

# On Bayesian workflow

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Talk partially based on

Andrew Gelman, *Aki Vehtari*, Daniel Simpson, Charles C. Margossian, Bob Carpenter, Yuling Yao, Lauren Kennedy, Jonah Gabry, Paul-Christian Bürkner, and Martin Modrák (2020).

**Bayesian workflow.**

*arXiv preprint arXiv:2011.01808.*

# Outline

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  - efficiency
  - reliability
  - reproducibility
  - etc.

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- Software assisted workflows

# Workflow term

- Saunders and Blundstone, 1921. Railway engineering.
- Started to get more popular in 1990s based on Google books ngram viewer

# Bioinformatics and scientific workflow in 2000's

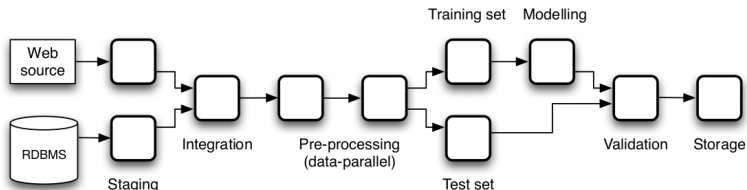


Fig. 1. Workflow example

Curcin & Ghanem (2008). Scientific workflow systems - can one size fit all?

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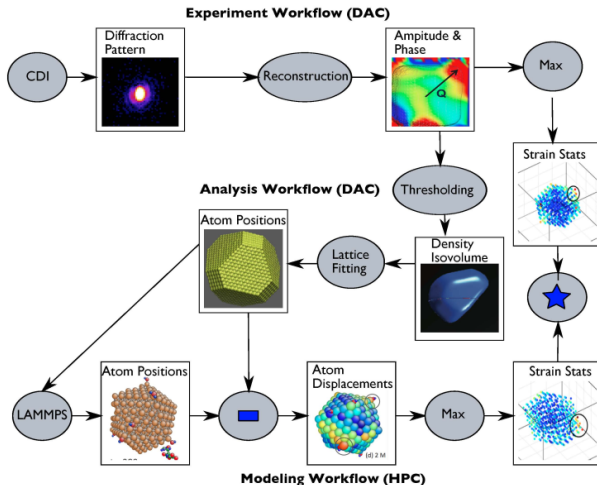


Figure 1: Science workflow for the comparison of a molecular dynamics simulation with a high-energy X-ray microscopy of the same material system includes three interrelated computational and experimental workflows.

Deelman et al (2017). The Future of Scientific Workflows

# Workflows in general

- Workflow frameworks improve
  - efficiency
  - reliability
  - reproducibility
  - etc.

# Bayesian workflow

- Savage (2016). An introduction to Bayesian modelling in Stan for economists.
  - “The Bayesian workflow”
- Gabry, Simpson, Vehtari, Betancourt, and Gelman (2017). Visualization in Bayesian workflow.

# Box & Youle, 1955

The Exploration and Exploitation of Response Surfaces: An Example of the Link between the Fitted Surface and the Basic Mechanism of the System

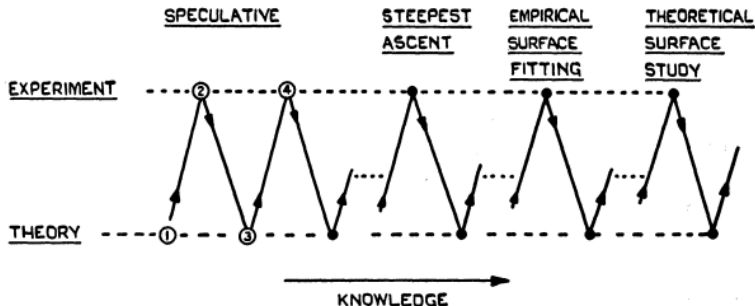


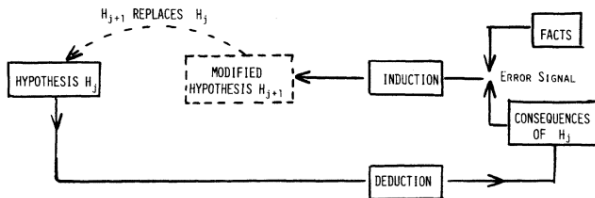
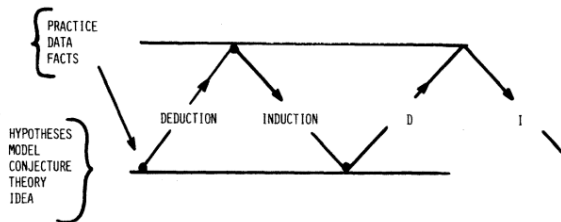
FIGURE 7. DIAGRAMATIC REPRESENTATION OF PROCESS OF EXPERIMENTAL ITERATION.

