Quantifying Uncertainty in Mathematical Models

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May 6, 2022

Outline

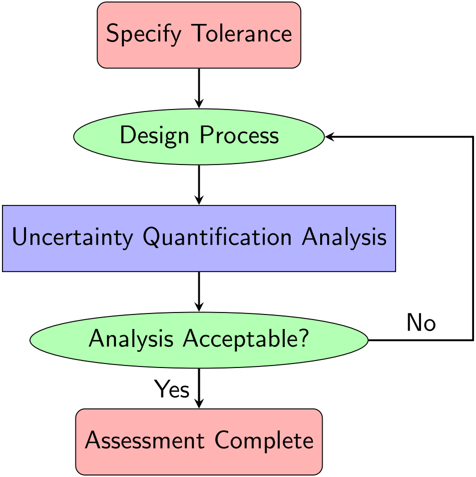
Goals of the Talk

- What *is* research in math?
- What kind of problems can you solve?
- How do classes apply?

The Goals of My Work

- Uncertainty Quantification
  - Tools
    - Probability & Statistics
    - Mathematical Modelling (Calculus, ODEs)
  - Applications
    - Machine Learning
    - Physical Problems (Fracture Mechanics)

An Example: Manufacturing



How We Model Uncertainty

We model (frequently) as distributions!

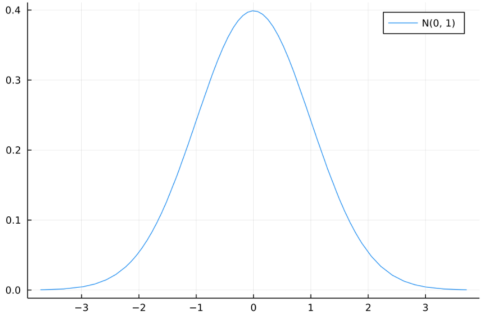


Figure: Standard Normal Distribution

Uncertain Parameters

What if we don't know mean or variance?

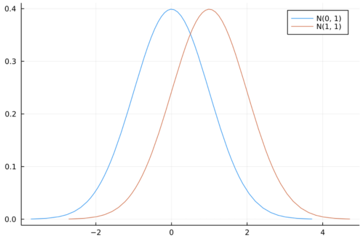


Figure: Changes in Mean

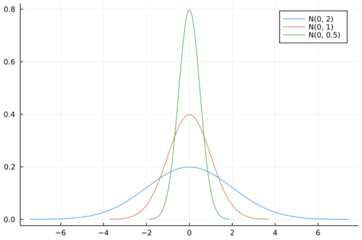


Figure: Changes in Variance

"Distances" Between Distributions

A notion of "distance" between (discrete) probability distributions is the *relative entropy* or *Kullback-Leibler Divergence*:

$$D_{\mathrm{KL}}(P||Q) = \sum_x P(x) \log \frac{P(x)}{Q(x)}$$

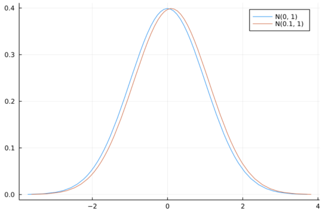


Figure: Low KL Divergence

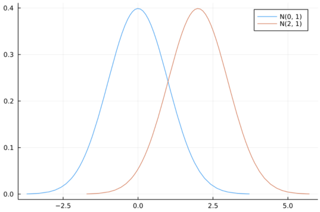


Figure: High KL Divergence

Usefulness of KL Divergence & Uncertainty Modelling

- Physics - Oscillating spring experiment: Model spring constant k as a distribution
- Social science - Bias in random sampling (e.g., polling voting preferences from a city that is skewed towards one party)

Example: Coin Toss

Result (x)	Probability
H	0.5
T	0.5

Table: Fair Coin (Truth/P)

Result (x)	Probability
H	0.6
T	0.4

Table: Biased Coin (Guess/Q)

$$
\begin{aligned}
D_{\mathrm{KL}}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\
&= 0.5 \log \frac{0.5}{0.6} + 0.5 \log \frac{0.5}{0.4} \\
&\approx 0.02041
\end{aligned}
$$

The Continuous Version

For continuous distributions (e.g., normal), we have

$$D_{\mathrm{KL}}(P||Q) = \int_{\mathcal{X}} \log\left(\frac{dP}{dQ}\right) dP.$$

Involves calculus, since now our random variable can be anything in a range of values! An example would be a number picked at random between 0 and 1.

