Uncertainty Quantification via Optimal Experimental Design and Bayesian Neural Networks for Aerospace Applications

Xun Huan
xhuan@umich.edu

University of Michigan
Mechanical Engineering

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Uncertainty in engineering and science

(Sources: 1. Argonne National Lab; 2. www.weather.com; 3. NASA Ames)
Uncertainty is everywhere

“Uncertainty is everywhere and you cannot escape from it.”

— Dennis Lindley

Uncertainty quantification (UQ) focuses on systematic approaches to bridge together data and models, and allows us to:

- characterize
- incorporate
- propagate
- reduce

...uncertainty in complex engineering systems

To what extent can we trust a simulation and its prediction? How can we continue to improve that trust?
UQ in engineering and science: big picture

Mathematical Model

Data Analysis & Assimilation

Theory

Uncertainty Propagation

Prediction

Product, Decision

Optimization Under Uncertainty

Experimental Design

Experiment

Data
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Huan (University of Michigan)
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Experimental Design

Experiment
UQ work in hypersonics research

UQ for scramjet design—supersonic turbulent reactive flow

HIFiRE: [Dolvin 08, Dolvin 09, Gruber 08, Jackson 11, Ferlemann 08, Gruber 09]; Scramjet UQ: [Witteveen 11, Constantine 15]
RAPTOR flow solver: [Oefelein 06, Oefelein 07, Lacaze 17]

Uncertainty propagation through flow-field


Bayesian inference of model-form uncertainty:

No model error treatment

With model error treatment

max $\eta_c$ design optimization:

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>QoI</th>
<th>Allowable</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_G$</td>
<td>$\phi_{\text{burn}}$</td>
<td>$\geq 0.1843$ (nominal d/8)</td>
</tr>
<tr>
<td>$\phi_R$</td>
<td>$\max P_{\text{rms}}$</td>
<td>$\leq 0.1677$ (nominal d/8)</td>
</tr>
<tr>
<td>$x_1$</td>
<td>$x_{\text{shock}}$</td>
<td>$\geq 32d$</td>
</tr>
<tr>
<td>$x_2$</td>
<td>$P_{\text{stagloss}}$</td>
<td>$\leq 0.3768$ (nominal d/8)</td>
</tr>
</tbody>
</table>


UQ in engineering and science: big picture
Outline

1. Optimal Experimental Design
2. Bayesian Neural Network Surrogate Models
3. Data-Driven Modeling of Turbulence Energy Spectrum
4. Summary
Some experiments are more useful than others

Experiments can be:

- Expensive
- Time-consuming
- Delicate to perform
- Dangerous or controversial

(Statistical) experimental design focuses on questions such as:

- Under what **conditions** (how) to perform the experiments?
- **What**, **where**, and **when** to measure?
- **How many** experiments?

Experimental design may have an entirely different meaning to experimentalists
Classical statistical **design of experiments** often non simulation-based (e.g. space-filling)  [Fisher 35, Box 87, Cox 00, Box 05, Santner 18]

**Optimal experimental design**: criterion based on a model/simulator

- Linear: information matrix (e.g., A-, D-optimal)  [Fedorov 72, Atkinson 07]
- Nonlinear: intractable  [Box 59, Ford 89, Chaloner 95, Müller 05, Ryan 16]
- Bayesian and decision-theoretic: maximize expected utility  
  [Lindley 56, Berger 85, Clyde 96, Müller 04, Amzal 06, Parmigiani 09, Santner 18]
- Recent numerical advances (and many more...)  
  [Ryan 03, Huan 13, Long 15, Weaver 16, Alexanderian 16, Tsilifis 17, Beck 18]

**Scope of this talk:**

- **Nonlinear** and expensive (e.g., physics-based) models
- **Continuous** parameter, design, and data spaces of multiple dimensions
- Bayesian information objective with non-Gaussian distributions
### Step 1: Define experimental goals

**What is a good experiment?**

Depends on the experimental goals

### Examples:

<table>
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<tr>
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<td>learn model parameter</td>
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<td>minimize a loss function</td>
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**Step 1: Define experimental goals**

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Step 2: Formulate objective function

Characterize uncertainty using Bayes’ Theorem:

\[
\frac{\text{posterior}}{\text{likelihood}} \cdot \text{prior} = \text{evidence}
\]

\[p(y|\theta, d) \cdot p(\theta|d) = \frac{p(\theta)}{p(y|d)}\]

\(\theta\) — parameters \quad y — noisy data

\[
p(\theta)
\]