# Box 1976: Science and Statistics

## A. The Advancement of Learning

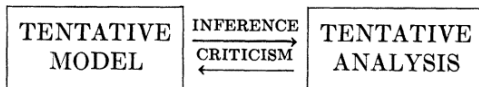
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### A(2) A Feedback Loop

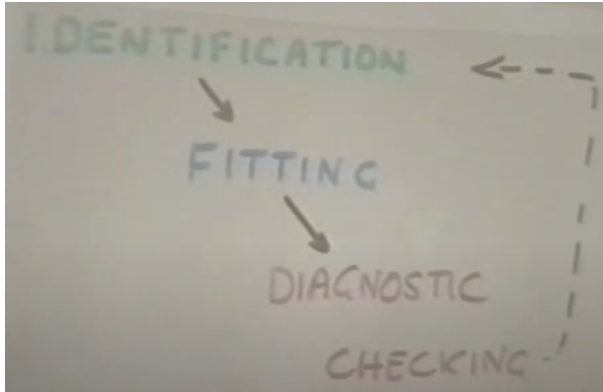


# Box 1976: Science and Statistics

Data analysis, a subiteration in the process of investigation, is illustrated here.



# Box 1987



From the talk slides ‘Some aspects of statistical design in quality improvement’

## StanCon 2018 intro

### Bayesian Workflow

#### Scope out your problem

What inputs and outputs can help you learn? What relationships can you see by eye?

#### Specify likelihood & priors

Use knowledge of the problem to construct a generative model and shape the scope of the parameters

#### Check the model with fake data

Generate data, fit model, and evaluate fit as a sanity check

#### Fit the model to real data

To recover parameters

#### Check diagnostics

Algorithms should come with diagnostics that let you know when they're not working

#### Graph fit estimates

Understand your inferences

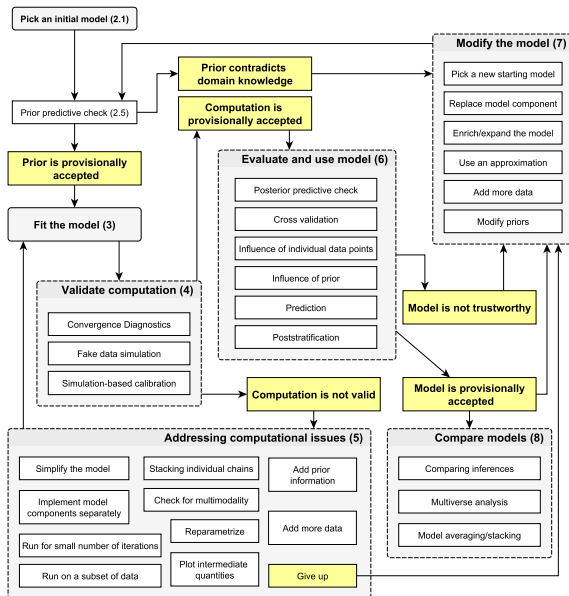
#### Check predictive posterior

Perform PPCs to understand predictions

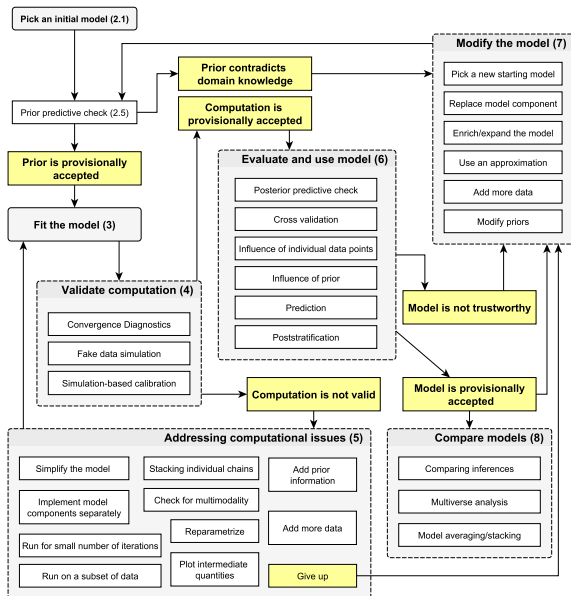
#### Compare models

Iterate on model design, choose a model!