An Important Inequality

Jensen's inequality says that

$$f(\mathbb{E}[x]) \leq \mathbb{E}[f(x)]$$

if f is convex. A visual plausibility argument:

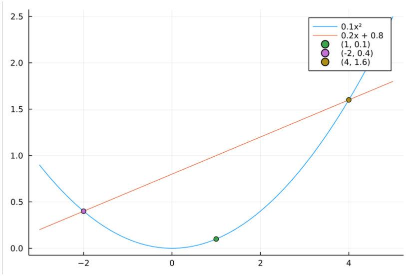


Figure: Illustration of Jensen's Inequality

A Use of Jensen

We can use Jensen's inequality to show the relative entropy is non-negative:

$$\begin{aligned} D_{KL}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= \mathbb{E}_P\left[\log \frac{P}{Q}\right] \\ &= \mathbb{E}_P\left[-\log \frac{Q}{P}\right] \\ &\geq -\log \mathbb{E}_P\left[\frac{Q}{P}\right] \\ &\geq -\log \sum_x P(x) \frac{Q(x)}{P(x)} = 0. \end{aligned}$$

A Game Example

A pair of (possibly unfair) dice are simultaneously rolled. The outcomes are either

- Sum is in between 5 and 10 (inclusive): You win \$1
- Otherwise: You lose \$1

Question: What is the *worst* that can happen for you, under the assumption that you can guess *how rigged* the dice are?

The Outcomes

Roll	1	2	3	4	5	6
1	2	3	4	5	6	7
2	3	4	5	6	7	8
3	4	5	6	7	8	9
4	5	6	7	8	9	10
5	6	7	8	9	10	11
6	7	8	9	10	11	12

- Green - Outcome of a roll
- Blue - Lose money
- Orange - Win money

Some Setup

- F - a function that returns 1 if we lose money, and 0 if we win money; our *Quantity of Interest* (QoI)
- Q - the true, unknown distribution
- P - our guess (assume fair dice)

Our question, mathematically: What is the *largest* that

$$\sum_x F(x)Q(x)$$

could be?

A Major Tool

We define the *exponential integral*

$$\Lambda_c = \frac{1}{c} \log \sum_x e^{cF(x)} P(x)$$

for $c > 0$ and with the restriction that $F \geq 0$.

The motivation for this definition is outside the scope of this talk. It is related to a field called *large deviation theory*.

The Punchline

The main reason for defining Λ_c is

$$\sum_x F(x)Q(x) \leq \Lambda_c + \frac{1}{c} D_{\mathrm{KL}}(P||Q),$$

which means now we have an upper bound for what we want (and can optimize the right hand side over c)!

A crude (but true) interpretation: True performance is no worse than a combination of approximated performance and the error of approximation.

The Game Example in Action

Suppose that both dice had distribution

$$Q = (.5, .1, .1, .1, .1, .1).$$

The probability matrix for the outcomes of a two-dice roll is

Roll	1	2	3	4	5	6
1	0.25	0.05	0.05	0.05	0.05	0.05
2	0.05	0.01	0.01	0.01	0.01	0.01
3	0.05	0.01	0.01	0.01	0.01	0.01
4	0.05	0.01	0.01	0.01	0.01	0.01
5	0.05	0.01	0.01	0.01	0.01	0.01
6	0.05	0.01	0.01	0.01	0.01	0.01

The Game Example in Action

Denote

- x - Outcome of roll 1
- y - Outcome of roll 2

The true performance (expected loss) is

$$\sum_{x,y} F(x,y)Q(x)Q(y) = 0.49.$$

Let's see what our bound can tell us, under the approximation of fair dice!

