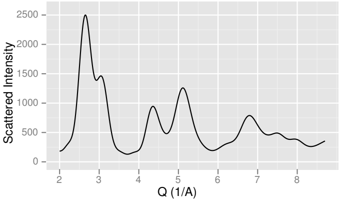
What do noisy datapoints tell us about the true signal?

C. R. Hogg

November 16, 2011

Outline

Overview



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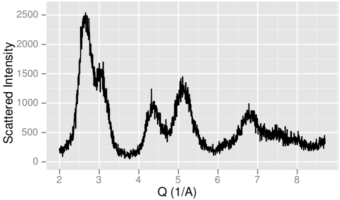

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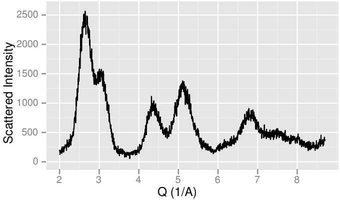

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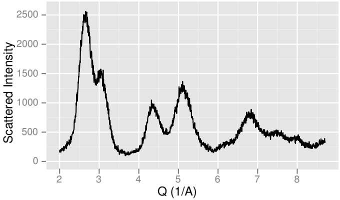

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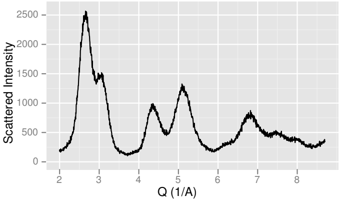

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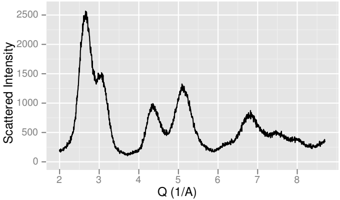

Ernest Rutherford (1871-1937)

"If your experiment needs statistics,

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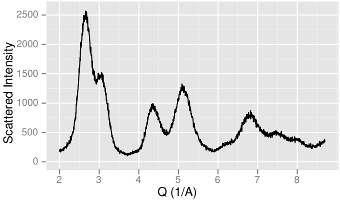

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“If your experiment needs statistics,

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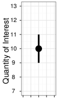
(Or: use better statistics!)

Goals for the talk

1. Explain **Bayesian analysis** at *conceptual* level

Goals for the talk

Uncertainty in single quantity:



1. Explain **Bayesian analysis** at *conceptual* level
2. Discuss *quantifying* uncertainty in **continuous functions**

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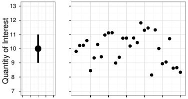

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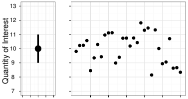

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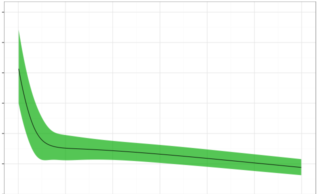

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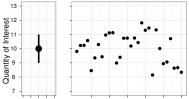

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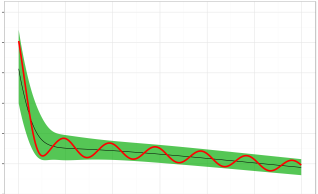

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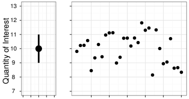

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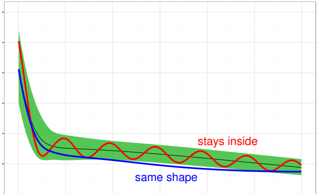

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Why Bayes at NIST?

NIST's mission:
To promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.

NIST's vision:
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- Which language to discuss uncertainty?
  - If "probabilities": *Bayesian analysis*

[a] NIST TN 1297

What is Bayesian Analysis?

