

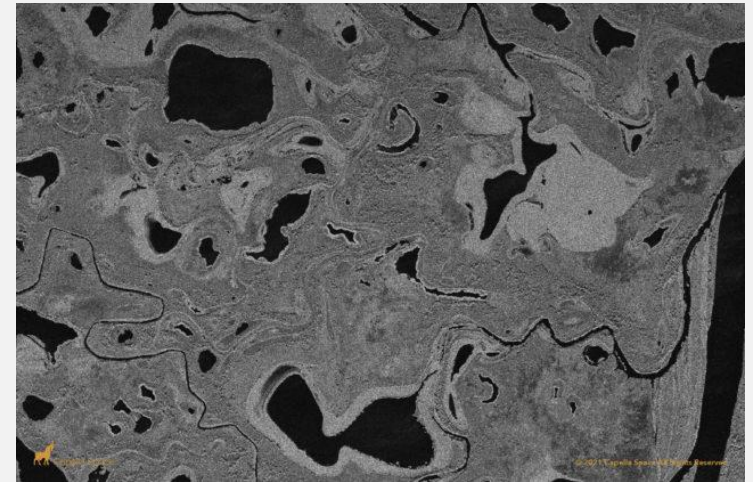
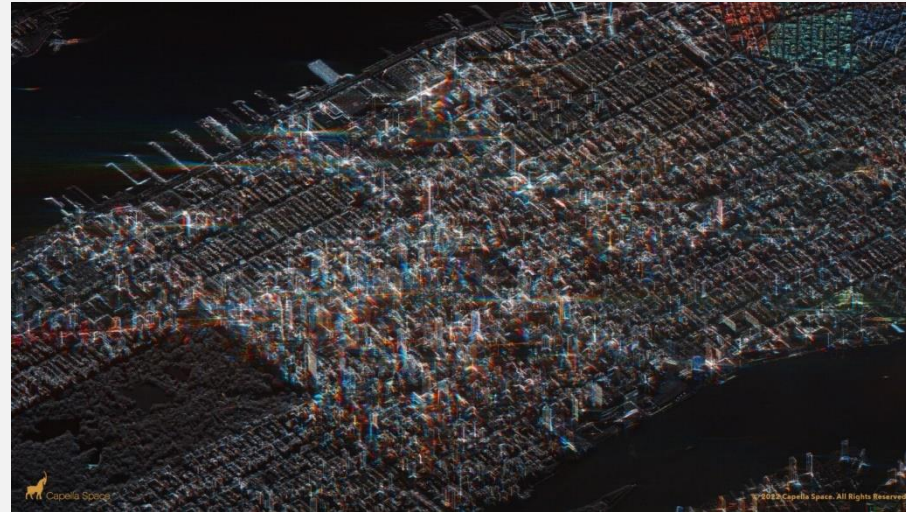
Monaco: Quantify Uncertainty and Sensitivities in Your Computational Models with a Monte Carlo Library

