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An investigation towards the Uncertainty Model calibration approaches for NASA-Langley UQ Challenge 2019

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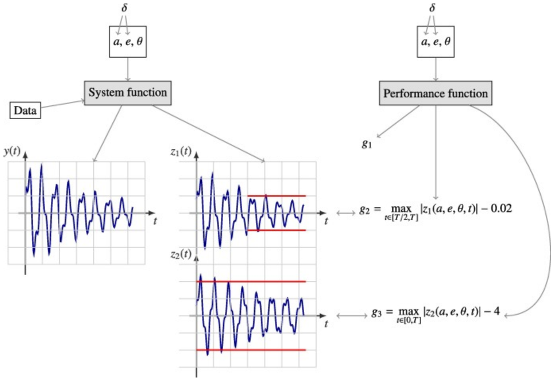
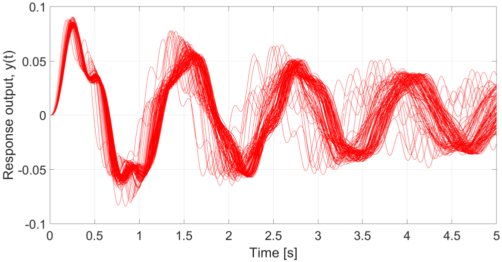
Research Objectives

- An extension to the investigation towards the Uncertainty Model (UM) calibration in the recent NASA-Langley UQ Challenge 2019 [1];
- The objective is to investigate the different calibration approaches to the UM and determine which of the following factors has significant contribution to the uncertainty on the UM:
  1. the choice of distribution model for $\boldsymbol{a}$;
  2. the choice of the stochastic distance metric to model the data variability; and
  3. the choice of data type to calibrate the UM.



Background

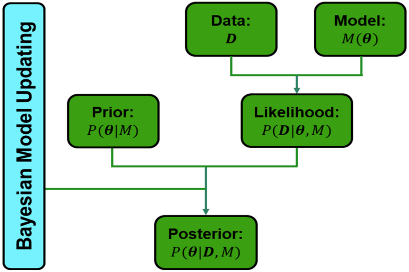
- A Black-box Uncertainty Model is to be calibrated [2];
- Consists of 5 aleatory parameters, $\boldsymbol{a}$, and 4 epistemic parameters, $\boldsymbol{e}$, such that: $\boldsymbol{a} \subseteq [0, 2]^5$ & $\boldsymbol{e} \subseteq [0, 2]^4$;
- By virtue of being aleatory, $\boldsymbol{a} \sim f_a(\boldsymbol{a})$, where $f_a(\boldsymbol{a})$ is a distribution function bounded between $[0, 2]$;
- For the calibration, we are given 100 sets of the sub-system's response data from $t = 0s$ to $t = 5s$ with $\Delta t = 0.001s$;
- The calibration is done via Bayesian Model Updating [3].

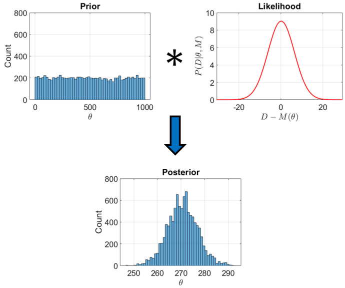


Conceptual Introduction:

- Bayesian Model Updating [3]:

$$P(\boldsymbol{\theta}|\boldsymbol{D}, M) = \frac{P(\boldsymbol{D}|\boldsymbol{\theta}, M) \cdot P(\boldsymbol{\theta}|M)}{P(\boldsymbol{D}|M)}$$





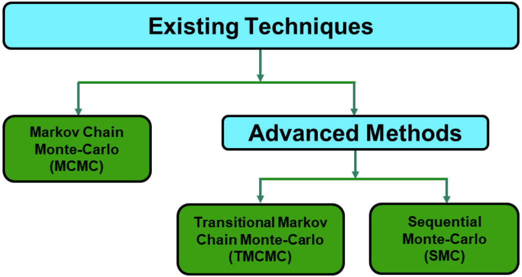
Methodology: Bayesian Model Updating

Conceptual Introduction:

- However, $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$ is usually un-normalised: [3]:

$$P(\boldsymbol{\theta}|\boldsymbol{D}, M) \propto P(\boldsymbol{D}|\boldsymbol{\theta}, M) \cdot P(\boldsymbol{\theta}|M)$$