# Bayesian workflows



# Workflows and sub-workflows



# Model building as software development process

Boehm (1996, 1988)

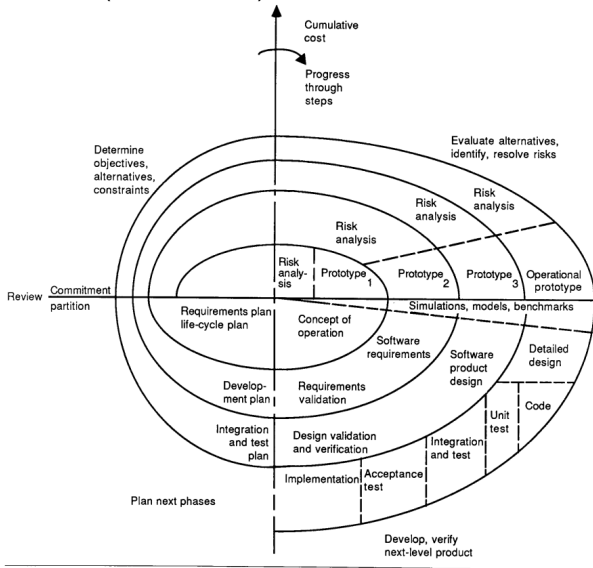
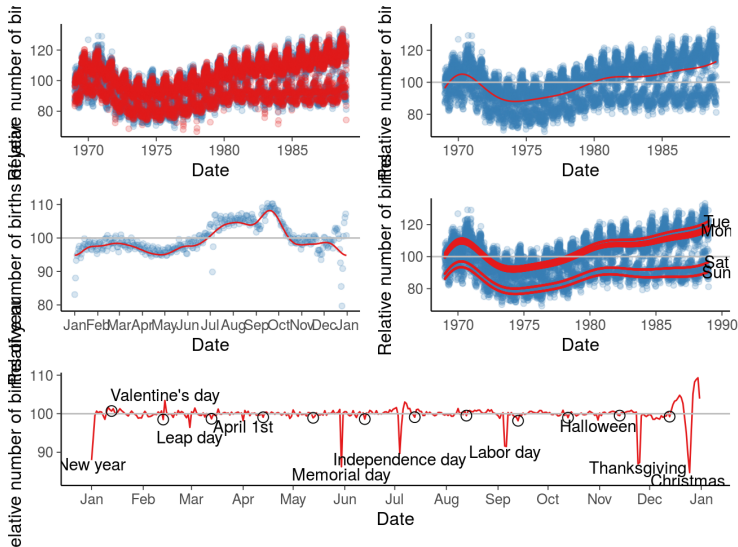


Figure 2. Spiral model of the software process.