SciPy 2022 Conference
Machine Learning and Data Science Track
Scott Shambaugh

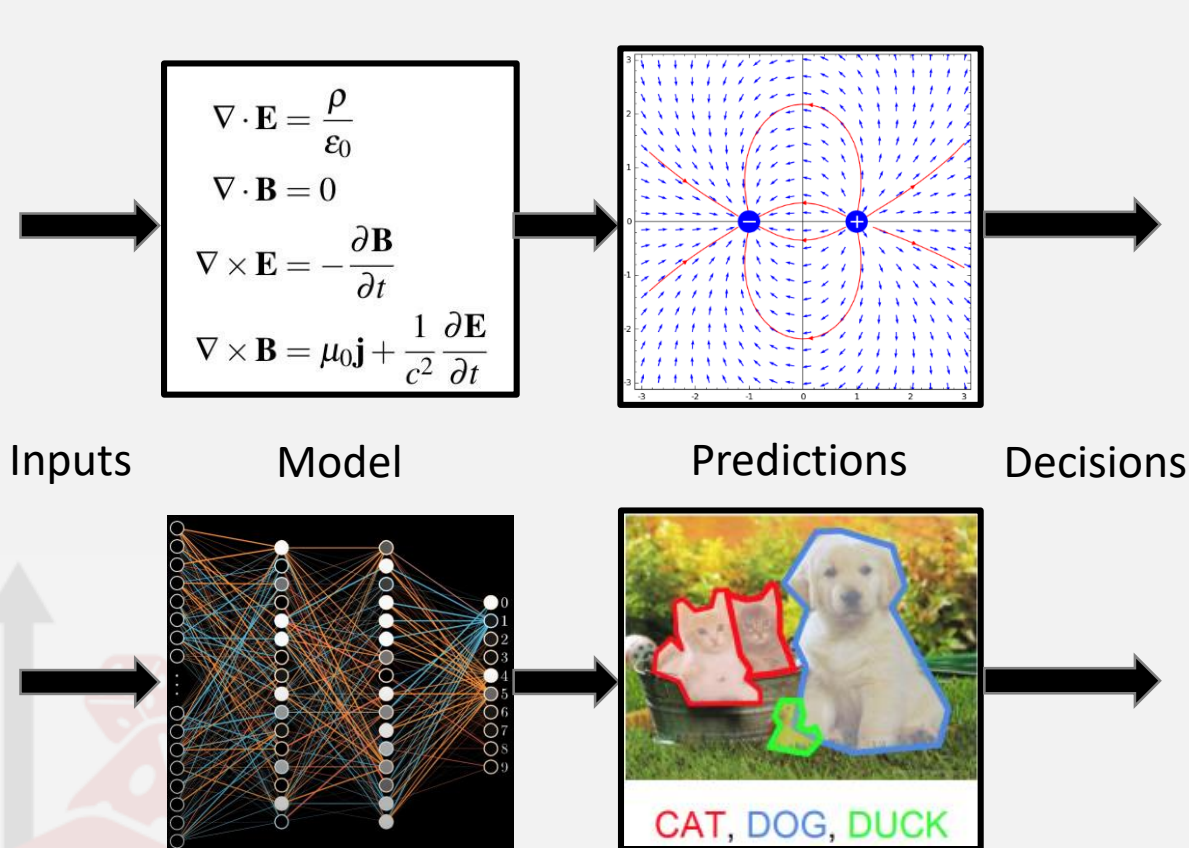


Acknowledgements

Thank you to Capella Space for sponsoring this talk



Mechanistic vs Empirical Models



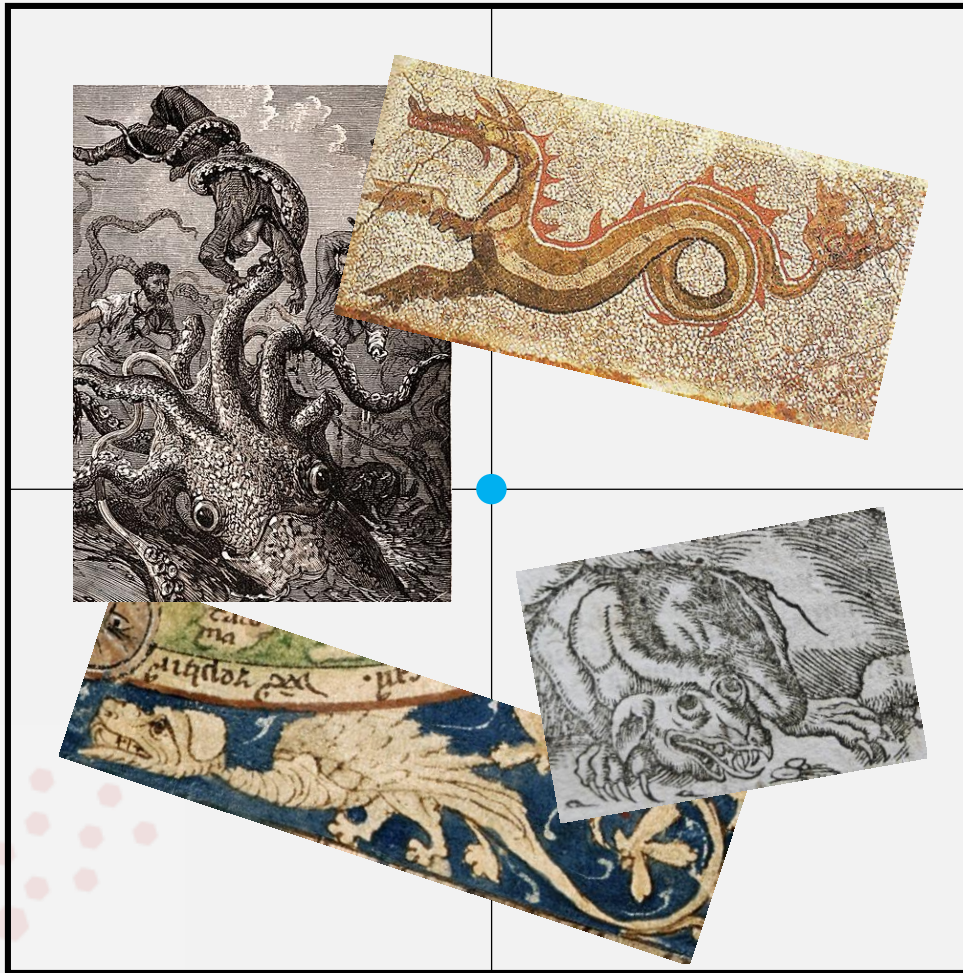
- Deterministic
- Debuggable & Auditable
- Encodes Human Knowledge
- No Need for Training Data
- Easy to Implement → Used Everywhere

“Too Perfect”

- Real world is noisy and messy!
- How sensitive are these predictions?
- What’s the range of outcomes?

