *Latin American J. Solids Struct.*, **13** (2016) 2316–2332.

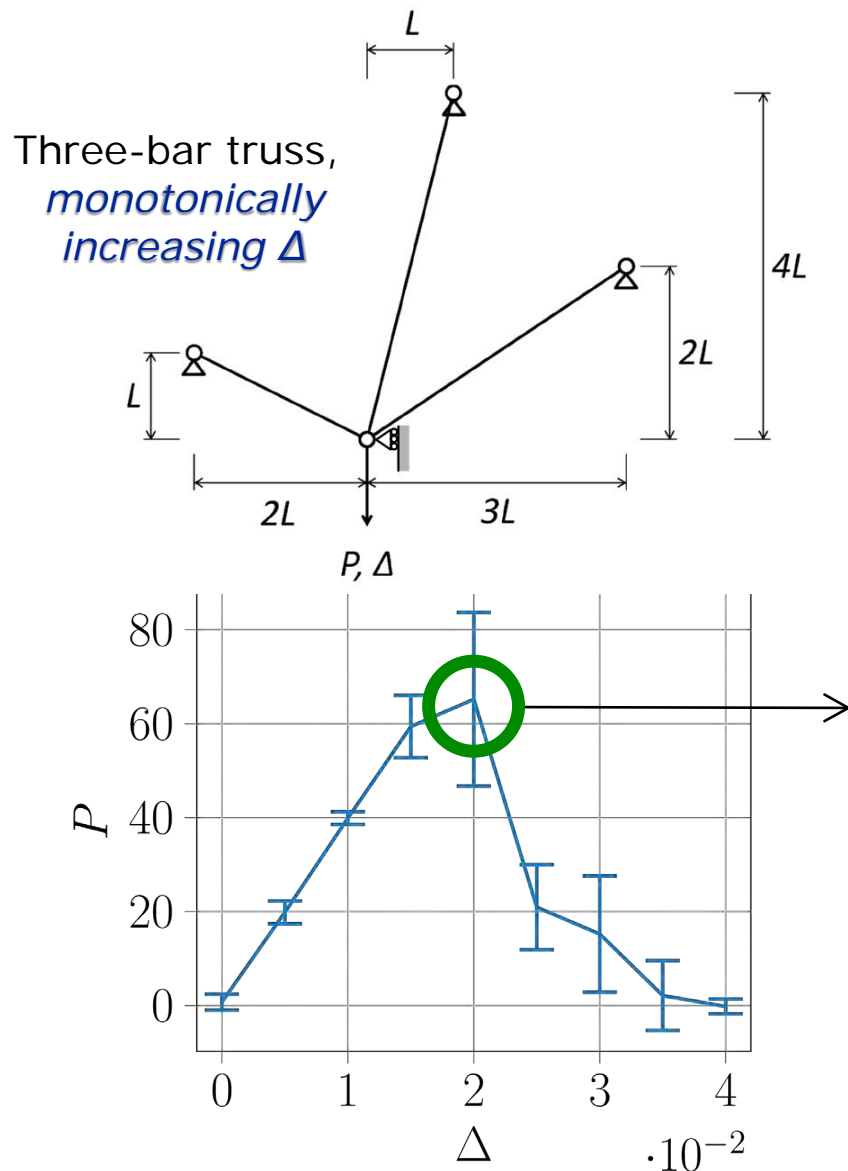


Left: Material likelihood,
Weibull tensile strength.