- Standard Monte-Carlo approach cannot work, we need something else!
- Detailed explanation to the respective samplers found in Review paper [3];
- For this work, the state-of-the-art Transitional Ensemble Markov Chain Monte Carlo (TEMCMC) is implemented [4]



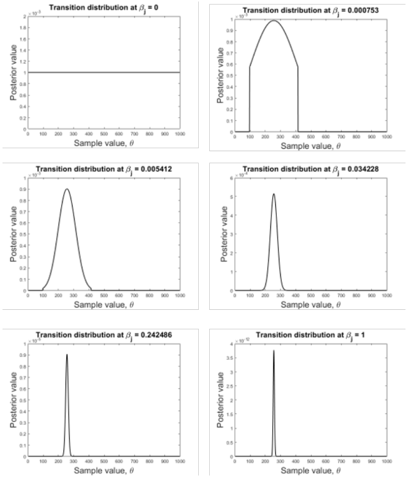
Methodology: TEMCMC

- A variant of the TMCMC algorithm, utilising the Affine-invariant Ensemble sampler as the MCMC kernel;
- Adopts the use "transitional" distributions, P^j:

$$P^j \propto P(\boldsymbol{D}, M|\boldsymbol{\theta})^{\beta_j} \cdot P(\boldsymbol{\theta}|M)$$

  where $j = 1, ..., m$ denotes the iteration number, and β_j is such that $\beta_0 = 0 < \beta_1 <, ..., < \beta_{m-1} < \beta_m = 1$

- Change in β_j has to be small to ensure smooth, gradual transition;
- Performs parallel sampling: N samples obtained per iteration;
- Generates the solution for $P(\boldsymbol{D}|M)$ as by-product;
- Details provided in [4].



Methodology: Uncertainty Model set-up

- We consider 2 different functions to model the Aleatory model parameters $\boldsymbol{a}$:

S/N:	Distribution:	Shape Parameters:
1	Beta	$\boldsymbol{\theta}_a = \{\alpha, \beta\}$
2	SDF	$\boldsymbol{\theta}_a = \{\underline{x}, \overline{x}, \mu, m_2, m_3\}$

- The Approximate Bayesian Computation (ABC) approach will be adopted to address the problem;
- An approximate "Gaussian" likelihood function $P(\boldsymbol{D}|\boldsymbol{\theta}, f_a)$ is adopted to compute the likelihood [5] :

$$P(\boldsymbol{D}|\boldsymbol{\theta}, f_a) \propto exp\left[\frac{d^2}{\epsilon^2}\right]$$

where d is the stochastic distance metric, and ϵ is the width parameter;

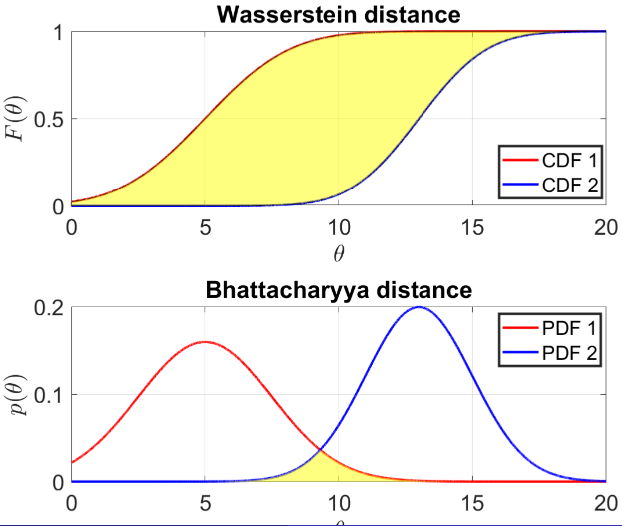
- We consider 2 stochastic distance metrics:

S/N:	Distance metric:	Formula:
1	Wasserstein distance	d $= \int_{\boldsymbol{\theta}} \lvert F_{yfun}(\boldsymbol{\theta}) - F_{\boldsymbol{D}}(\boldsymbol{\theta})\rvert \cdot d\boldsymbol{\theta}$
2	Bhattacharyya distance	d $=$ -log $\left[\int_{\boldsymbol{\theta}} \sqrt{p_{yfun}(\boldsymbol{\theta}) \cdot p_{\boldsymbol{D}}(\boldsymbol{\theta})} \cdot d\boldsymbol{\theta}\right]$