Prior

\[
\theta
\]
Step 2: Formulate objective function

Characterize uncertainty using **Bayes’ Theorem**:

\[
p(y|\theta) p(\theta)
\]

\(\theta\) — parameters \(y\) — noisy data

\[p(\theta)\]

\[
\text{Prior} \quad \text{Likelihood (inference)}
\]
Step 2: Formulate objective function

Characterize uncertainty using **Bayes’ Theorem**:

$$p(\theta|y) = \frac{p(y|\theta) \cdot p(\theta)}{p(y)}$$

- **posterior**
- **likelihood**
- **prior**
- **evidence**

\(\theta\) — parameters  \(y\) — noisy data

![Graph showing prior, likelihood, and posterior distributions]
Step 2: Formulate objective function

Characterize uncertainty using **Bayes’ Theorem**:

\[
p(\theta | y, d) = \frac{p(y | \theta, d) p(\theta | d)}{p(y | d)}
\]

\(\theta\) — parameters \(y\) — noisy data \(d\) — design (experimental conditions)

\[p(\theta)\]

Prior

\[p(\theta | y)\]

Posterior

Likelihood

(inference)
Step 2: Formulate objective function

Expected **Kullback-Leibler (KL)** divergence between posterior and prior ($\iff$ **mutual information** between data and parameters)

$$
U(d) = \mathbb{E}_{y|d} \left[ D_{KL}(p(\theta|y, d)||p(\theta|d)) \right] \\
= \int_y \left[ \int_\Theta \ln \left( \frac{p(\theta|y, d)}{p(\theta)} \right) p(\theta|y, d) d\theta \right] p(y|d) dy \\
\approx \frac{1}{N} \sum_{i=1}^{N} \left\{ \ln \left[ p(y^{(i)}|\theta^{(i)}, d) \right] - \ln \left[ p(y^{(i)}|d) \right] \right\} \\
p(y^{(i)}|d) \approx \frac{1}{M} \sum_{j=1}^{M} p(y^{(i)}|\theta^{(i,j)}, d) \quad \text{(nested Monte Carlo!)}
$$

$U$ — expected utility

$\theta$ — parameters of interest

$y$ — noisy data

$d$ — design variables
Step 3: Approximate objective function numerically

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\(U\) — expected utility

\(\theta\) — parameters of interest

\(y\) — noisy data

\(d\) — design variables
Step 3: Approximate objective function numerically

Likelihood evaluation is the most expensive part:

\[ p(y|\theta, d) \]

Need to specify a likelihood model:

- statistical description of mismatch between model prediction vs. observed data
- e.g., additive Gaussian noise \( \epsilon \sim \mathcal{N}(0, \sigma^2_\epsilon) \)

\[ y = G(\theta, d) + \epsilon \]

Each evaluation \( p(y|\theta, d) = p_\epsilon(y - G(\theta, d)) \) requires a model solve

\( U \) — expected utility

\( \theta \) — parameters of interest
\( y \) — noisy data
\( d \) — design variables
Step 4: Perform stochastic optimization

Find optimal design:  
\[ d^* = \arg\max_{d \in \mathcal{D}} U(d) \]

\[ \Rightarrow \textbf{noisy} \text{ objective function due to Monte Carlo} \]

**Robbins-Monro** stochastic approximation  \[ [\text{Robbins 51}] \]

- Needs to derive gradient
- Can approximate by building certain types of surrogate models
Example: polynomial chaos expansions \[g(\theta(\xi)) = \sum_{\beta \in \mathcal{I}} c_\beta \psi_\beta(\xi)\]

- \(c_\beta\): coefficients (\(\beta\) polynomial order multi-index)
- \(\xi\): reference random vector (e.g., uniform, Gaussian)
- \(\psi_\beta\): multivariate orthonormal polynomial (e.g., Legendre, Hermite)

Non-intrusive approach to compute coefficients

\[c_\beta = \langle G\psi_\beta \rangle = \int G(\theta(\xi), d(\xi))\psi_\beta(\xi)p(\xi) \, d\xi\]

Integrate using adaptive sparse quadrature \[\text{[Gerstner 98, Barthelmann 00, Gerstner 03]}\]
Design of shock tube experiment for combustion kinetics

$\text{H}_2-\text{O}_2$ homogeneous ignition, no transport, constant pressure, adiabatic

**Goal:** learn 2 kinetic parameters in a 19-reaction mechanism \[\text{[Yetter } 91\text{]}\]

- $\ln A$ of $R1: \; H + \text{O}_2 \leftrightarrow O + \text{OH}$
- $E_a$ of $R3: \; \text{H}_2 + \text{OH} \leftrightarrow \text{H}_2\text{O} + \text{H}$