# Example: Birthdays

<https://avehtari.github.io/casestudies/Birthdays/birthdays.html>

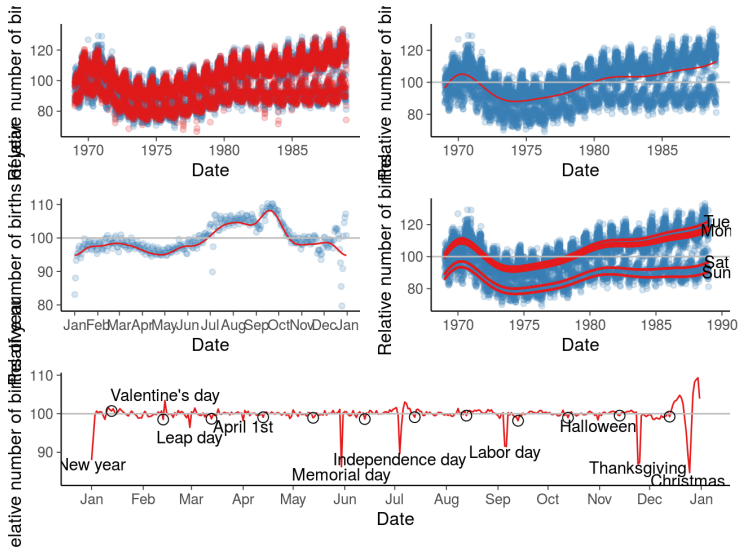


# Prototypes, shortcuts, and workflow as engineering

- When building prototypes or making initial experiments, we can use shortcuts
  - the final models tested with sufficient rigor

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# Different requirements and workflow as cooking

- Make a sandwich out of available ingredients
  - a generic model that is useful for almost any data
  - normal linear model is not probably the best dish given the ingredients, but can be delicious anyway

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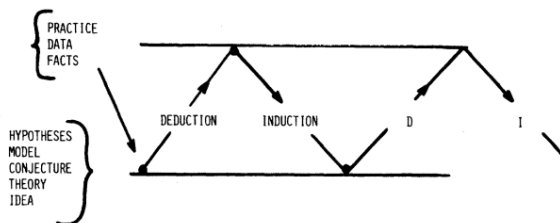
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  - many different pre-described models that match your data and task
  - e.g. rstanarm, brms, shinybrms
- Develop a new recipe to be used in a fine dining restaurant
  - may require several iterations (depending on how much the customers are willing to pay)
  - write the model in probabilistic programming language

# Iterative workflow as a learning process

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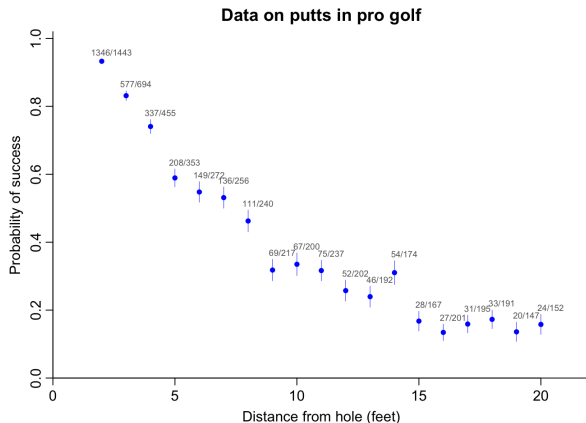
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Box (1976)

- Incremental learning reduces cognitive load

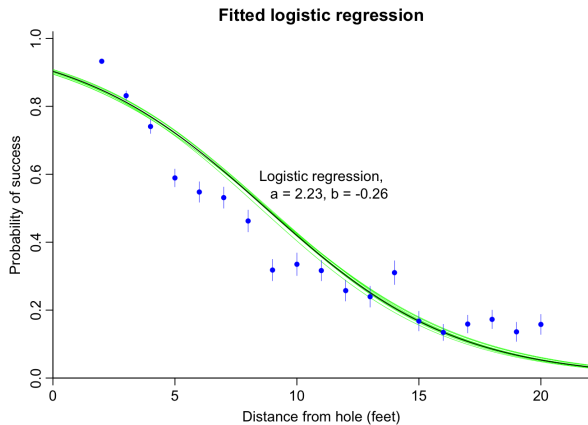
# Example: Golf putting



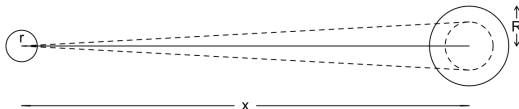
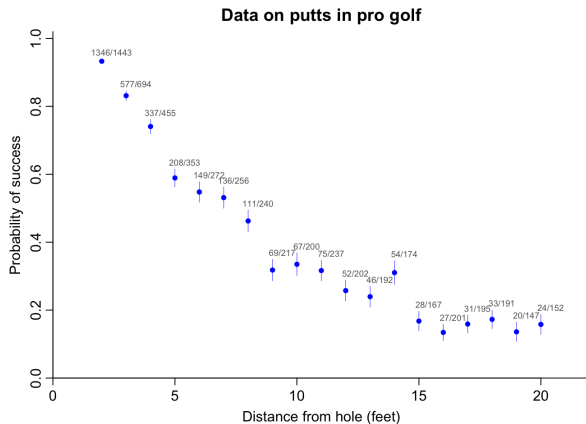
Example by Andrew Gelman CC-BY-NC 4.0