Wasserstein vs Bhattacharyya Distances

Illustrative Example:

- Consider 2 distinct distributions:
  1. $P_1(\theta) \sim N(5, 2.5)$;
  2. $P_2(\theta) \sim N(13, 2)$;



Methodology: Uncertainty Model set-up

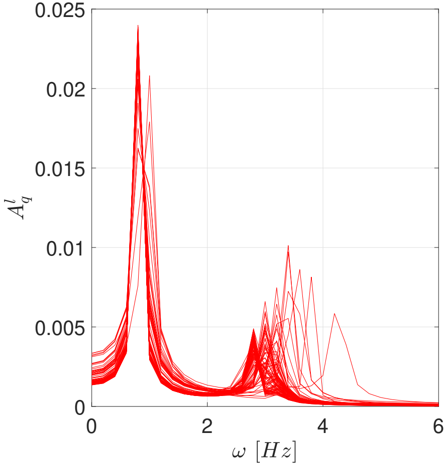
We consider 2 types of data to use for calibration [1]:

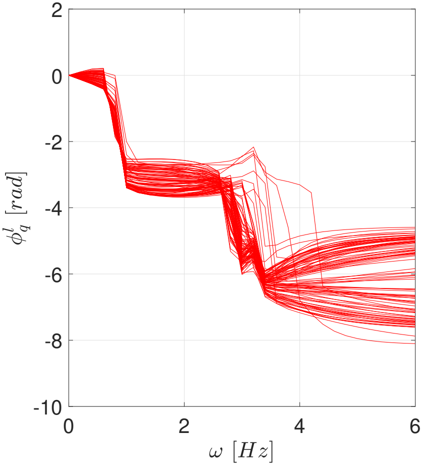
- 1) Time-domain data:
  - Set window length $L_w = 50$ and divide $\{y^l(t)\}_{l=1,\dots,100}$ into 101 distinct windows;
  - Compute the Root Mean Squared (RMS) values of each interval $\boldsymbol{R} = \left[R_1, \dots, R_{\frac{N_t}{L_w}}\right]$ and generate the sample set of the RMS values $\boldsymbol{R}_D \in \mathbb{R}^{100 \times \frac{N_t}{L_w}}$ where:

$$\boldsymbol{R}_D = \left[\boldsymbol{R}_D^1, \dots, \boldsymbol{R}_D^{\frac{N_t}{L_w}}\right], \text{ with } \boldsymbol{R}_D^{\nu} = [R_{1,\nu}, \dots, R_{100,\nu}]^T$$

    for $\nu = 1, \dots, \frac{N_t}{L_w}$ while $\boldsymbol{R}_{\hat{y}} \in \mathbb{R}^{N_{sim} \times \frac{N_t}{L_w}}$ where $N_{sim} = 1000$ the number of model evaluations by $\hat{y}$ per given set of model inputs $\{\boldsymbol{a}, \boldsymbol{e}\}$;
  - Evaluate the corresponding stochastic distance d between sample sets $\boldsymbol{R}_D^{\nu}$ and $\boldsymbol{R}_{\hat{y}}^{\nu}$ for all ν;
  - Obtain the corresponding RMS values R_d and use it as the distance metric.
- 2) Frequency-domain data:
  - Perform Fast Fourier Transform (FFT) on the Time-domain data and identify the Amplitude and Phase angles;
  - Discard data corresponding to frequencies with insignificant perturbations.

Methodology: Uncertainty Model set-up





Methodology: Uncertainty Model set-up

- In the NASA-Langley Challenge investigation, the following set-ups were used to derive 2 distinct UMs:

UM:	Aleatory model:	Distance metric:	Data:
UM^1_{y0}	Beta	Wasserstein	Frequency-based
UM^2_{y0}	Staircase Density Function (SDF)	Bhattacharyya	Time-based

- In the work, it was found that UM^2_{y0} yielded tighter epistemic bounds and aleatory P-boxes compared to UM^1_{y0} and this investigation seeks to identify which aspect of the set-up is responsible for the effectiveness of the Bayesian model updating results;
- UM^2_{y0} will be used as the "Control experiment", whose results will serve as reference to other set-ups:

Investigation:	Aleatory model:	Distance metric:	Data:
UM^1_{y0}	Beta	Wasserstein	Frequency-based
UM^2_{y0} (Control)	SDF	Bhattacharyya	Time-based
UM^I_{y0}	SDF	Wasserstein	Frequency-based
UM^{II}_{y0}	Beta	Bhattacharyya	Frequency-based
UM^{III}_{y0}	Beta	Wasserstein	Time-based
UM^{IV}_{y0}	Beta	Bhattacharyya	Time-based

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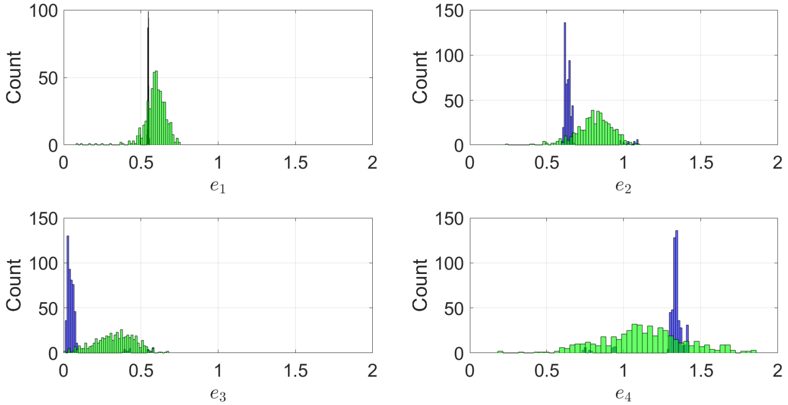
Results: Epistemic model parameter Uncertainty

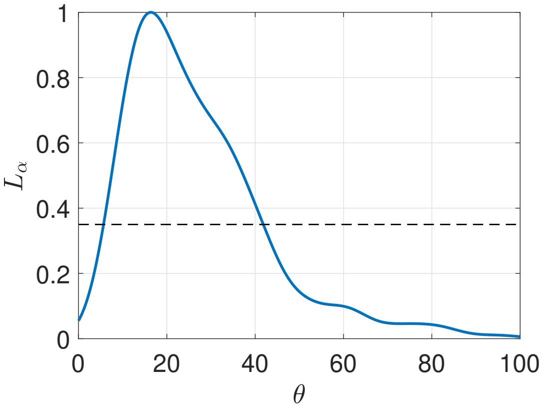


UM_{y0}^{IV} (blue) vs UM_{y0}^{2} (green).

Results: Epistemic model parameter Uncertainty

Fuzzy-set and Alpha-cut [6]:

- The histograms are converted into probability distribution functions using Kernel density estimation with a Gaussian kernel;
- The resulting distribution is normalized such that the distribution peak equals to 1;
- The distribution can be interpreted as Fuzzy sets where different levels of confidence L_α would yield distribution-free intervals of varying width;
- Following the work in [1], we set $L_\alpha = 0.025$.



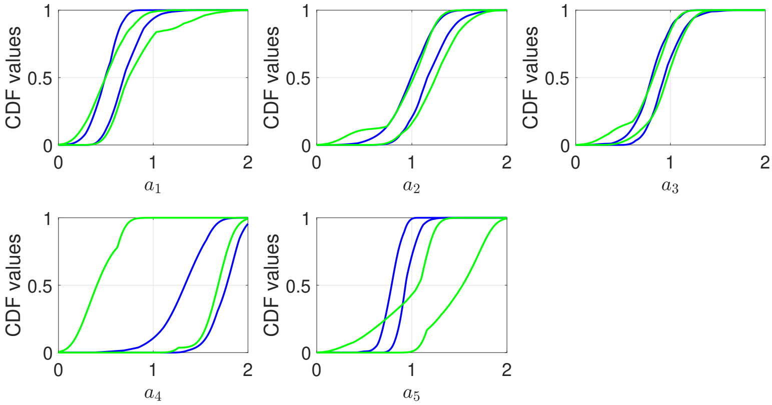
Results: Epistemic model parameter Uncertainty

