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

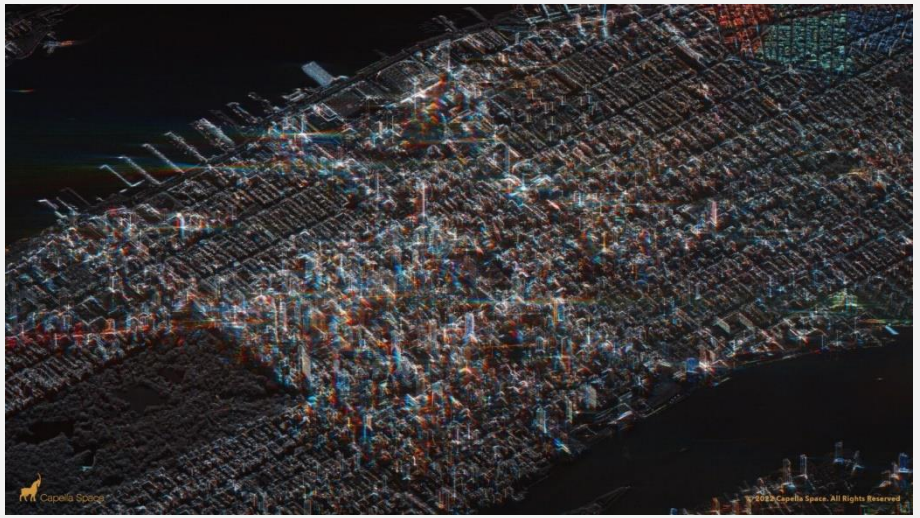
SciPy 2022 Conference

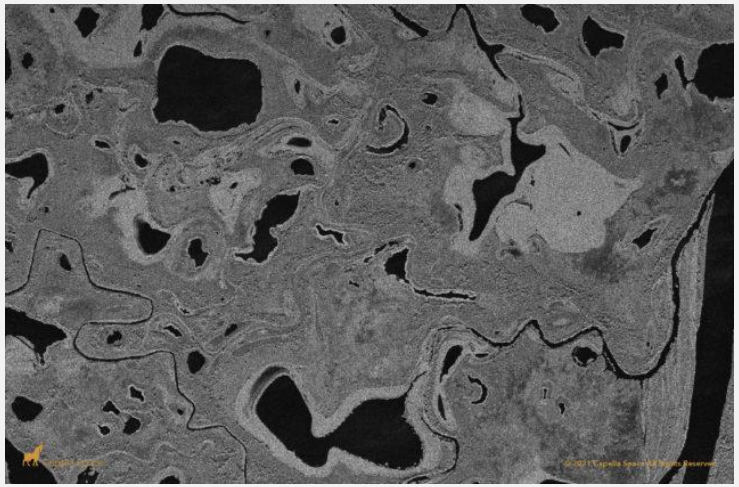
Machine Learning and Data Science Track

Scott Shambaugh

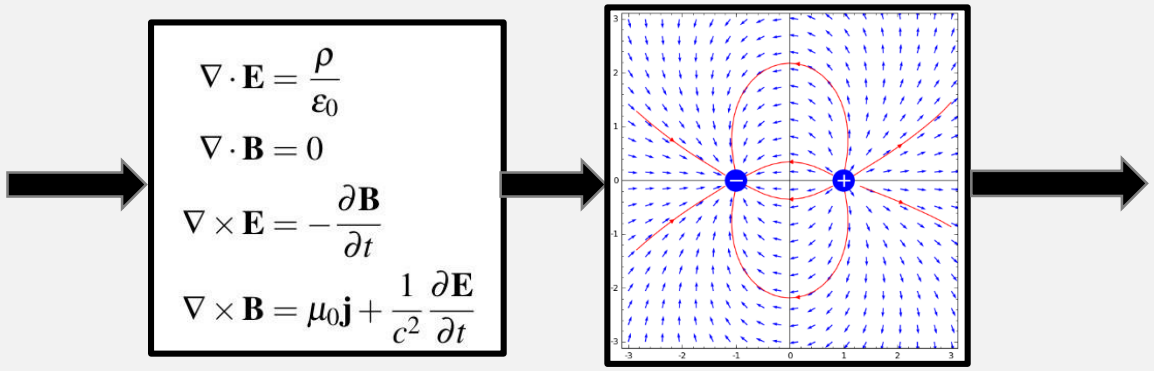
Acknowledgements

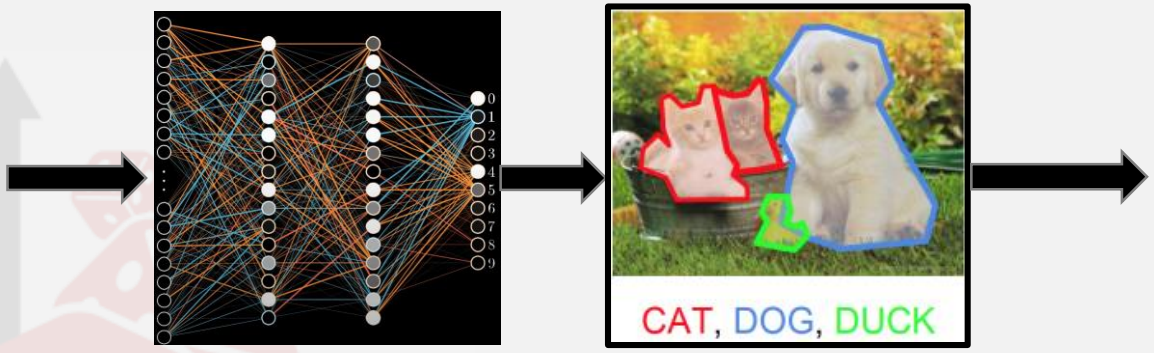