<https://mc-stan.org/users/documentation/case-studies/golf.html>

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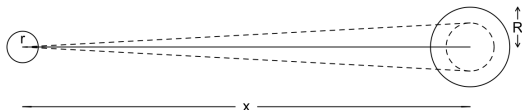
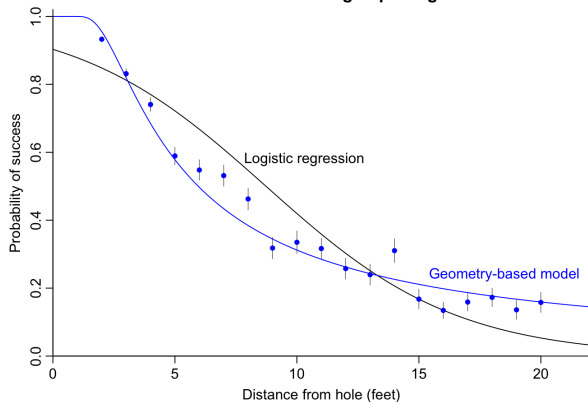


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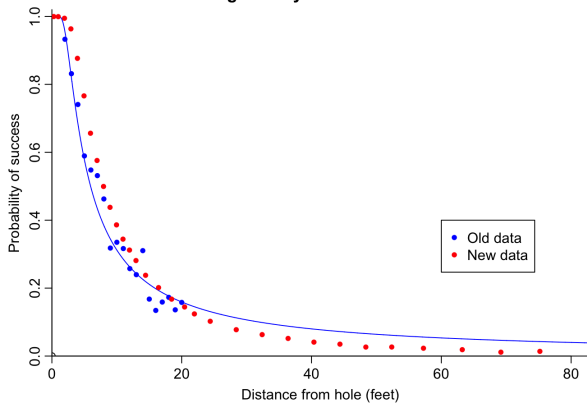
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Two models fit to the golf putting data



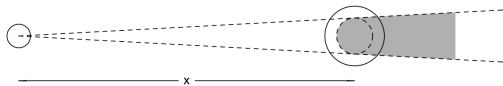
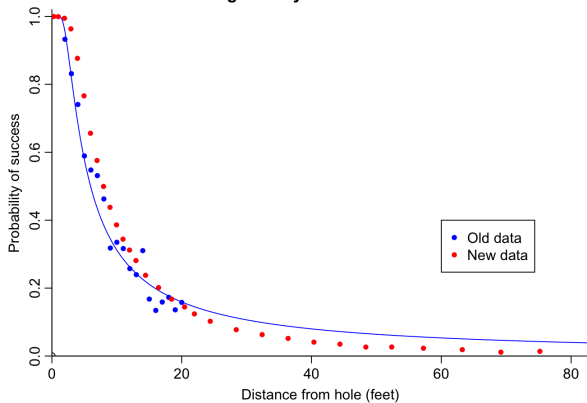
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Checking already-fit model to new data



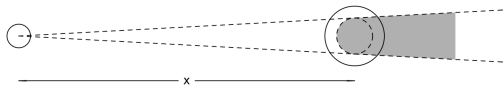
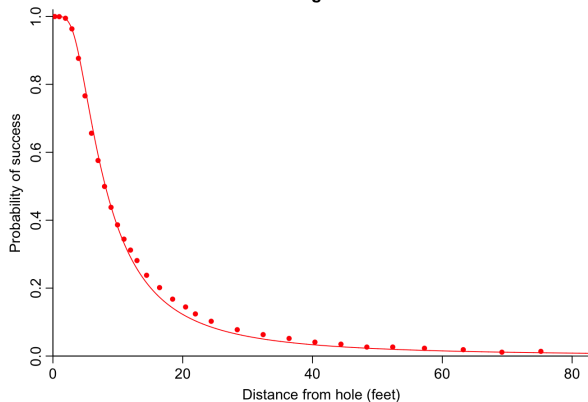
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Checking model fit