θ: what we **care** about

y: **data**

$p(\theta|y)$

(**fullest possible** information about θ, **in light of** y)

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

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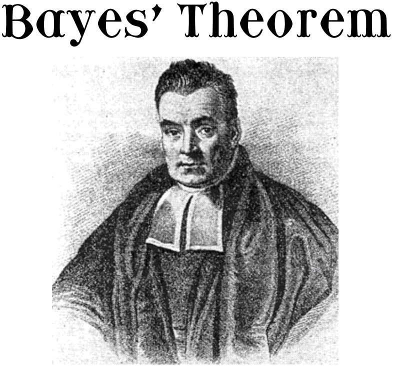

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function f: what **I** care about
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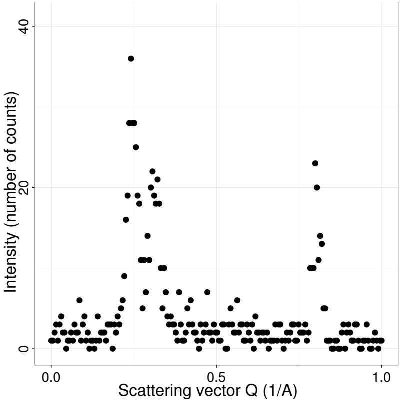
Likelihood of function $p(y|f)$



- Example: artificial dataset
- Noise model: **Poisson**

$$p(y|f) = \frac{f^y e^{-f}}{y!}$$

- Assume *independent pixels*

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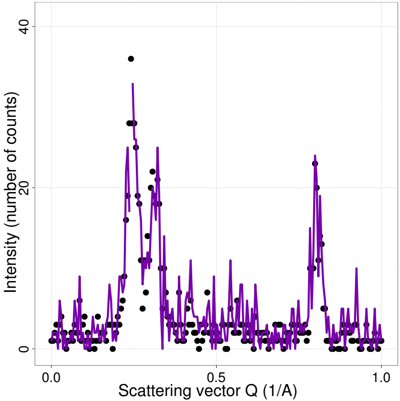

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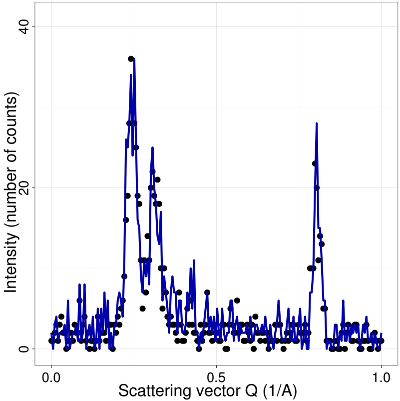

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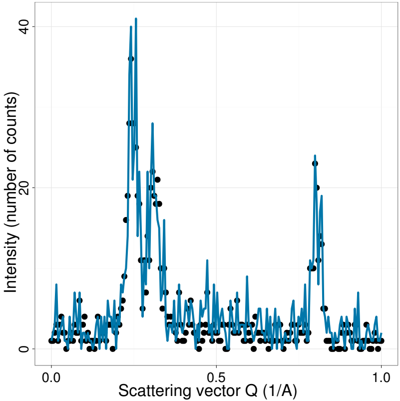

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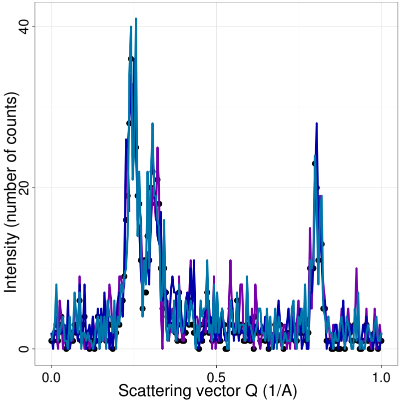

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- Problem: not **plausible**
  - (What makes a function "plausible"?)

“Plausibility” of function $p(f)$

- Assume *smooth* and *continuous*
- ***No*** *functional form* assumed

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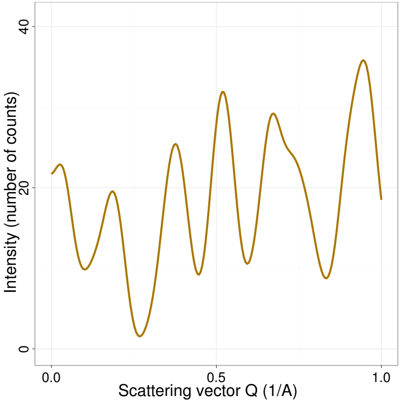