System of stiff ODEs, numerically solved using Cantera with CVODE

**Measurement:** ignition delay time

**Design variables:** initial $T$ and $\phi$ (fuel amount used)

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**Huan & Marzouk, “Simulation-based optimal Bayesian experimental design for nonlinear systems,”**

*Journal of Computational Physics, 232(1):288–317, 2013.* \[\text{[Huan } 13\text{]}\]
Sensor placement for source inversion

2D scalar diffusion PDE in a square domain with a time-limited source

**Goal:** infer uncertain source location

**Measurements:** concentrations at 5 equally spaced sample times

**Design variables:** sensor coordinates

---

Sensor placement for source inversion: 1 sensor

Posterior PDFs: \( x_{\text{src}} = (0.39, 0.52) \)

\( x_{\text{sensor}} = (0, 0) \)

\( x_{\text{sensor}} = (0, 1) \)

\( x_{\text{sensor}} = (0.5, 0.5) \)
Sensor placement for source inversion: 1 sensor

Posterior PDFs: $x_{src} = (0.39, 0.52)$ (row 1) and $x_{src} = (0.09, 0.22)$ (row 2):

- $x_{sensor} = (0, 0)$
- $x_{sensor} = (0, 1)$
- $x_{sensor} = (0.5, 0.5)$
Sensor placement for source inversion: 2 sensors

Posterior PDFs: $x_{src} = (0.39, 0.52)$ (row 1) and $x_{src} = (0.09, 0.22)$ (row 2):

$x_{sensors} = (0, 0), (0, 0)$

$x_{sensors} = (0, 0), (0, 1)$

$x_{sensor} = (0.5, 0.5), (0.5, 0.5)$
Planning measurements: batch (non-sequential) design

Location of contaminant?

Wind
Planning measurements: sequential design

Location of contaminant?

Wind
Planning measurements: sequential design

Sequential experimental design much more challenging

- Greedy (myopic) design generally sub-optimal
- Incorporate 1. feedback and 2. lookahead
- Utilize dynamic programming and reinforcement learning

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Motivation: in-flight rotorcraft icing


- In-flight rotorcraft icing is extremely dangerous:
  - alters leading-edge shape of rotor blades
  - severely degrades aerodynamic performance
  - is difficult to escape from/recover
- Many icing-induced fatal accidents in recent years
- Real-time in-flight ice detection system is of paramount importance

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Source: BBC NEWS, Mar 2nd 2006

Source: NASA Glenn Icing Research Wind Tunnel
Motivation: in-flight rotorcraft icing

In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using acoustic signals enabled by simulations

- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)
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**But:** physics-based solutions very expensive (min/hours)

⇒ accelerate via **machine-learning (ML)** models
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Numerical modeling and simulations

Key components (omitting much details, please see [Zhou 19a]):

- PoliDrop, PoliMIce—ice seeding and accretion
- URANS/DES—turbulent flow solve for near field
- FW-H (Ffowcs Williams-Hawking)—acoustics solver propagate signals to far field
- Coupled through open-source software SU2 [Zhou 15]
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Deep Learning

Huan (University of Michigan)  Experimental Design & Bayesian NNs  August 27, 2019
Deep neural networks (DNNs)

A neural network (NN) is a function \( f : x \in \mathbb{R}^m \rightarrow \hat{y} \in \mathbb{R}^n : \)

\[
\hat{y} = f(x)
\]

- \( \hat{y} \) here denotes DNN prediction
- Example below: fully connect feed-forward NN
- NN generally considered “deep” with 2+ hidden layers
Deep neural networks (DNNs)

Computation at node $j$ in layer $\ell$:

$$a_{\ell,j} = \phi_\ell \left( \sum_i W_{\ell,ij} a_{\ell-1,i} + b_{\ell,j} \right)$$

- $a_{\ell,j}$: nodal output
- $a_{\ell-1,i}$: nodal input from previous layer
- $W_{\ell,ij}$: weight on $a_{\ell-1,i}$
- $b_{\ell,j}$: bias (offset) term
- $\phi_\ell$: activation function (e.g., rectified linear unit, tanh)
Deep neural networks (DNNs)

In this example:

\[ a_0 = x \]
\[ a_1 = \phi_1(W_1^T a_0 + b_1) \]
\[ a_2 = \phi_2(W_2^T a_1 + b_2) \]
\[ a_3 = \phi_3(W_3^T a_2 + b_3) = \hat{y} \]