Crucial for effective & responsible use of
models in decision-making

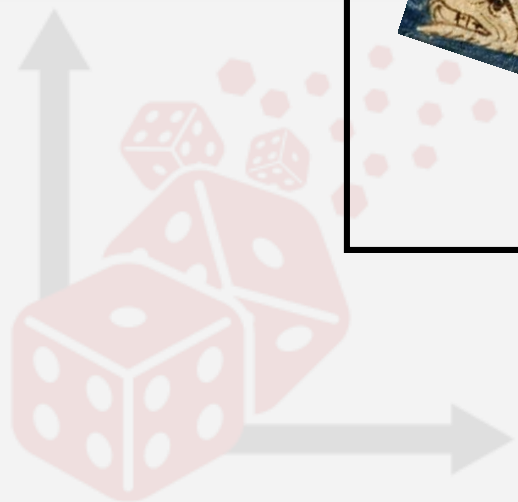
Variable 2

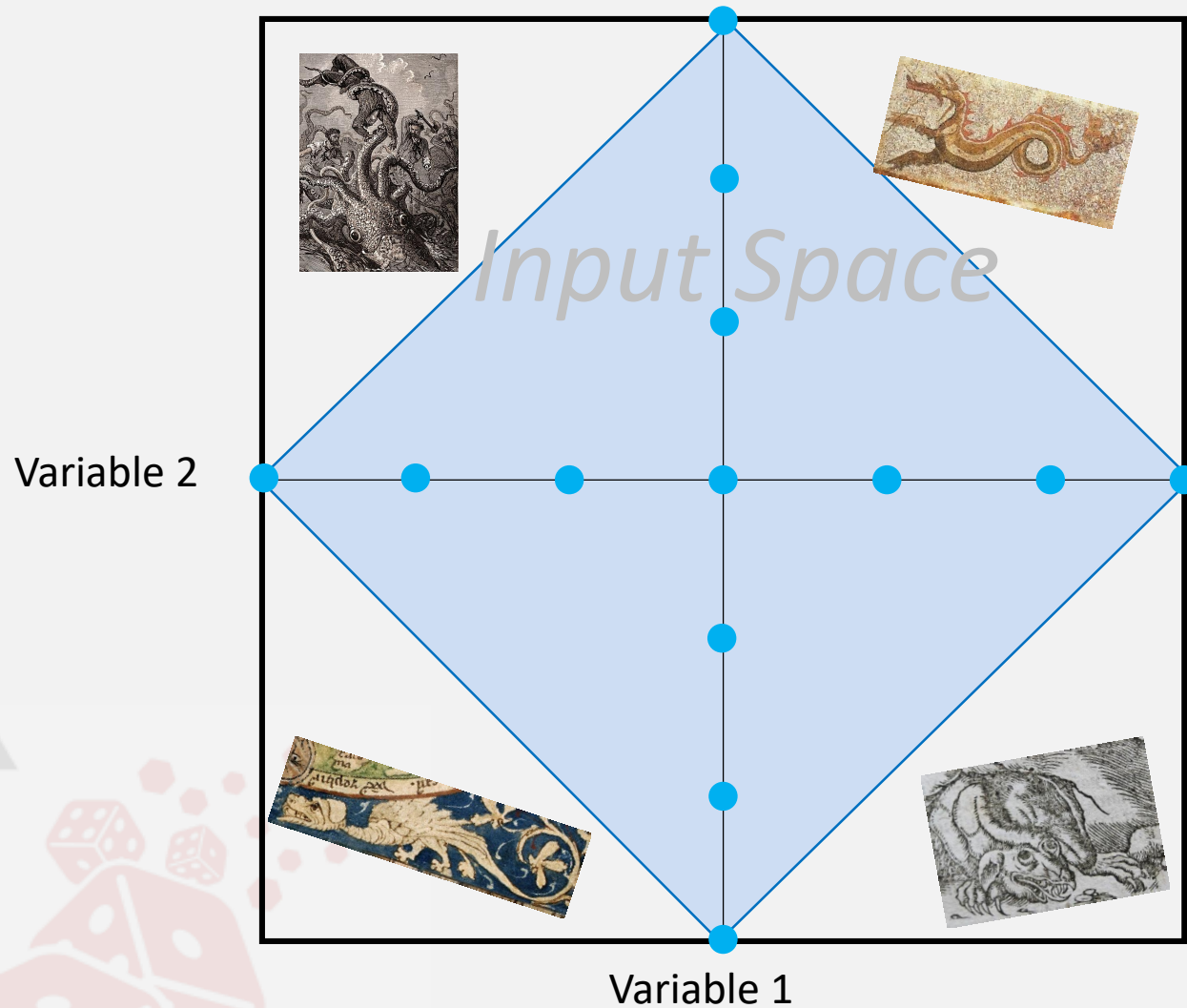


Variable 1

Best Point Estimate

*Here be
dragons!*



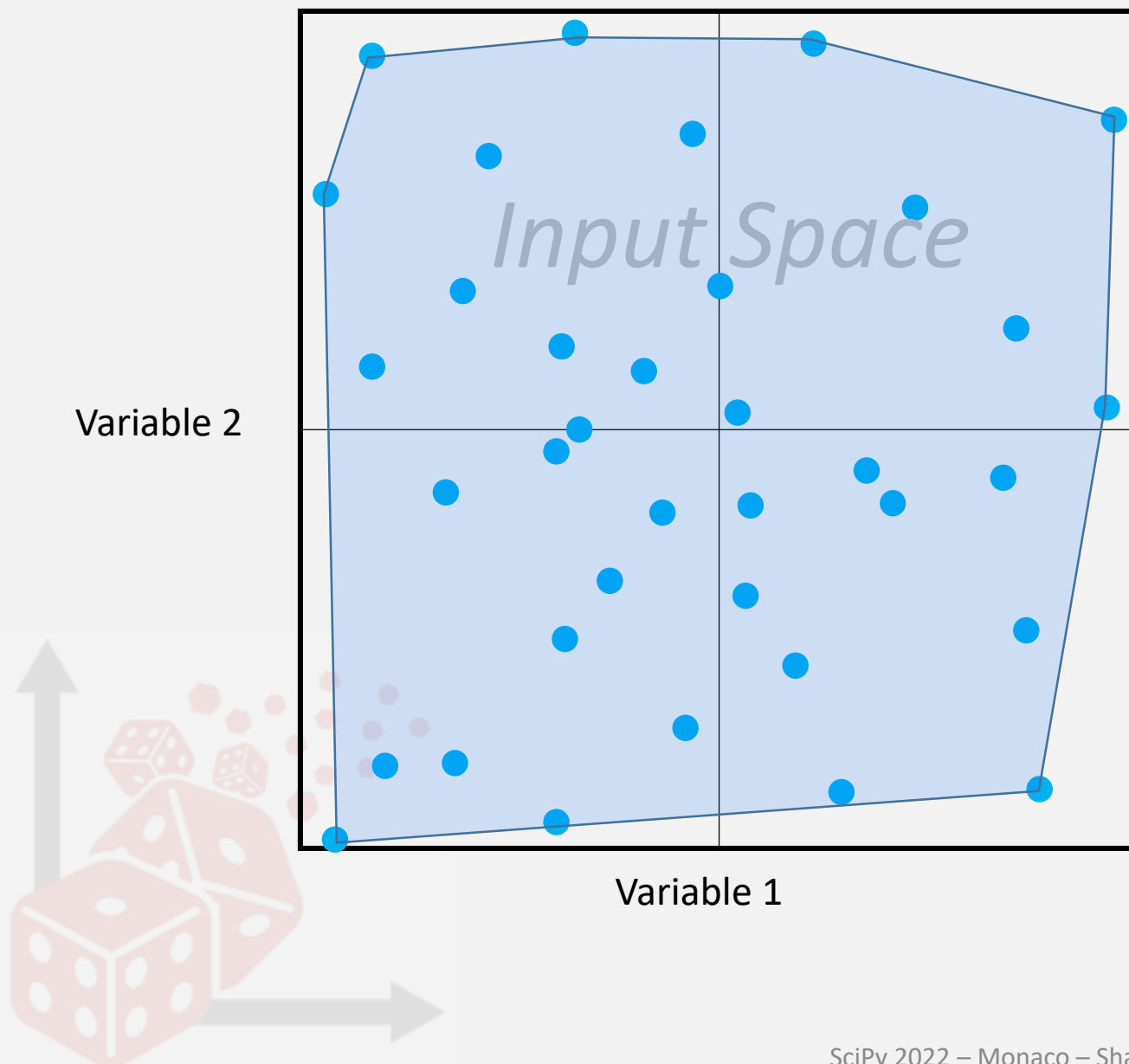


Varying Inputs One-At-A-Time

- Covered volume (convex hull)
 $= \frac{1}{2}$

***Here still be
dragons!***

- As # of variables increase,
volume $= \frac{1}{k!}$
- Doesn't scale!



Random Points