Investigation:	Aleatory model:	Distance metric:	Data:
UM_{y0}^{2} (Control)	SDF	Bhattacharyya	Time-based
UM_{y0}^{1}	Beta	Wasserstein	Frequency-based
UM_{y0}^{I}	SDF	Wasserstein	Frequency-based
UM_{y0}^{II}	Beta	Bhattacharyya	Frequency-based
UM_{y0}^{III}	Beta	Wasserstein	Time-based
UM_{y0}^{IV}	Beta	Bhattacharyya	Time-based

UM	e_1	e_2	e_3	e_4	V_E
UM_{y0}^{1}	$[0.2307, 1.4567]$	$[0.3155, 1.4810]$	$[0.0411, 1.4123]$	$[0.0641, 1.9417]$	3.6772
UM_{y0}^{2} (Control)	$[0.4351, 0.7082]$	$[0.5583, 1.0000]$	$[0.0721, 0.5511]$	$[0.6066, 1.6893]$	0.0626
UM_{y0}^{I}	$[0.0149, 1.6714]$	$[0.1245, 1.2491]$	$[0.1441, 1.9873]$	$[0.0083, 1.5558]$	5.3139
UM_{y0}^{II}	$[0.2054, 1.6552]$	$[0.3158, 1.3241]$	$[0.0204, 0.8553]$	$[0.0247, 1.7999]$	1.2855
UM_{y0}^{III}	$[0.4024, 0.6671]$	$[0.6191, 1.2870]$	$[0.0161, 0.6122]$	$[0.1487, 1.9641]$	0.1914
UM_{y0}^{IV}	$[0.4864, 0.6336]$	$[0.7415, 0.9850]$	$[0.1746, 0.4911]$	$[0.1511, 0.5023]$	0.0040

Intervals for $\boldsymbol{e}$ obtained for the respective UM.

Results: Aleatory model parameter Uncertainty



UM_{y0}^{IV} (blue) vs UM_{y0}^{2} (green).

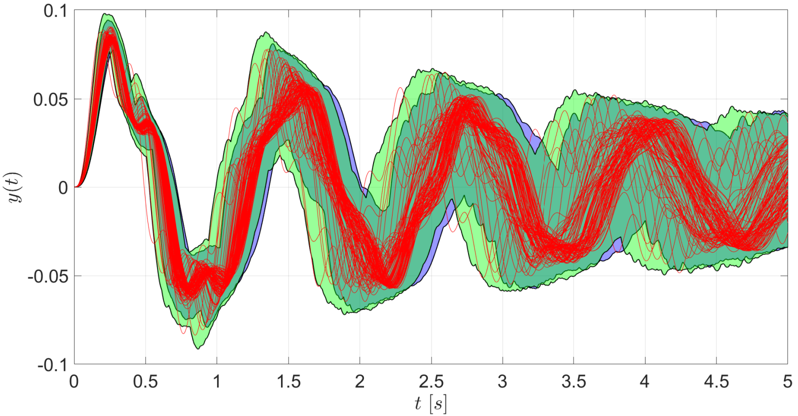
Results: Aleatory model parameter Uncertainty

Investigation:	Aleatory model:	Distance metric:	Data:
UM^{1}_{y0}	Beta	Wasserstein	Frequency-based
UM^{2}_{y0} (Control)	SDF	Bhattacharyya	Time-based
UM^{I}_{y0}	SDF	Wasserstein	Frequency-based
UM^{II}_{y0}	Beta	Bhattacharyya	Frequency-based
UM^{III}_{y0}	Beta	Wasserstein	Time-based
UM^{IV}_{y0}	Beta	Bhattacharyya	Time-based

UM	a_1	a_2	a_3	a_4	a_5
UM^{1}_{y0}	0.6849	1.2786	0.4638	0.8690	0.7655
UM^{2}_{y0} (Control)	0.3200	0.2946	0.1783	1.2531	0.7159
UM^{I}_{y0}	0.5902	1.0410	0.4886	0.8699	0.5617
UM^{II}_{y0}	1.0101	1.1212	0.7176	0.8109	0.7250
UM^{III}_{y0}	0.5789	0.8208	0.3011	1.0734	0.8568
UM^{IV}_{y0}	0.2217	0.2023	0.1501	0.4416	0.1614

Area enclosed by the P-box of each component of $\boldsymbol{a}$ given the respective UM set-up.

Results: Model output Uncertainty



UM_{y0}^{IV} (blue) vs UM_{y0}^{2} (green).