Thank you to Capella Space for sponsoring this talk





Mechanistic vs Empirical Models





Inputs Model Predictions Decisions

- 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?

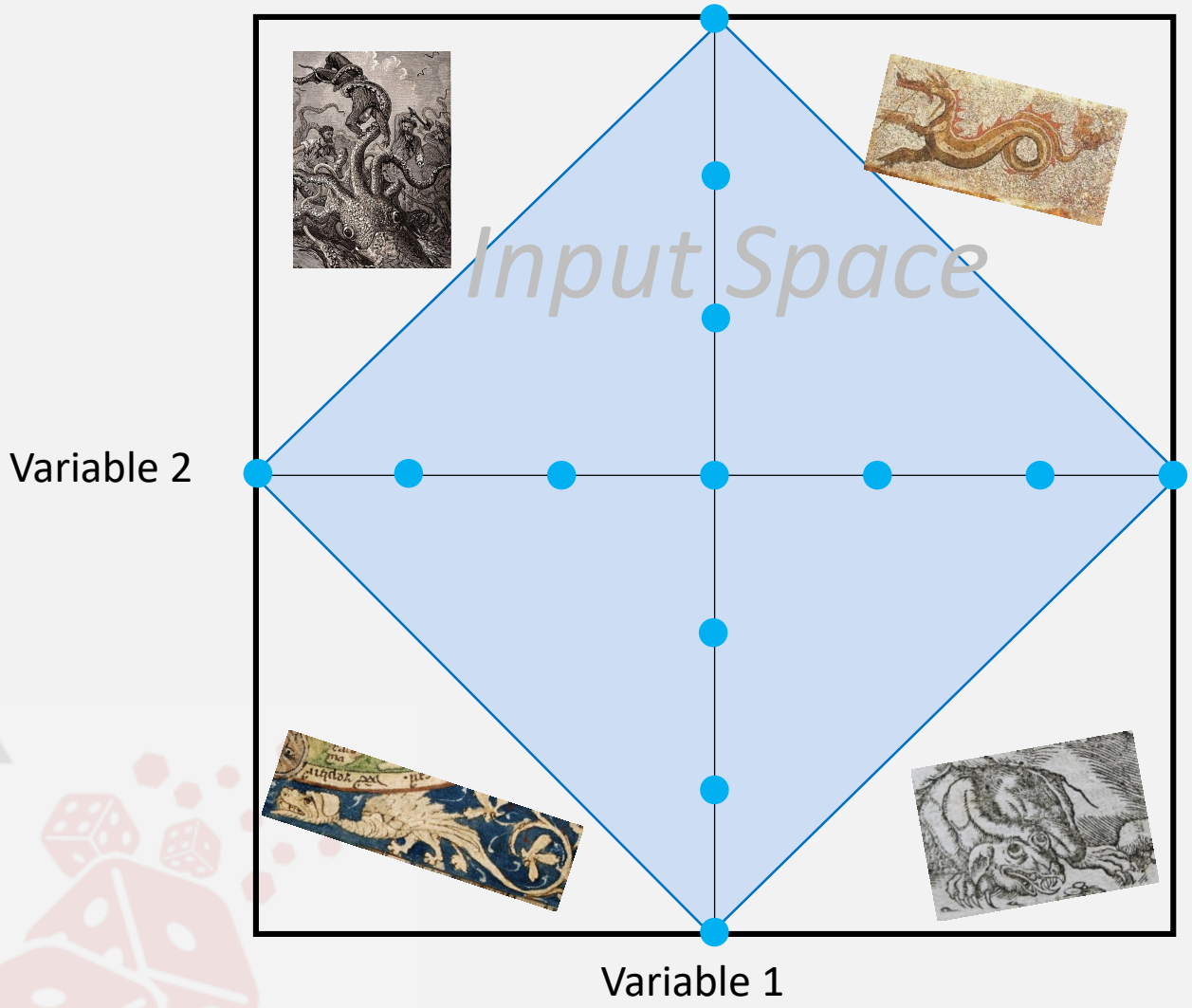
Crucial for effective & responsible use of models in decision-making

Variable 2

Variable 1

Best Point Estimate

Here be dragons!