“Monte Carlo” approach

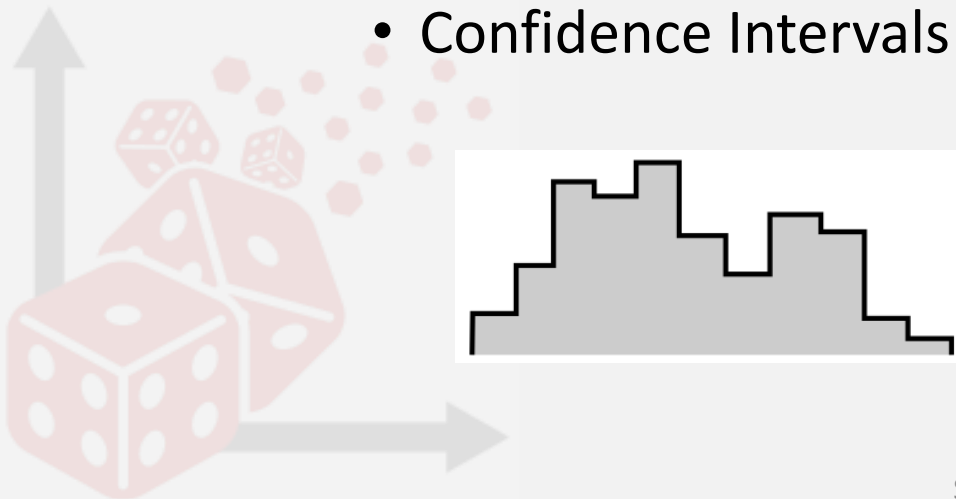
- Covered volume $\rightarrow 1$ as $n \rightarrow \infty$ for any dimension hypercube
- Good coverage inside that volume
- Full exploration of the input space

Uncertainty & Sensitivity Analysis

“What is the range of possible outcomes?”

Uncertainty Analysis

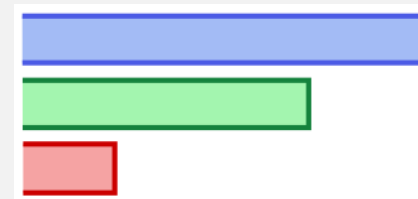
- Histograms
- Spaghetti Plots
- Confidence Intervals



“Which parameters most affect these outcomes?”