Results: Model output Uncertainty

Investigation:	Aleatory model:	Distance metric:	Data:
UM^{1}_{y0}	Beta	Wasserstein	Frequency-based
UM^{2}_{y0} (Control)	SDF	Bhattacharyya	Time-based
UM^{I}_{y0}	SDF	Wasserstein	Frequency-based
UM^{II}_{y0}	Beta	Bhattacharyya	Frequency-based
UM^{III}_{y0}	Beta	Wasserstein	Time-based
UM^{IV}_{y0}	Beta	Bhattacharyya	Time-based

UM	UM^{1}_{y0}	UM^{2}_{y0}	UM^{I}_{y0}	UM^{II}_{y0}	UM^{III}_{y0}	UM^{IV}_{y0}
Area	0.4117	0.4114	0.4452	0.4210	0.3710	0.3518

Area enclosed by the P-box of each component of $\boldsymbol{a}$ given the respective UM set-up.

Conclusion

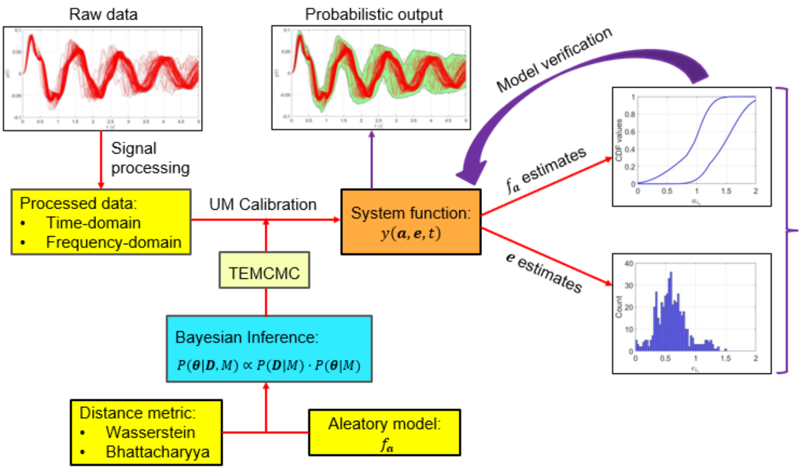
Research Outcome:

- Significant decrease in the uncertainty of the results in $\boldsymbol{e}$ between UM_{y0}^{III} and UM_{y0}^{1};
    - The type of data used for the calibration plays a significant role.
- Improvement in the precision of the estimates from UM_{y0}^{III} to UM_{y0}^{IV} due to the choice in the stochastic distance metric;
    - The Bhattacharyya's distance is a better metric than the Wasserstein's distance in this context;
    - Such improvement, however, is less significant than that due to the choice of data-type.
- The choice of f_a is of the least relative significance as there is little improvement in the interval estimates for each component of $\boldsymbol{e}$ and the P-box estimates of f_a;
- Hence, in order of descending significance on the uncertainty of the Uncertainty Model estimates is:

Rank	1	2	3
Factor	Data	Distance metric	Aleatory model

Conclusion

Presentation Summary:



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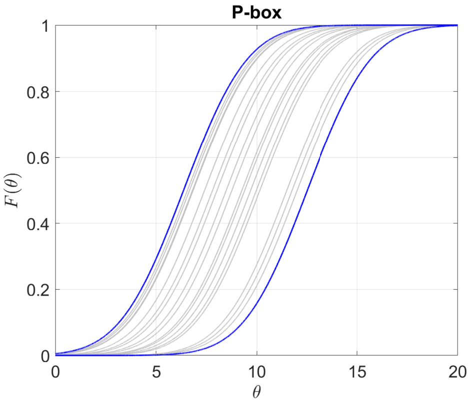
Q & A: P-box

Illustrative Example:

- Consider a Normal distribution with $\mu = [5, 13]$ and $\sigma = 2.5$;
- We will obtain a collection of distributions for different values of μ;
- Consider only the extreme bounds and this gives an interval distribution;
- Quantifies our uncertainty over the true distribution.



Q & A: Staircase Density Function

- A class of random variables for uncertainty modelling;
- The variables of interest have a bounded support set and prescribed values for the first 4 moments;
- These variables satisfy a set of feasibility conditions whose distributions are obtained via Convex optimization according to several optimality criteria;
- The term "Staircase" is due the density of the variables being a piece-wise constant function;
- Provides flexibility in modelling skewed and/or multi-modal response at a low computational cost;
- An efficient and robust meta-modelling tool to model epistemic and aleatory uncertainties.