Training a DNN: find the best \( \mathbf{w} \equiv \{W_\ell, b_\ell\} \)
Deep neural networks (DNNs)

Given training data \((x_T, y_T) = \{x_n, y_n\}_{n=1}^{N}\), solve regression problem:

\[
    w^* = \arg\min_w \left\{ \frac{1}{N} \sum_{n=1}^{N} \| f(x_n; w) - y_n \|_2^2 \right\}
\]

- Popular algorithm: stochastic gradient descent [LeCun 12, Robbins 51]
- Gradient \(\nabla_w f\) computed from chain rule (back-propagation)
Deep neural networks (DNNs)

**However**, after training, only single-valued predictions available:

\[
\hat{y} = f(x; w^*)
\]

- DNN does not offer uncertainty information to indicate the quality and credibility of output value
- We expect the prediction uncertainty to vary depending on:
  - architecture of the DNN
  - quantity, quality, and informativeness of the training data
  - input/operating regime, etc.

---

**How much can we trust this DNN prediction?**

This question is crucial for mission- and safety-critical scenarios, and must be addressed before certifying and deploying ML-based technology

⇒ need UQ for ML
Bayesian neural networks (BNNs): treat $w$ as random variables

[MacKay 92, Neal 96, Graves 11, Blundell 15, Gal 16]

- $w$ now has distribution of values
- $\hat{y} = f(x; w)$ then is also a distribution of predictions
  - $\Rightarrow$ uncertainty information for each prediction
- Update distribution of $w$ from training data, via Bayes’ theorem:

$$p(w|x_T, y_T) = \frac{p(y_T|x_T, w)p(w)}{p(y_T|x_T)}$$
**Variational Bayesian inference**

**Major challenge:** # of DNN weight parameters $\sim \mathcal{O}(10^3 - 10^6 +)$:
- extremely high dimensional inference problem
- mainstream Markov chain Monte Carlo (MCMC) methods intractable

**Variational inference (VI) more scalable:**
- approximate posterior $p(w|x_T, y_T)$ with parametric family $q(w; \lambda)$
- e.g., mean-field (independent) 1D Gaussians

\[
q(w; \lambda) = \prod_{k=1}^{K} q(w_k; \lambda_k) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi}\sigma_k} \exp \left[-\frac{(w_k - \mu_k)^2}{2\sigma_k^2}\right]
\]

- find best approximation: inference problem $\rightarrow$ optimization
Variational Bayesian inference

Find best approximation by minimizing KL divergence:

\[
\lambda^* = \arg\min_{\lambda} D_{KL} [q(w; \lambda) \parallel p(w|x_T, y_T)]
\]

\[
\approx \arg\min_{\lambda} \left\{ \frac{1}{M} \sum_{m=1}^{M} \left[ \log q\left(w^{(m)}; \lambda \right) - \log p\left(y_T|x_T, w^{(m)}\right) \right] - \log p\left(w^{(m)}\right) \right\}
\]

where \( w^{(m)} \sim q(w; \lambda) \)

- above known as the **evidence lower bound (ELBO)**
- for DNN, gradient available through chain rule
  \[ \rightarrow \text{can use stochastic gradient descent} \]
Results

**Input:** power spectral density of noise signal, discretized into 151 bins covering the frequency range 0–140 Hz

**Output:** minimum, maximum, and mean values of $C_L$ and $C_M$

<table>
<thead>
<tr>
<th>Layer</th>
<th>Name</th>
<th>No. of Neurons</th>
<th>Activation Fcn.</th>
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<tbody>
<tr>
<td>1</td>
<td>input</td>
<td>151</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>hidden 1</td>
<td>50</td>
<td>tanh</td>
</tr>
<tr>
<td>3</td>
<td>hidden 2</td>
<td>50</td>
<td>tanh</td>
</tr>
<tr>
<td>4</td>
<td>output</td>
<td>6</td>
<td>linear</td>
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- Total 10,456 weight parameters
- $M = 1000$ samples in computing ELBO
- ADAM optimizer [Kingma 15] (variant of stochastic gradient descent)
- Database: 101 CFD-CAA simulations available, trained on subsets
Predictive uncertainty intervals (all validation runs)

1 training datum

![Graph showing predicted vs measured C values with uncertainty intervals]

- BNN Predicted C
- Measured C
- CL, min
- CL, max
- CL, mean
- CM, min
- CM, max
- CM, mean
Predictive uncertainty intervals (all validation runs)