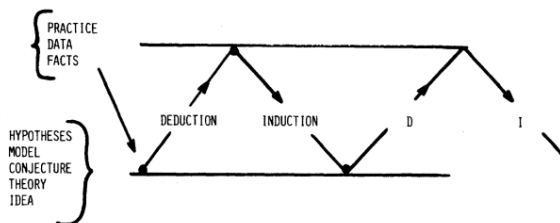


# Models as experiments

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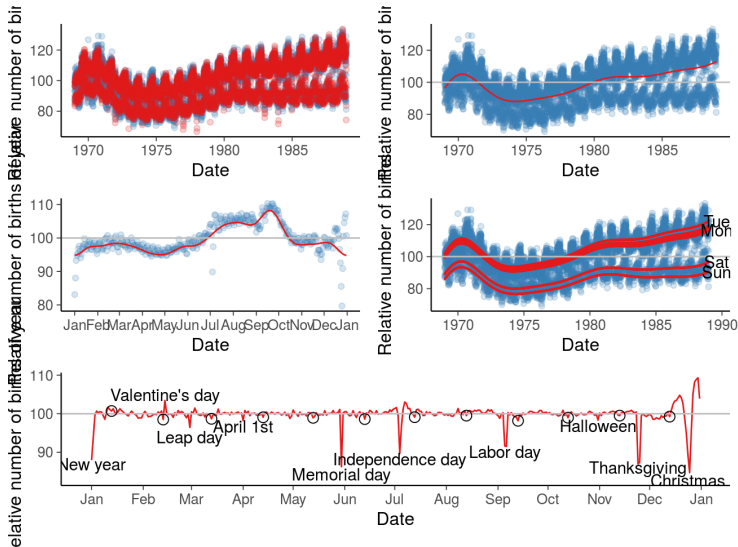


Box (1976)

- New facts are learned by using the models
- New learned facts can be used to choose the next model

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# Software development process vs. Models as experiments

- The end result may also be a series of models
  - it may be useful to report results of simpler experiments, too
  - presenting the results of many models is also part of the workflow

# Cost and benefit of model building

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Stick figure and silhouette from Weech et al. (2014) doi:10.1167/14.12.10. Photo CC0.

# Cost and benefit of model building

- Sufficient accuracy for model and computation

# Argument against iterative model building

- Double dipping, inference after model selection, etc.

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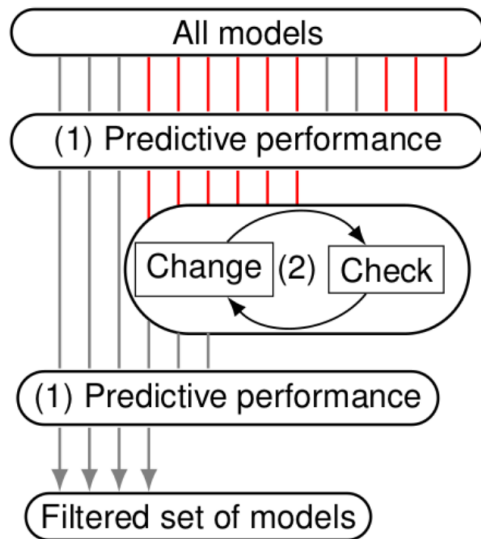
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Watch and listen more (4.5h) in

- Model assesment, selection and averaging  
<https://www.youtube.com/watch?v=Re-2yVd0Mqk>
- Use of reference models in variable selection  
<https://www.youtube.com/watch?v=N0ce8J8slFY>
- These are a few of my favorite inference diagnostics  
<https://www.youtube.com/watch?v=vLx6lUIZ0fc>

# Filtering



from Riha, Siccha & Vehtari (2023)

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- See also “What do we need from a PPL to support Bayesian workflow?” by Bob Carpenter [statmodeling.stat.columbia.edu/2021/10/22/carpenter-slides-papers-prob-prog-2021/](https://statmodeling.stat.columbia.edu/2021/10/22/carpenter-slides-papers-prob-prog-2021/)

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# Computer assisted workflows

- There are software for sub-workflows
- Software for the whole is very challenging as there are so many possibilities
  - LLMs (e.g. ChatGPT) can only help when there has been enough material in the internet for them to learn, and even then they may provide misleading recommendations

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