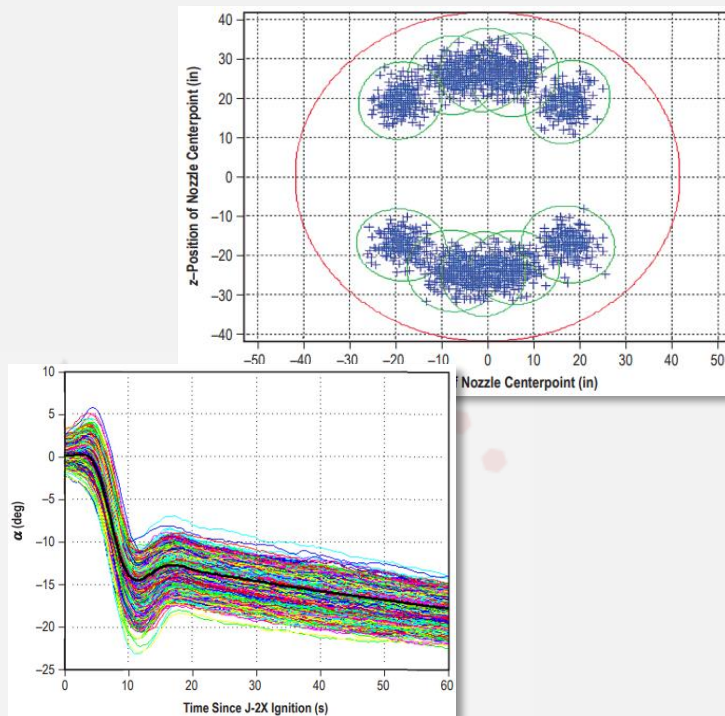
Sensitivity Analysis

- Scatter Plots
- Sensitivity Indices
- Regressions

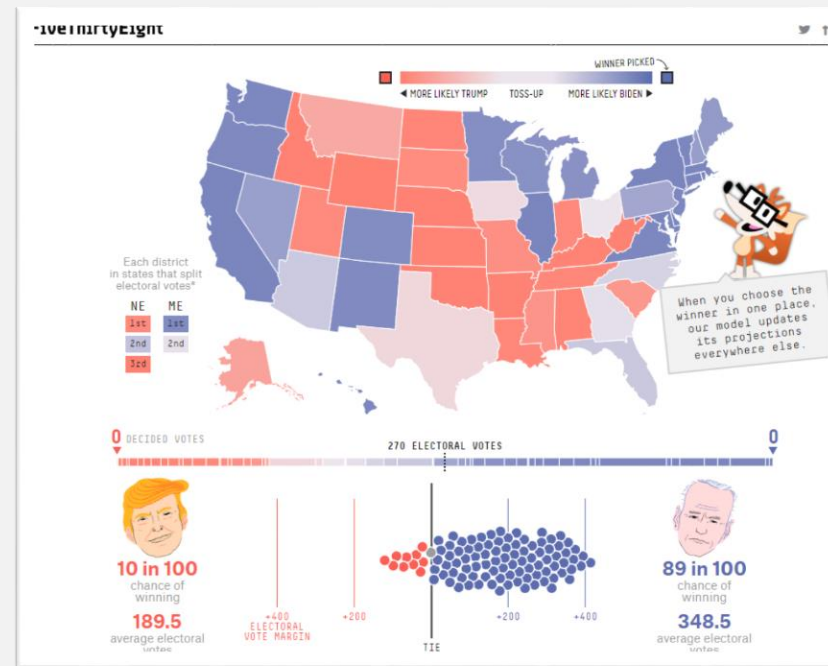


What this looks like in practice

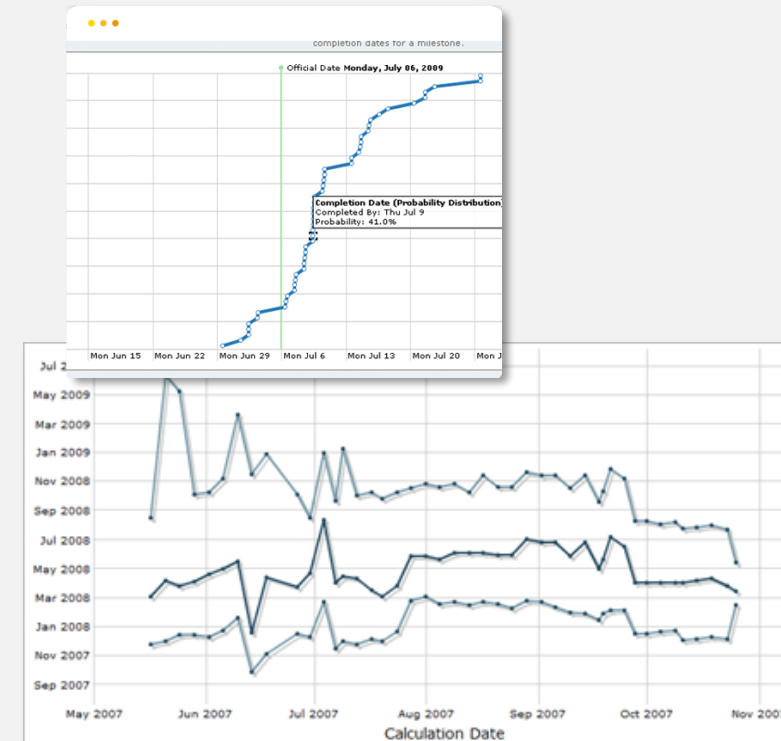
NASA: Ares I Flight Simulations



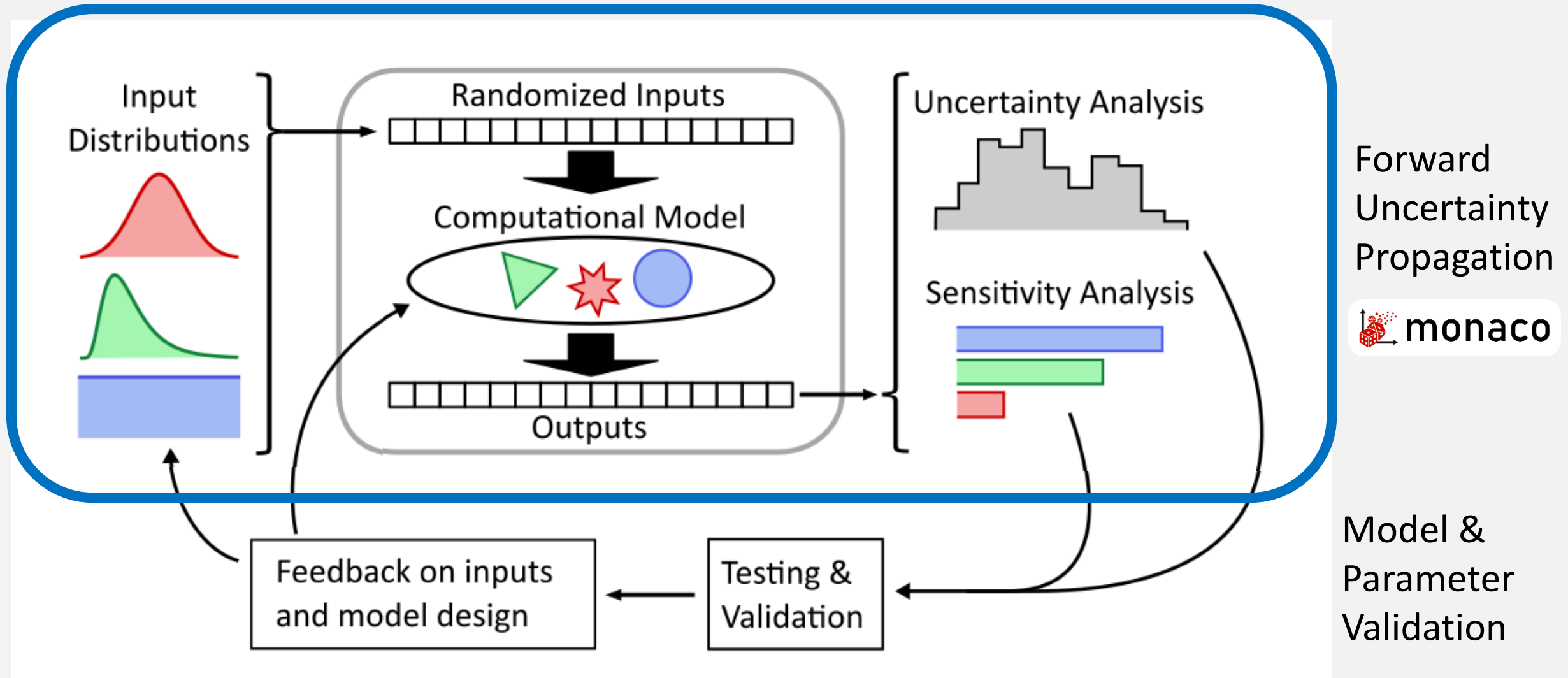
FiveThirtyEight: Election Forecasting



FogBugz: Evidence-Based Scheduling



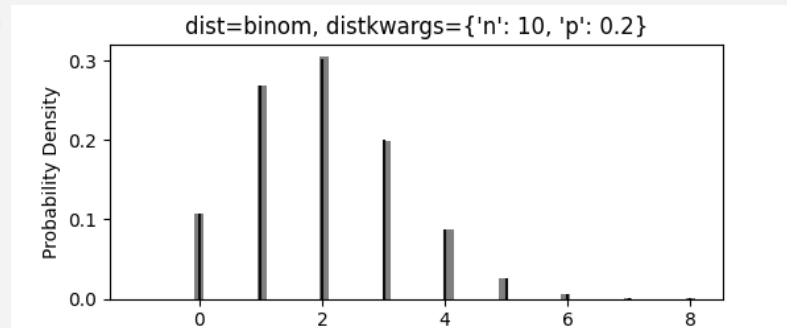
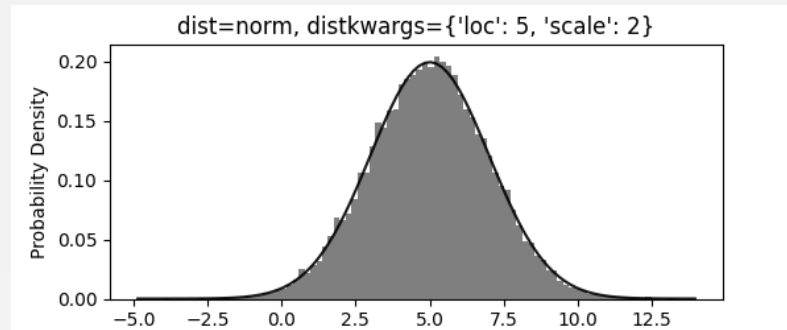
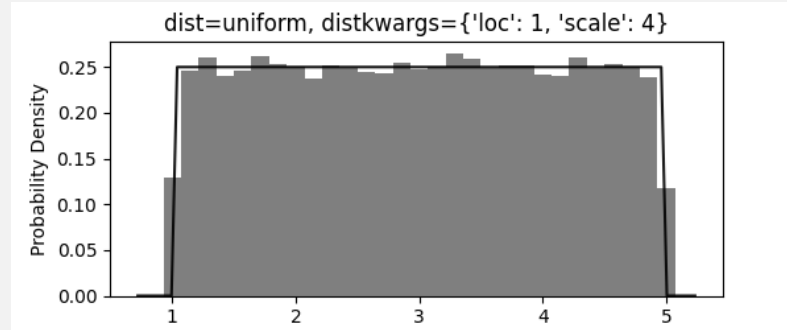
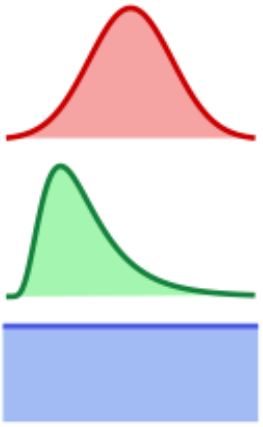
Workflow





monaco – Input Distributions

Input Distributions

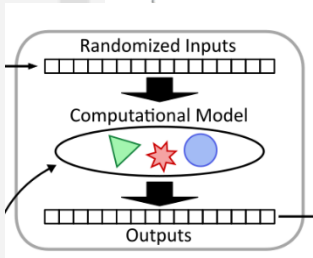


Pass in any of `scipy.stats`' probability distributions

- Or, define a custom one

Input ranges come from:

- Observed / experimental data
- Physical limits
- Spec sheets
- Best guesses



Preprocess

- Run

- ## Postprocess

- Grabs raw outputs from *run* function and extracts output values for each case



monaco – Analyzing Results

Plotting!