20 training data

![Graph showing Predictive uncertainty intervals for BNN Predicted versus Measured C]
Predictive uncertainty intervals (all validation runs)

80 training data

BNN Predicted C vs Measured C

- $C_{L,\text{min}}$
- $C_{L,\text{max}}$
- $C_{L,\text{mean}}$
- $C_{M,\text{min}}$
- $C_{M,\text{max}}$
- $C_{M,\text{mean}}$
Predictive uncertainty distributions (specific runs)

1 training datum
Predictive uncertainty distributions (specific runs)

20 training data
Predictive uncertainty distributions (specific runs)

80 training data
Given noise signal input, perform 1000 DNN evaluations to generate these 6 prediction distributions: \( \sim 3.8 \text{ ms} \) (MacBook Pro)

- Positive outlook for meeting real-time detection requirements
- Plan to seek higher-fidelity simulations, and bigger databases
- Will investigate other ML architectures for feature detection, e.g.
  - recurrent neural network (RNN): suitable for time-dependent data
  - convolutional neural network (CNN): suitable for image-like signals
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Motivation: stochastic noise generation


Preliminary work (mainly formulation currently)

- Aircraft noise is important for design optimization
- High number of design variables motivates adjoint-based approaches
- Dilemma:
  - Scale-resolving simulations required for noise prediction, but adjoint diverges due to chaotic turbulent content [Blonigan 12]
  - Adjoint divergence benign in RANS, but noise generation suppressed

Approach: reconstruct turbulent fluctuations through stochastic noise generation (SNG) [Bechara 94, Bailly 99, Rossignol 13]

\[ \ddot{u}'(\vec{x}, t) = 2 \sum_{n=1}^{N_F} \hat{u}_n \cos \left[ \vec{k}_n \cdot (\vec{x} - \vec{U}t) + \psi_n \right] \hat{\sigma}_n \]

where \( \vec{k}_n, \psi_n, \hat{\sigma}_n \) randomly generated, and Fourier mode magnitudes are

\[ \hat{u}_n = \sqrt{E(k_n, K, \epsilon) \Delta k_n} \]

and \( K \) and \( \epsilon \) are computed from RANS
Turbulence energy spectrum generally adopts (isotropic) Von Kármán-Pao energy spectrum:

\[ E(k, K, \epsilon) = \frac{2A}{3} \frac{K}{k_e} \left( \frac{k}{k_e} \right)^4 \exp \left[ -2 \left( \frac{k}{k_\eta} \right)^2 \right] \left[ 1 + \left( \frac{k}{k_e} \right)^2 \right]^{-\frac{17}{6}} \]

RANS-SNG: demonstrated design for noise reduction with weakly anisotropic cases  

Turbulence energy spectrum generally adopts (isotropic) Von Kármán-Pao energy spectrum:

\[ E(k, K, \epsilon) = \frac{2A K}{3 k_e} \left( \frac{k}{k_e} \right)^4 \exp \left[ -2 \left( \frac{k}{k_{\eta}} \right)^2 \right] \left[ 1 + \left( \frac{k}{k_e} \right)^2 \right]^{-\frac{17}{6}} \]

...however, isotropic assumption may not hold in scenarios with strong shear layers (e.g., jet flow in NASA Acoustic Research Nozzle 2)
Machine learning (data-driven) idea:

- learn scenario-specific energy spectrum $E_{\text{DNN}}(k, K, \epsilon)$ from relevant (and low number of) LES run(s), then use it in RANS-SNG
- e.g., construct $E_{\text{DNN}}(k, K, \epsilon)$ by minimizing loss function

$$\min_{\theta} \| E_{\text{LES}}(k, K, \epsilon) - E_{\text{DNN}}(k, K, \epsilon; \theta) \|_2^2$$

- lots of data points from a single LES run (each $\vec{x}$ can provide a $E_{\text{LES}}(k, K, \epsilon)$ datum)
- ongoing work: plan to start with feed-forward DNN
- hypothesis: hybrid isotropic-DNN form may provide more accurate representations (combining physics with ML)
1. Optimal Experimental Design

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4. Summary
Enabled tractable computation of optimal experimental designs targeting nonlinear and computationally intensive models

Demonstrated design of combustion experiments for learning kinetic parameters, sensor placement for source inversion

Advanced towards real-time in-flight rotorcraft icing detection using aeroacoustic computations

Constructed Bayesian neural network machine learning models that achieve rapid online predictions with uncertainty information

Presented plans for data-driven ML modeling of turbulence energy spectrum to improve RANS-SNG under anisotropic turbulence
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