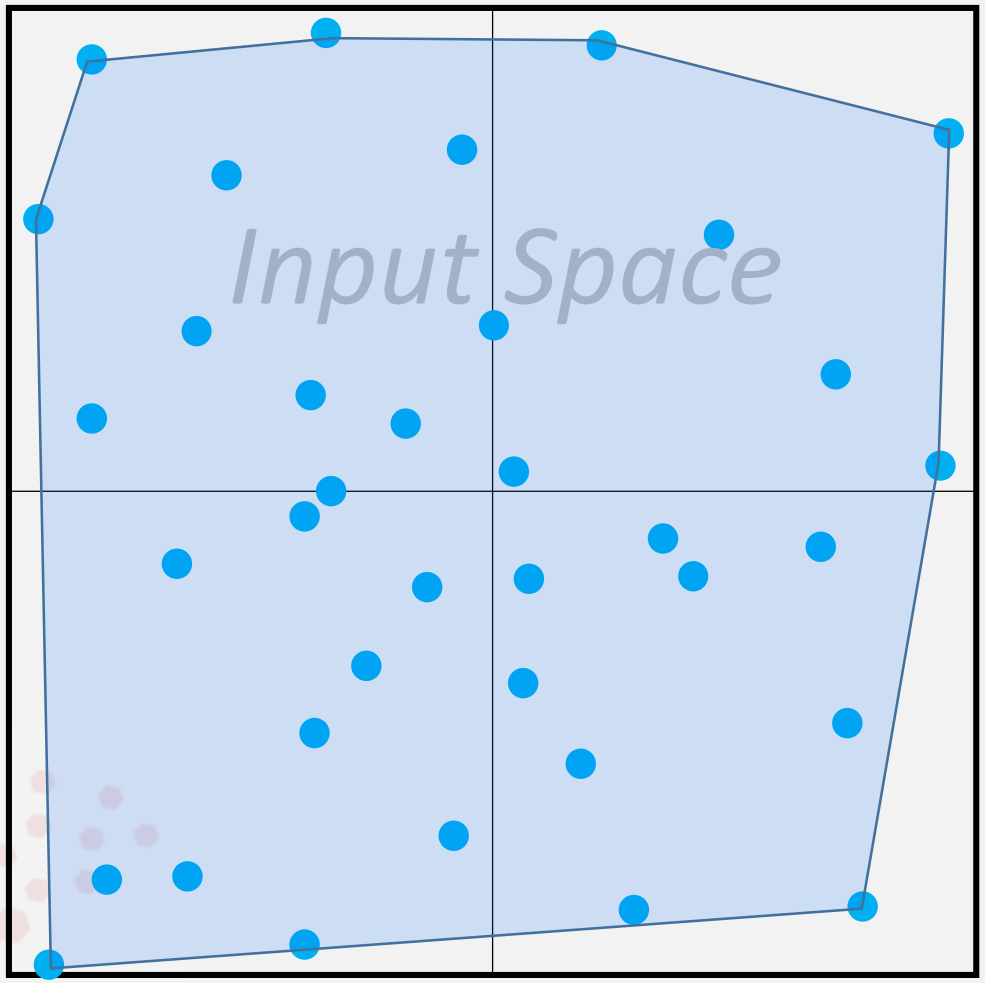


Varying Inputs
One-At-A-Time

- Covered volume (convex hull) = ½

Here still be dragons!

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



Random Points

"Monte Carlo" approach

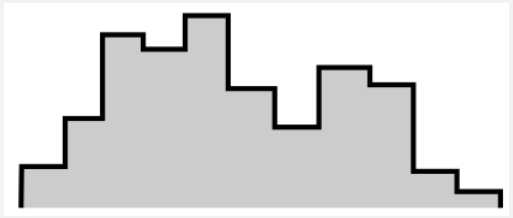
- Covered volume $\rightarrow 1$ as $n \rightarrow \infty$ for any dimension hypercube
- Good coverage inside that volume
- Full exploration of the input space

Uncertainty & Sensitivity Analysis

"What is the range of possible outcomes?"