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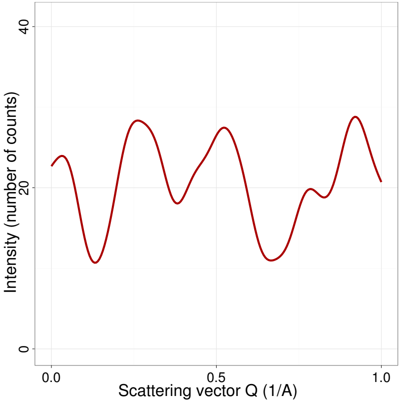

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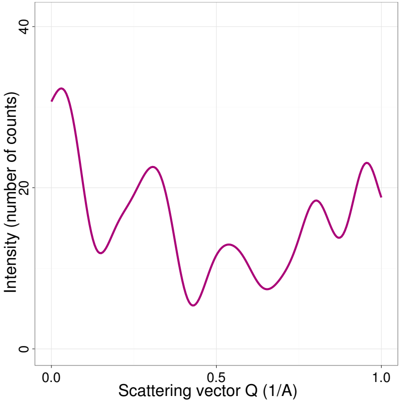

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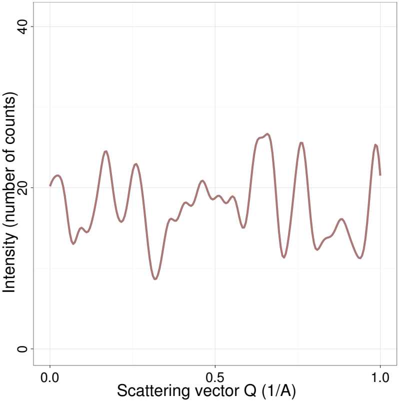

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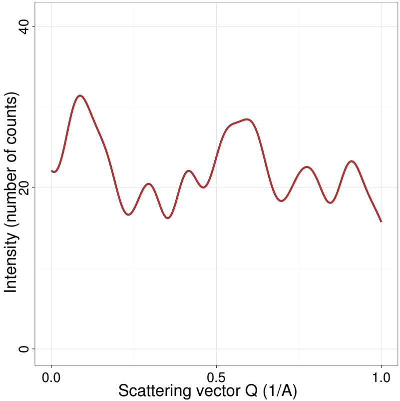

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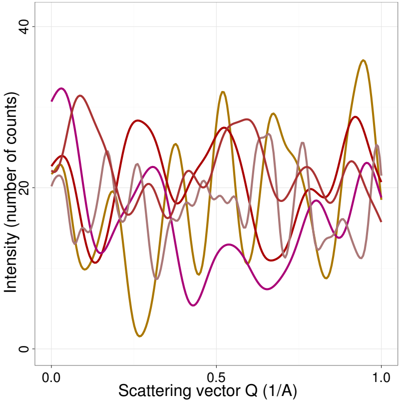

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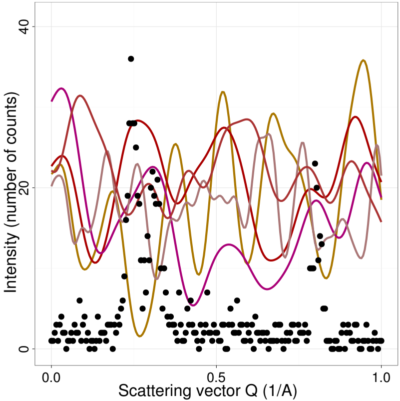
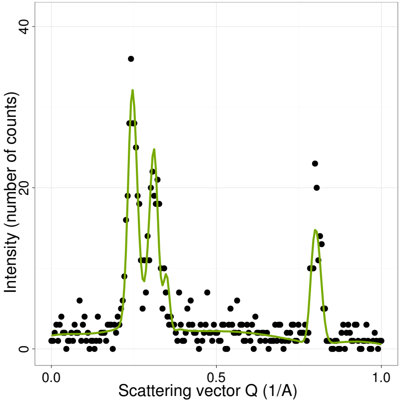


- Assume *smooth* and *continuous*
- ***No** functional form* assumed
- Naturally: unrelated to data