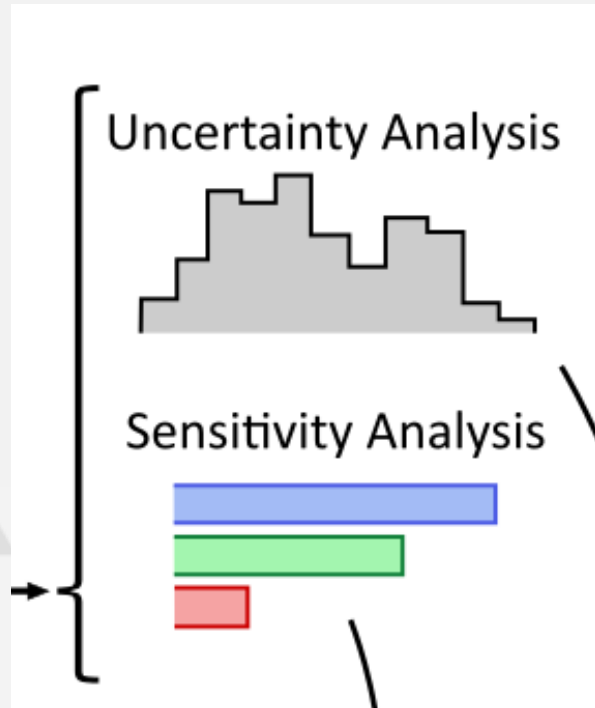
- `monaco.plot()` on one or more *Vars* will automatically choose best plot type to show
- Histograms, empirical CDFs, 2D/3D scatter plots, 2D/3D spaghetti plots

Variable Statistics

- Calculate mean, percentiles, etc, or any custom statistic
- Bootstrapped to specified confidence levels

Sensitivity Indices

- Measures contribution to output variance from variance of inputs
- Includes first-order as well as nonlinear interaction effects



Live Demo: Dice Roll



Live Demo: Baseball





monaco – Other Features

Parallel Processing

- Run workflow serially or in parallel with *dask.distributed*



How Many Cases to Run?

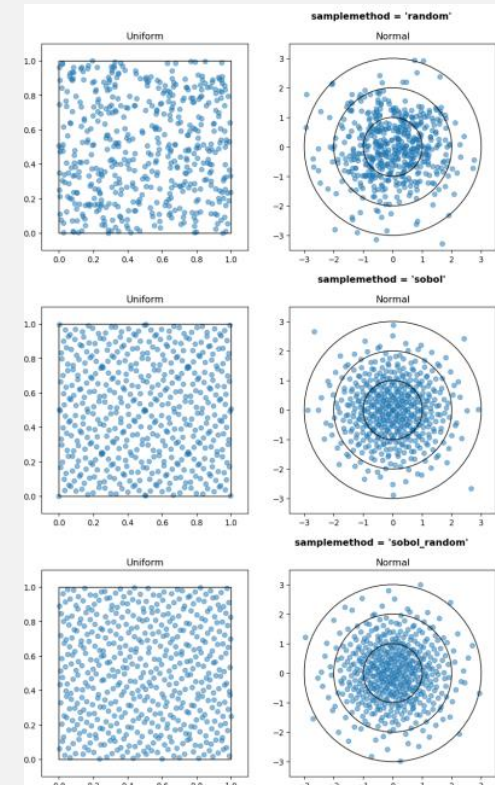
- Order statistics determine cases needed to rigorously reach confidence level for variable statistics

File I/O

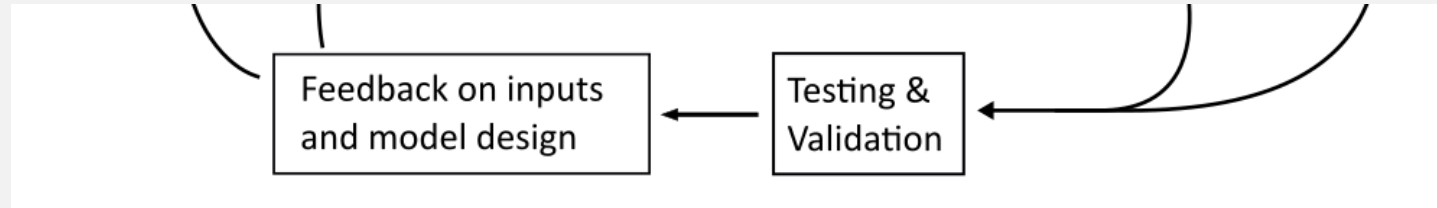
- Save and load *Sim* and *Case* objects to file to avoid repeating expensive computations
- Import and export variables to *.csv* or *.json* to trade out any part of the workflow with external tooling

Quasi Monte-Carlo Sampling

- Fills space more efficiently than pure random sampling

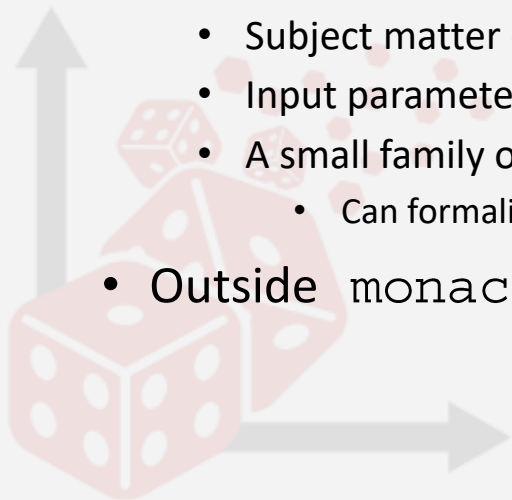


Model & Parameter Validation



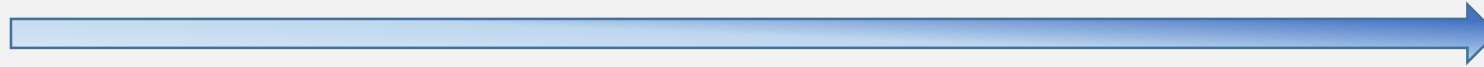
Very important, but genuinely difficult

- A rigorous treatment requires:
 - Lots of test data
 - Moving to a full probabilistic programming framework
- A more typical treatment looks like:
 - Subject matter expert validates model behavior (corners of input space often reveal bugs!)
 - Input parameters are anchored and defined conservatively
 - A small family of test data is compared to expected results
 - Can formalize with hypothesis testing or probabilistic scoring measures
- Outside monaco's scope