Uncertainty Analysis

- Histograms
- Spaghetti Plots
- Confidence Intervals



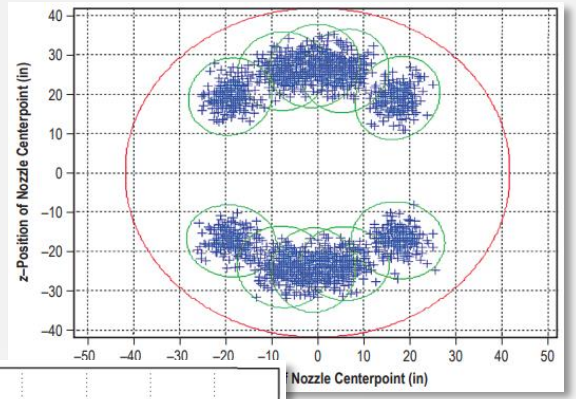
"Which parameters most affect these outcomes?"

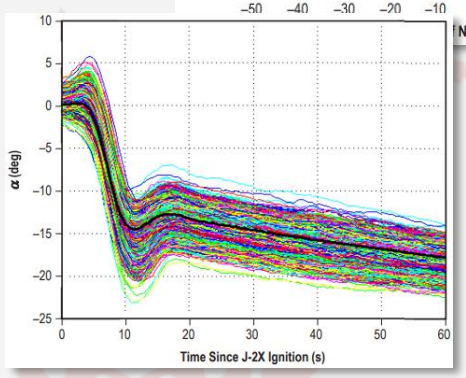
Sensitivity Analysis

- Scatter Plots
- Sensitivity Indices
- Regressions

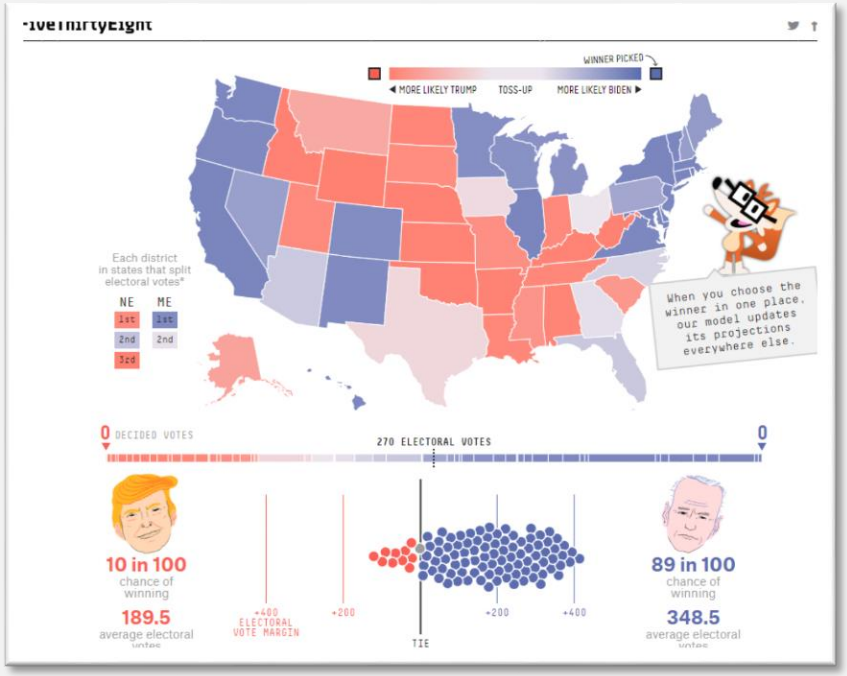
What this looks like in practice