Posterior probability $p(f|y)$



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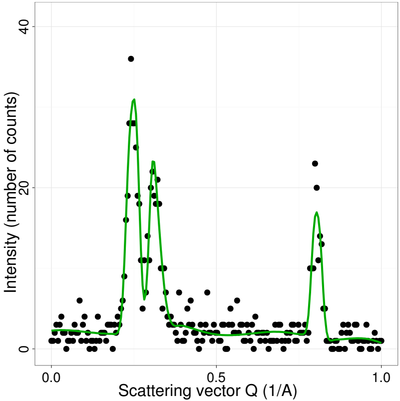

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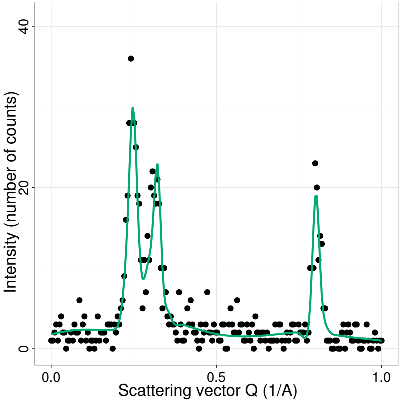

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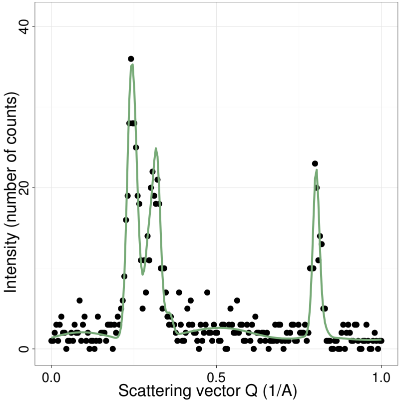

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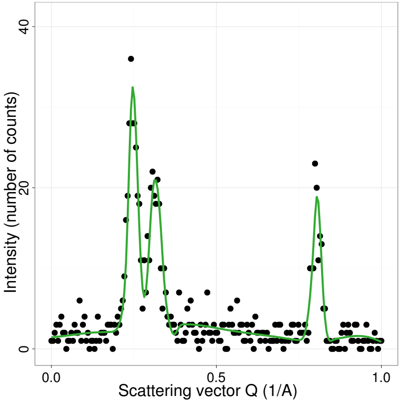

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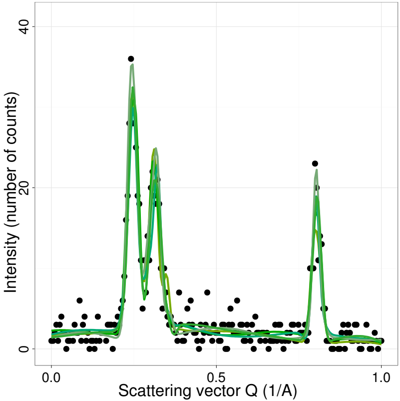

- "Best of both worlds":
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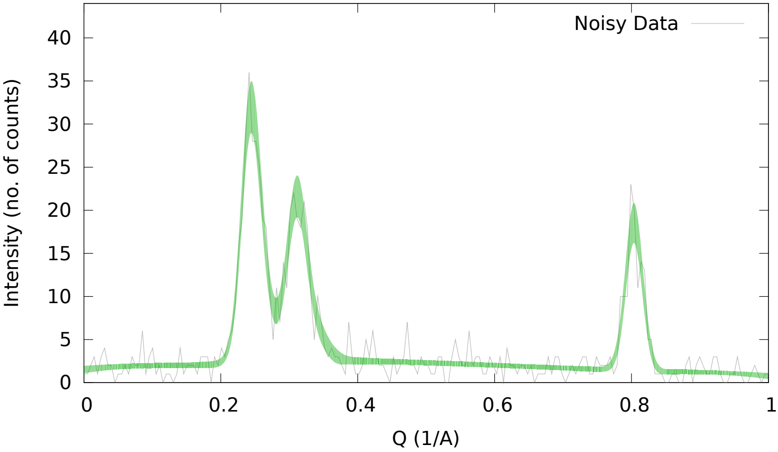
- To represent uncertainty: show *many guesses*
  - (Or, summarize them...)