Recommended Tools

Basic



Advanced

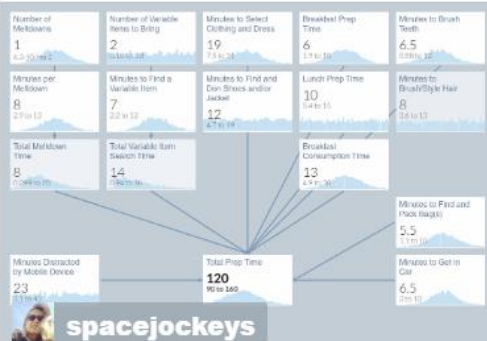
Guesstimate

Web-based tool for simple models

Guesstimate

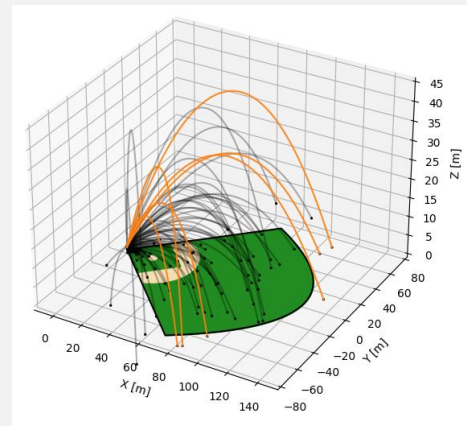
How Long It Takes To Get Ready for Preschool

Updated Jun 11, 2016



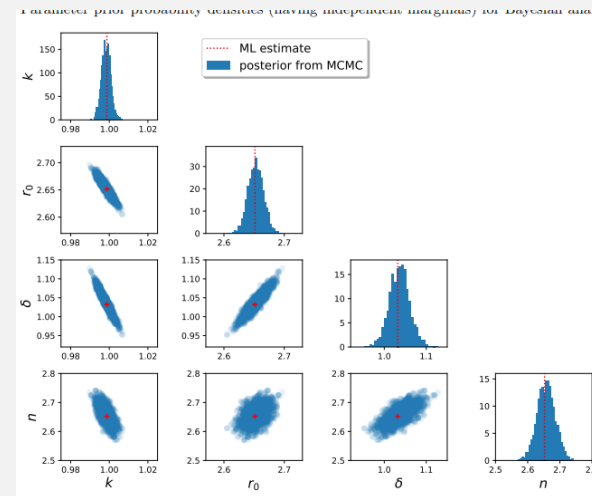
Monaco

Single-Shot
Uncertainty & Sensitivity
Analysis



UQpy

More Advanced
Uncertainty & Sensitivity
Analysis



Stan, PyMC

Probabilistic
Programming



Miscellanea

Links

- Project repo: github.com/scottshambaugh/monaco
- Lots of examples: github.com/scottshambaugh/monaco/tree/main/examples
- API Documentation: monaco.readthedocs.io
- Conference paper: conference.scipy.org/proceedings/scipy2022/pdfs/scott_shambaugh.pdf
- These slides and notebooks: github.com/scottshambaugh/monaco-scipy2022
- Video of conference talk: youtube.com/watch?v=yB539OIol_s

Recommended Reading:

- [“Applying Monte Carlo Simulation to Launch Vehicle Design and Requirements Analysis”](#)
- [“The Future of Sensitivity Analysis: An essential discipline for systems modeling and policy support”](#)
- [“Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices”](#)

Short-Term Roadmap – currently alpha software

- Single variable and pairwise regressions: linear, polynomial, custom, with confidence intervals
- Sensitivity Indices: confidence intervals and scale-dependent effects
- Dask: link task graph and confirm working on remote server
- Pairwise variable statistics



```
pip install monaco
```


Thank You

Questions?



Image Sources

- <https://www.capellaspace.com/>
- <https://www.youtube.com/watch?v=IHZwWFHWa-w>
- <https://www.cantorsparadise.com/maxwells-equations-7484212839b1>
- http://www.cs.cornell.edu/courses/cs4670/2016sp/lectures/lec41_recowrapup_web.pdf
- https://en.wikipedia.org/wiki/File:Reggio_calabria_museo_nazionale_mosaico_da_kaulon.jpg
- https://en.wikipedia.org/wiki/Dragon#/media/File:M%C3%BCnster_wawelski.jpg
- https://commons.wikimedia.org/wiki/File:Psalter_World_Map,_c.1265_dragons.jpg
- https://commons.wikimedia.org/wiki/File:20000_squid_holding_sailor.jpg
- <https://ntrs.nasa.gov/citations/20100038453>
- <https://projects.fivethirtyeight.com/2020-election-forecast/>
- <https://www.joelonsoftware.com/2007/10/26/evidence-based-scheduling/>
- <https://distributed.dask.org/en/stable/>
- <https://www.getguesstimate.com/models>
- <https://uqpyproject.readthedocs.io/en/latest/#>
- <https://mc-stan.org/>
- <https://www.pymc.io/welcome.html>