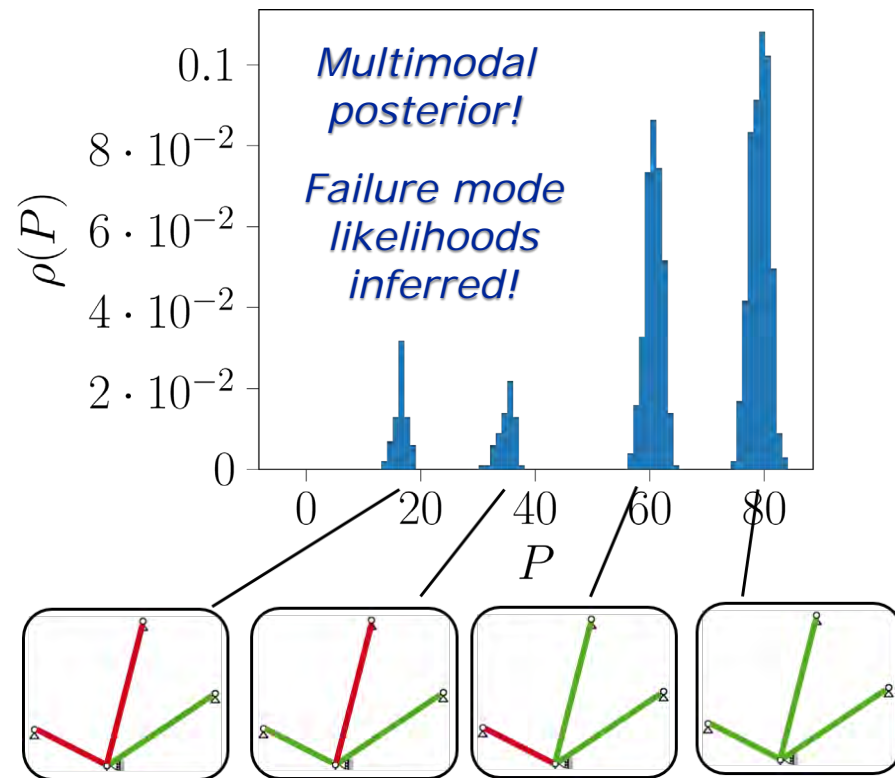
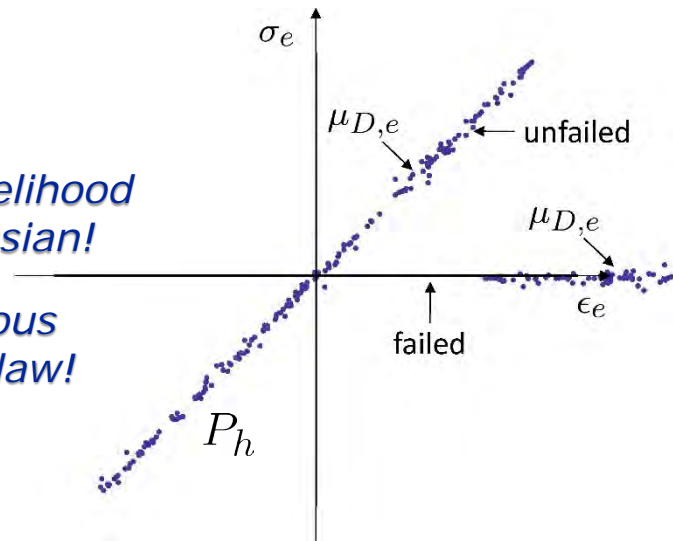
Right: Typical empirical
point data set sample.