NASA: Ares I Flight Simulations

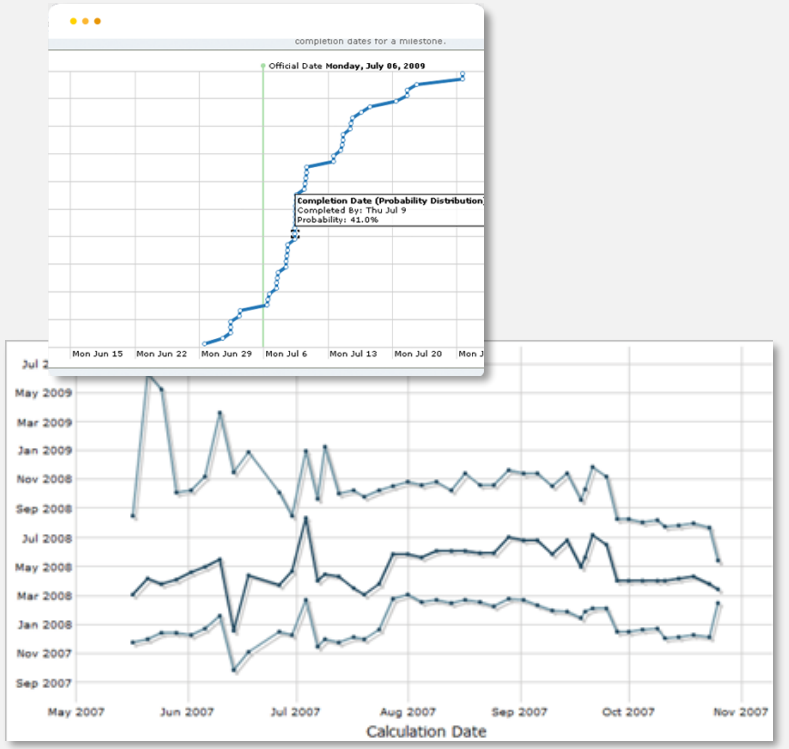




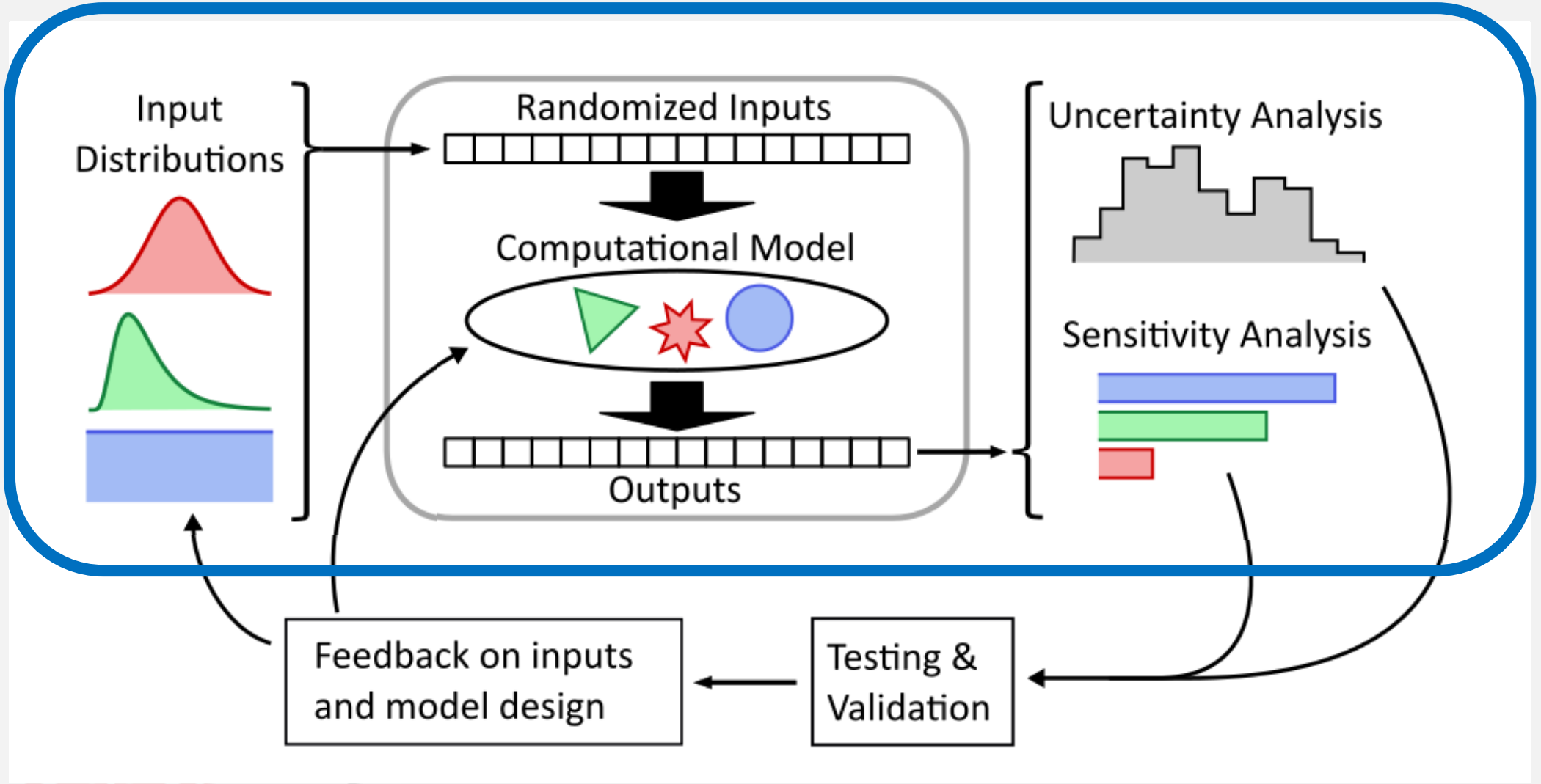
FiveThirtyEight: Election Forecasting



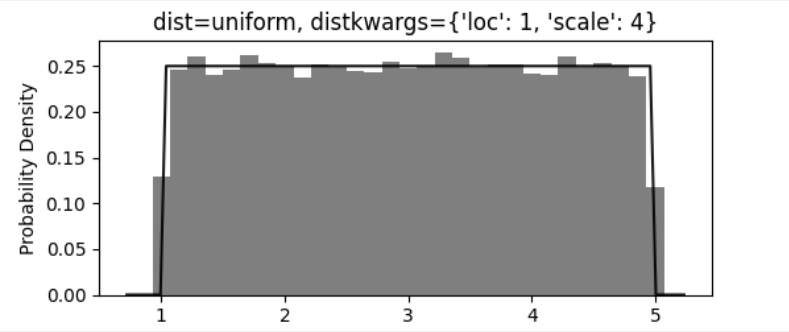
FogBugz: Evidence-Based Scheduling

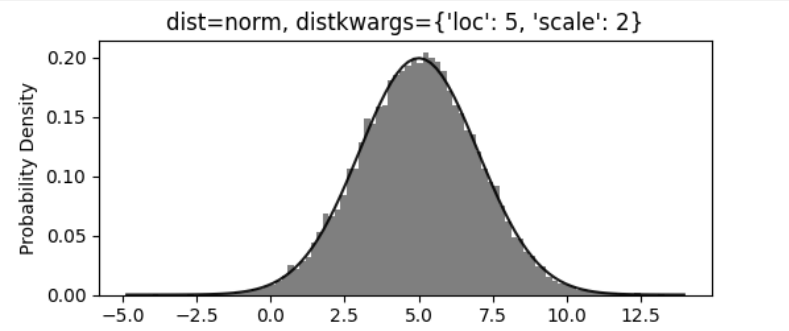


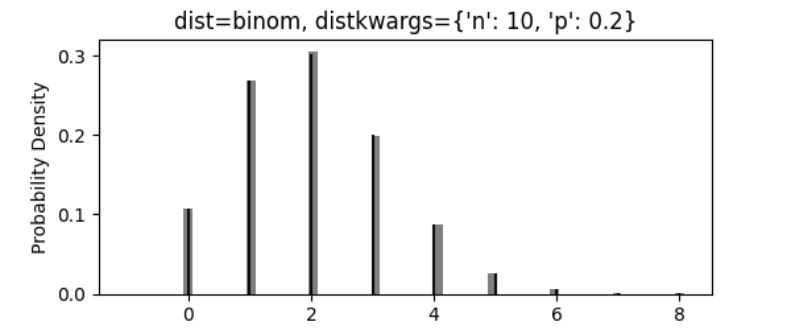
Workflow


Input Distributions