The Game Example in Action

Assume the fair distribution

$$P = (1/6, 1/6, 1/6, 1/6, 1/6, 1/6).$$

Then we have the true relative entropy (with a slight abuse of notation)

$$D_{\mathrm{KL}}(P||Q) \approx 0.485.$$

Let's say for sake of argument (since Q is supposed to be unknown) that we estimate $D_{\mathrm{KL}}(P||Q) \leq 0.5 = B$. What happens to $\Lambda_c + \frac{1}{c}B$?

The Game Example in Action

It isn't sharp, but it captures the upper bound on performance, as expected! We could optimize the bound over c to obtain the tightest bound at about 0.727.

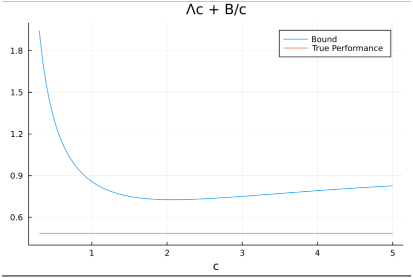


Figure: Performance Bound and True Performance

A (More) Realistic Problem

Consider the initial value problem (ODE problem)

$$\frac{d}{dt}u(t) = -\lambda u(t), \quad u(0) = 1,$$

where $\lambda \sim U[0,1]$. Our goal is to obtain bounds on the average of the quantity of interest

$$F(k) = u(1;\lambda).$$

Simulated Solutions

For a fixed λ, the solution is $u(t;\lambda) = e^{-\lambda t}$.

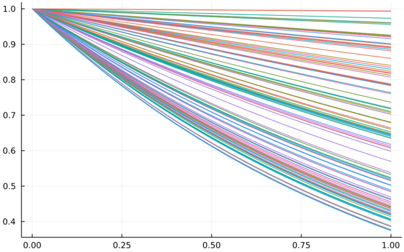


Figure: Some solutions of the ODE

A Different Underlying Distribution

Suppose that the "true" distribution is $\lambda \sim \text{beta}(\alpha = 1.5, \beta = 1.5)$:

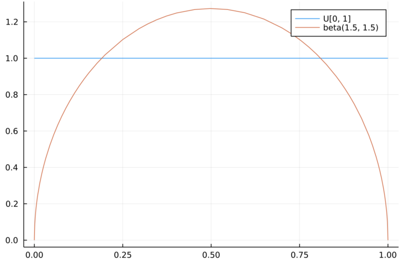


Figure: True and Approximated Distribution

The True Performance & The Bound

True performance: $\int_0^1 e^{-\lambda} \frac{1}{B(1.5,1.5)} \sqrt{\lambda(1-\lambda)} d\lambda \approx 0.626$.
Bound on relative entropy: 0.05 (True relative entropy ≈ 0.484).

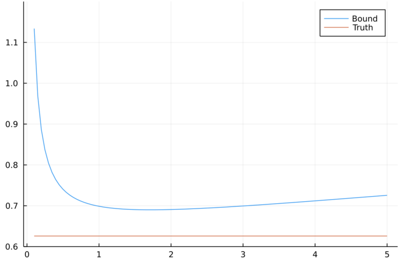


Figure: Performance Bound for ODE Model

Conclusions

In this talk, we:

- Addressed the modelling of uncertainty in mathematical models
- Considered some concrete models in which we are interested in uncertainty analysis
- Showed empirically we can obtain performance measures on these models under assumptions about the underlying uncertainty

References

- Kamaljit Chowdhary and Paul Dupuis, *Distinguishing and Integrating Aleatoric and Epistemic Variation in Uncertainty Quantification*
- P. Dupuis, M. Katsoulakis, Y. Pantazis, P. Plecháč, *Path-Space Information Bounds for Uncertainty Quantification and Sensitivity Analysis of Stochastic Dynamics*

Thank You!

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