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Random variables with moment-matching staircase density functions

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ABSTRACT

This paper proposes a family of random variables for uncertainty modeling. The variables of interest have a bounded support set, and prescribed values for the first four moments. We present the feasibility conditions for the existence of any of such variables, and propose a class of variables that conforms to such constraints. This class is called staircase because the density of its members is a piecewise constant function. Convex optimization is used to calculate their distributions according to several optimality criteria, including maximal entropy and maximal log-likelihood. The flexibility and efficiency of staircases enable modeling phenomena having a possibly skewed and/or multimodal response at a low computational cost. Furthermore, we provide a means to account for the uncertainty in the distribution caused by estimating staircases from data. These ideas are illustrated by generating empirical staircase predictor models. We consider the case in which the predictor matches the sample moments exactly (a setting applicable to large datasets), as well as the case in which the predictor accounts for the sampling error in such moments (a setting applicable to sparse datasets). A predictor model for the dynamics of an aeroelastic airfoil subject to flutter instability is used as an example. The resulting predictor not only describes the system's response accurately, but also enables carrying out a risk analysis for safe flight.

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Mathematical Preliminaries

- Consider the continuous random variable x with support set: $\Delta x = [\underline{x}, \overline{x}]$ and density $f(x)$, we define the r^{th} moment:

$$m_r = \int_{\Delta x} (x - \mu)^r \cdot f(x) \cdot dx, \quad r = 0, 1, 2, \ldots$$

  where μ is the expected value of x;

- Define the variables of the SDF as $\boldsymbol{\theta}_x \in \mathbb{R}^6$ whereby:

$$\boldsymbol{\theta}_x = [\underline{x}, \overline{x}, \mu, m_2, m_3, m_4]$$

- Note that $m_0 = 1$, $m_1 = 0$, m_2 is the variance, m_3 is the 3^{rd}-central moment, and m_4 is the 4^{th}-central moment.

Mathematical Preliminaries

- Feasibility conditions for $\boldsymbol{\theta}_x$ are given by $g_{1:14}(\boldsymbol{\theta}_x) \leq 0$ whereby [7, 8]:

$$g_1 = \underline{x} - \overline{x}$$

$$g_2 = \underline{x} - \mu$$

$$g_3 = \mu - \overline{x}$$

$$g_4 = -m_2$$

$$g_5 = m_2 - v$$

$$g_6 = {m_2}^2 - m_2 \cdot (\mu - \underline{x})^2 - m_3 \cdot (\mu - \underline{x})$$

$$g_7 = m_3 \cdot (\overline{x} - \mu) - m_2 \cdot (\overline{x} - \mu)^2 + {m_2}^2$$

$$g_8 = 4{m_2}^3 + {m_3}^2 - {m_2}^2 \cdot (\overline{x} - \underline{x})^2$$

$$g_9 = 6\sqrt{3} \cdot m_3 - (\overline{x} - \underline{x})^3$$

$$g_{10} = -6\sqrt{3} \cdot m_3 - (\overline{x} - \underline{x})^3$$

$$g_{11} = -m_4$$

$$g_{12} = 12 \cdot m_4 - (\overline{x} - \underline{x})^4$$

$$g_{13} = (m_4 - v \cdot m_2 - u \cdot m_3) \cdot (v - m_2) + (m_3 - u \cdot m_2)^2$$

$$g_{14} = {m_3}^2 + {m_2}^3 - m_2 \cdot m_4$$

- Here, $u = \overline{x} - \underline{x} - 2 \cdot \mu$, and $v = (\mu - \underline{x}) \cdot (\overline{x} - \mu)$;
- We define the variables which satisfy these constraints: $\boldsymbol{\Theta}_x = \{\boldsymbol{\theta}_x : g_{1:14}(\boldsymbol{\theta}_x) \leq 0\}$