Randomized Inputs
Computational Model
Outputs
Uncertainty Analysis
Sensitivity Analysis
Forward Uncertainty Propagation
monaco
Feedback on inputs and model design
Testing & Validation
Model & Parameter Validation

monaco – Input Distributions







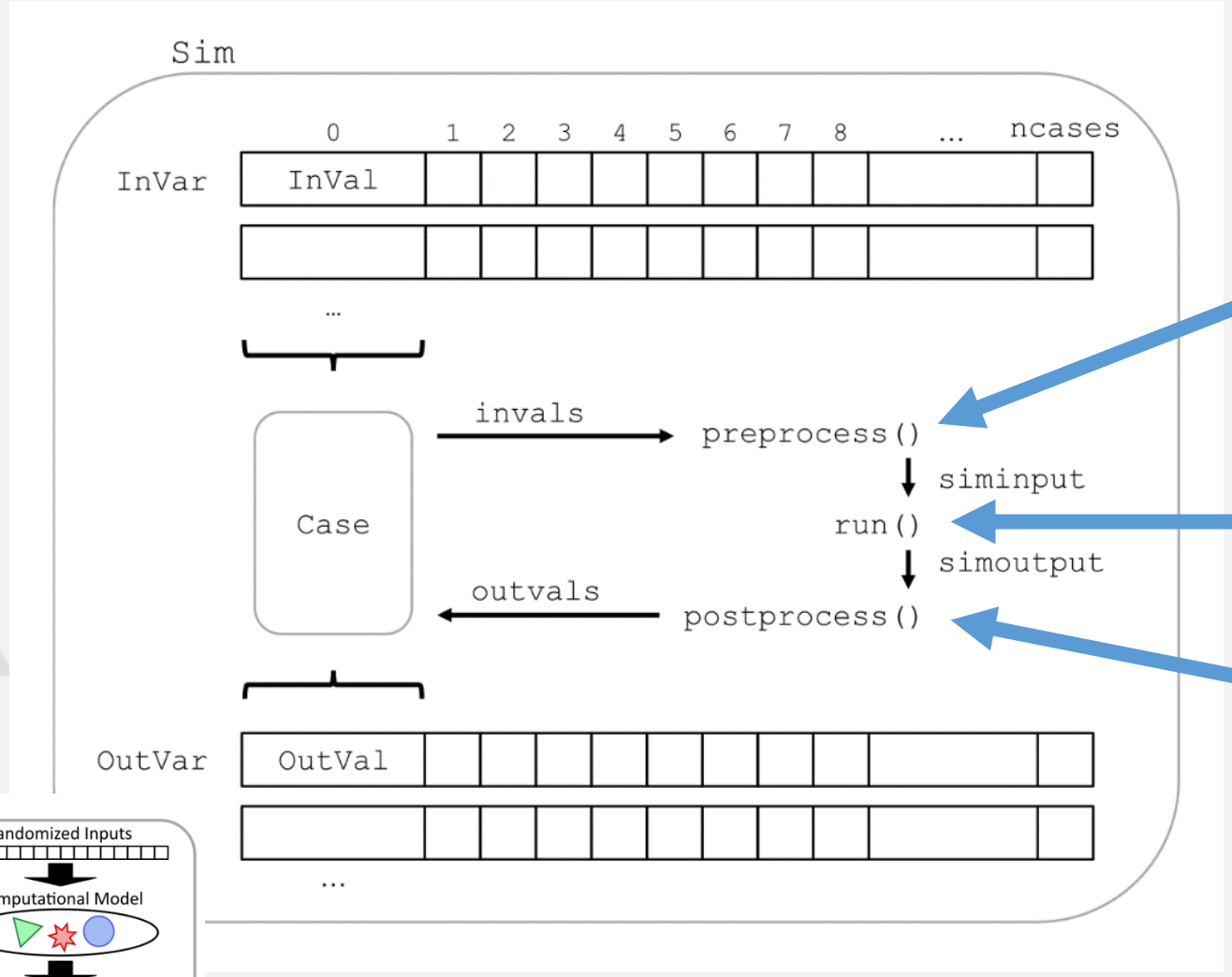
Pass in any of scipy.stats' probability distributions