Full Data-Driven inference – Scope

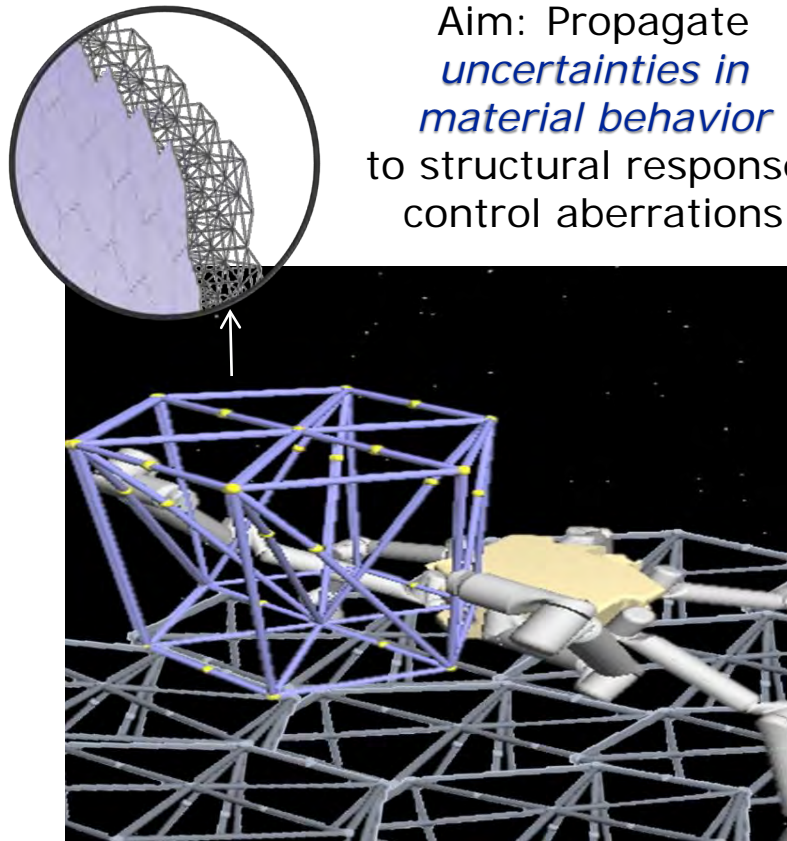


Material likelihood non-Gaussian!

No obvious material law!



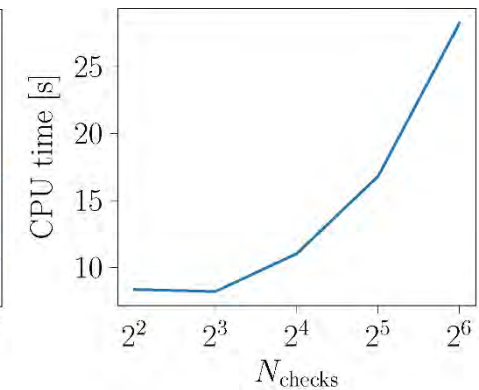
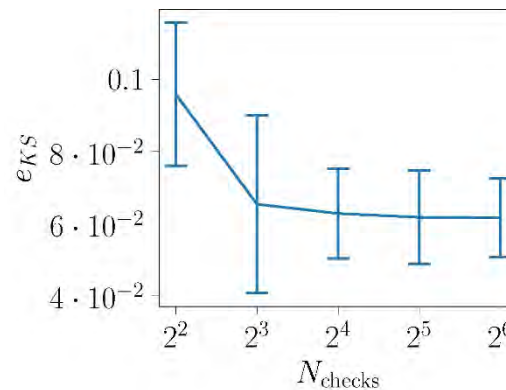
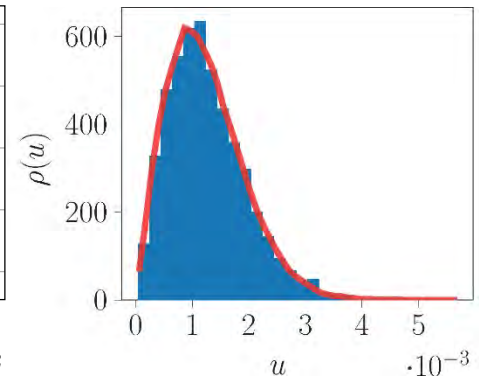
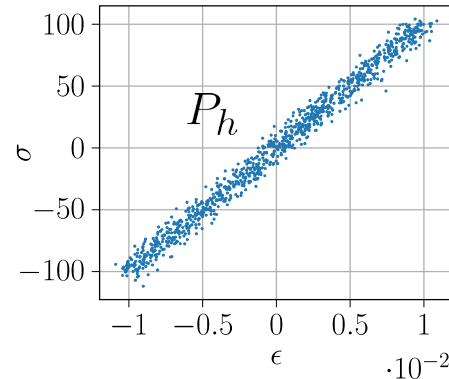
Full Data-Driven inference – Lightweight space structures



Aim: Propagate *uncertainties in material behavior* to structural response, control aberrations

Modular space telescope structure
In-Space Telescope Assembly
Robotics (ISTAR)

Hogstrom *et al.*, 65th International
Astronautical Congress, Toronto, CA: 2014



- Material data, sliding Gaussian.
- Posterior distribution of hub displacement.
- Accuracy vs. number of backtracks in approximate k -means search.
- CPU time in seconds on 12-Core AMD Ryzen 9 3900X computer.

to be continued...