Mathematical Preliminaries

- Problem: There might be indefinitely many random variables that realize a point in $\boldsymbol{\Theta}_x$;
- Solution: Staircase Random Variables (SRVs);
- Consider a random variable with density $f(x, h)$, where h is a hyper-parameter to be prescribed such that:

$$\hat{h} = \arg\min_{h} \left\{ J(h) : \int_{\Delta x} x \cdot f(x, h) \cdot dx = \mu, \;\; \int_{\Delta x} (x - \mu)^r \cdot f(x, h) \cdot dx = m_r, \;\; r = 0, 2, 3, 4 \right\} \tag{1}$$

where J is an arbitrary cost function [2]:

$$J(l) = \begin{cases} -E(l) = -\kappa \cdot log(l)^T l & \text{, the Differential Entropy} \\ H(l, Q, f) = l^T Q l + f^T l & \text{, the Hamiltonian with } Q \in \mathbb{R}^{n_b \times n_b} \text{ semi-positive definite} \\ -L(l, \{D_j\}_{j=1,\ldots,N}) = -\omega^T log(l) & \text{, the negative Log-likelihood where } D \text{ is the data} \end{cases}$$

for which $\omega \in \mathbb{R}^{n_b}$ where $\omega_i = \sum_{j=1}^{N} I\{D_j \in [z_i, z_{i+1}]\}$, and I is the indicator function.

Mathematical Preliminaries

- Next, to identify the staircase variable which realizes the parameters in $\boldsymbol{\theta}_x$, we define $n_b \geq 1$ as the number of equal partitions in interval $[\underline{x}, \overline{x}]$ where each sub-interval has width $\kappa = \frac{(\overline{x} - \underline{x})}{n_b}$;
- From which, we have the points $x_i = \underline{x} + (i-1) \cdot \kappa$ (for $1 \leq i \leq n_b + 1$);
- The staircase heights are then given by $l \in \mathbb{R}^{n_b}$ with $l \geq 0$ and $\kappa \cdot \sum_{i=1}^{n_b} l_i = 1$ which yields:

$$f(x, h) = \begin{cases} l_i & , \forall \; x \in (x_i, x_{i+1}] \text{ for } 1 \leq i \leq n_b \\ 0 & , \text{otherwise} \end{cases} \tag{2}$$

- Applying Eq. (1) to a staircase variable, $h = [\boldsymbol{\theta}_x, n_b]$, where $\boldsymbol{\theta}_x \in \boldsymbol{\Theta}$, and the resulting staircase variable is denoted as:

$$x \sim S_x(\boldsymbol{\theta}_x, n_b, J)$$

which has the staircase density prescribed by Eq. (2), where l is defined as:

$$\hat{l} = \underset{l \geq 0}{\arg\min} \left\{ J(l) : \boldsymbol{A}(\boldsymbol{\theta}_x, n_b) \cdot l = \boldsymbol{b}(\boldsymbol{\theta}_x), \quad \boldsymbol{\theta}_x \in \boldsymbol{\Theta} \right\}$$

where $\boldsymbol{A} \in \mathbb{R}^{5 \times n_b}$ and $\boldsymbol{b} \in \mathbb{R}^5$.

Mathematical Preliminaries

- The matrix $\boldsymbol{A}$ and vector $\boldsymbol{b}$ are defined as:

$$\boldsymbol{A} = \begin{bmatrix} \kappa\boldsymbol{e} \\ \kappa\boldsymbol{c} \\ \kappa\boldsymbol{c}^2 + \frac{\kappa^3}{12} \\ \kappa\boldsymbol{c}^3 + \frac{\kappa^3\boldsymbol{c}}{4} \\ \kappa\boldsymbol{c}^4 + \frac{\kappa^3\boldsymbol{c}^2}{2} + \frac{\kappa^5}{80} \end{bmatrix}, \text{ and } \boldsymbol{b} = \begin{bmatrix} 1 \\ \boldsymbol{\mu} \\ \boldsymbol{\mu}^2 + \boldsymbol{m}_2 \\ \boldsymbol{m}_3 + 3\boldsymbol{\mu}\boldsymbol{m}_2 + \boldsymbol{\mu}^3\boldsymbol{m}_4 + 4\boldsymbol{m}_3\boldsymbol{\mu} + 6\boldsymbol{m}_2\boldsymbol{\mu}^2 + \boldsymbol{\mu}^4 \end{bmatrix}$$

where $\boldsymbol{c} \in \mathbb{R}^{n_b}$ is a vector of the centre of the bins, $\boldsymbol{c}^p$ is the component-wise p^{th} power of $\boldsymbol{c}$, and $\boldsymbol{e}$ is a vector of ones.