- Or, define a custom one

Input ranges come from:

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

monaco – Simulation Structure



3 User-Defined Functions

Preprocess

- Grabs input values from each case, structures it into format *`run`* expects

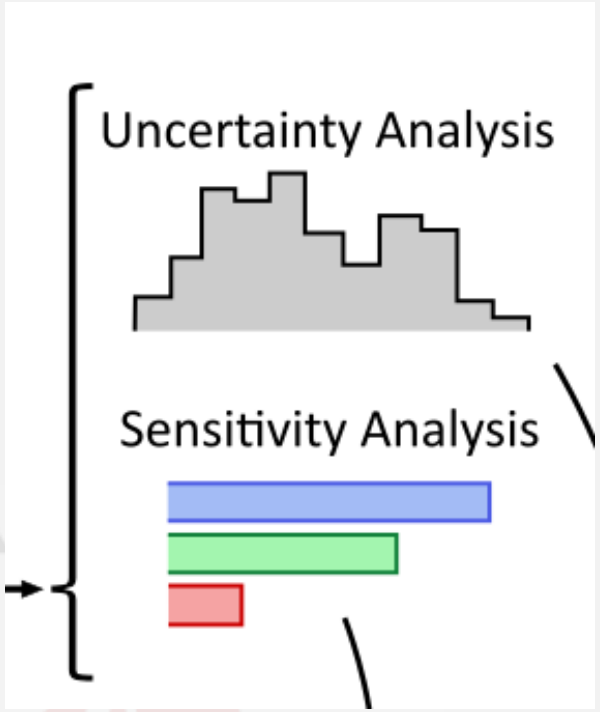
Run

- Wraps or directly implements your model

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

github.com/scottshambaugh/monaco-scipy2022/blob/main/dice_roll.ipynb

Live Demo: Baseball

github.com/scottshambaugh/monaco-scipy2022/blob/main/baseball.ipynb

monaco – Other Features

Parallel Processing

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

How Many Cases to Run?

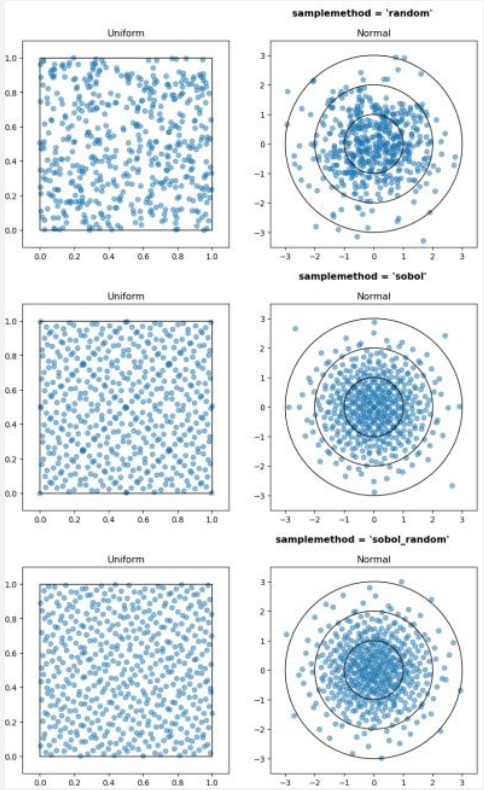
- Order statistics determine cases needed to rigorously reach confidence level for variable statistics

File I/O

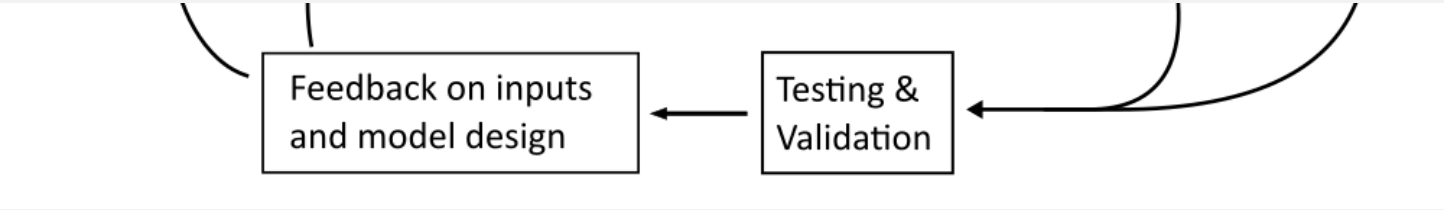
- Save and load *Sim* and *Case* objects to file to avoid repeating expensive computations
- Import and export variables to *.csv* or *.json* to trade out any part of the workflow with external tooling

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

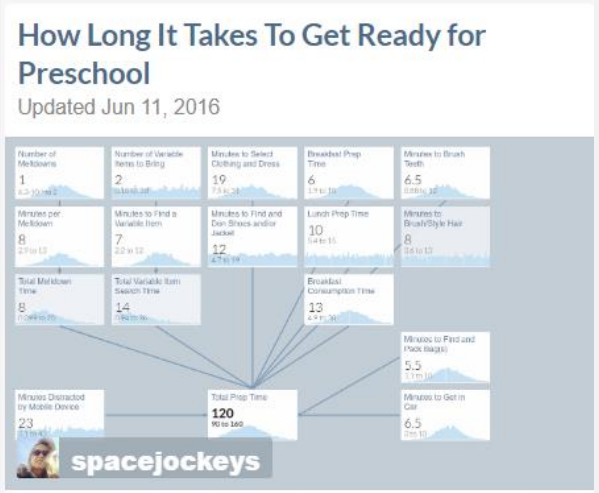
Recommended Tools

Basic → Advanced

Guesstimate

Web-based tool for simple models

Guesstimate



Monaco

Single-Shot Uncertainty & Sensitivity Analysis

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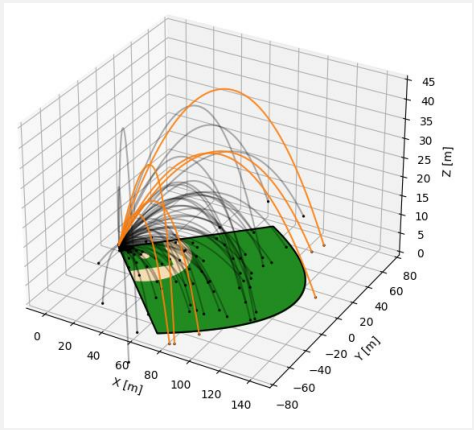
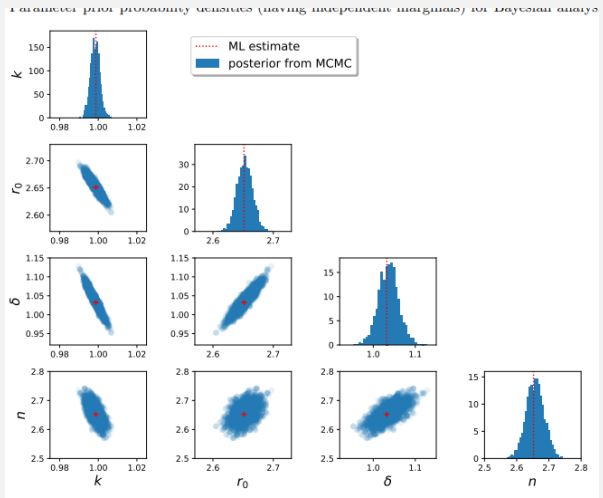


UQpy

More Advanced Uncertainty & Sensitivity Analysis

UQpy



Stan, PyMC

Probabilistic Programming

Stan

PyMC

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


```
pip install monaco
```

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

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