Posterior probability $p(f|y)$

Quantitative uncertainty visuals



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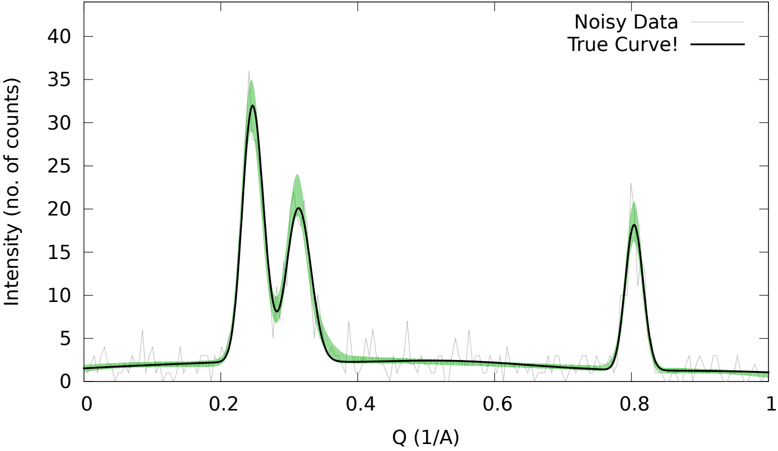
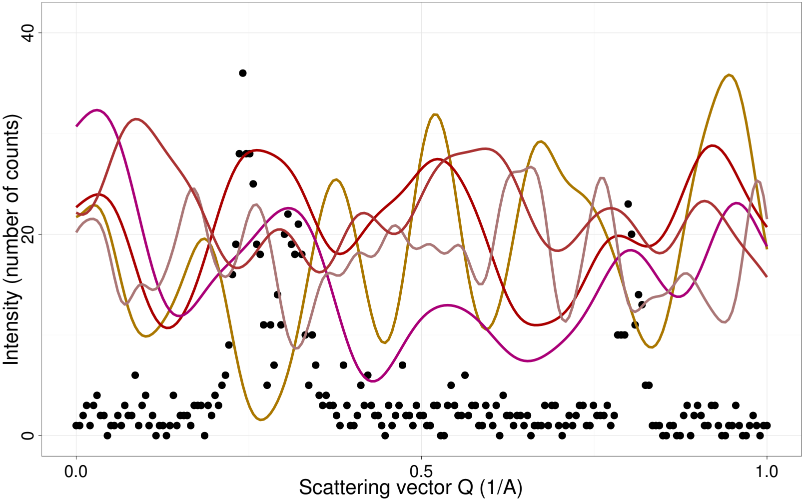


Recap: Bayesian denoising

Plausible curves



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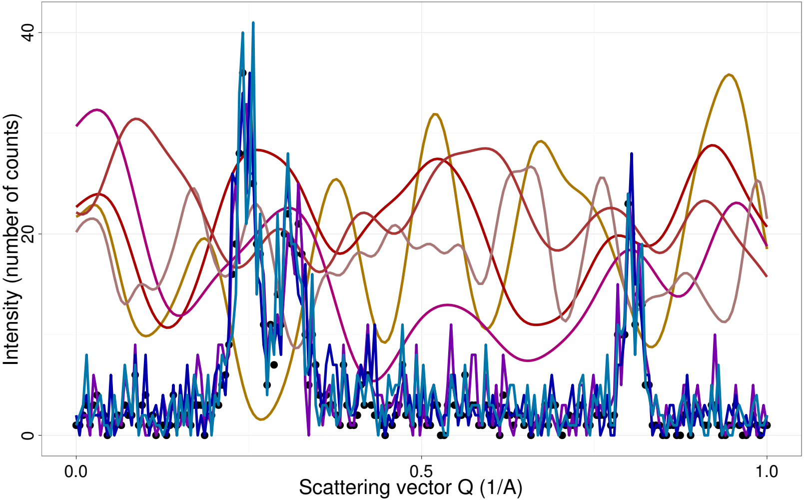

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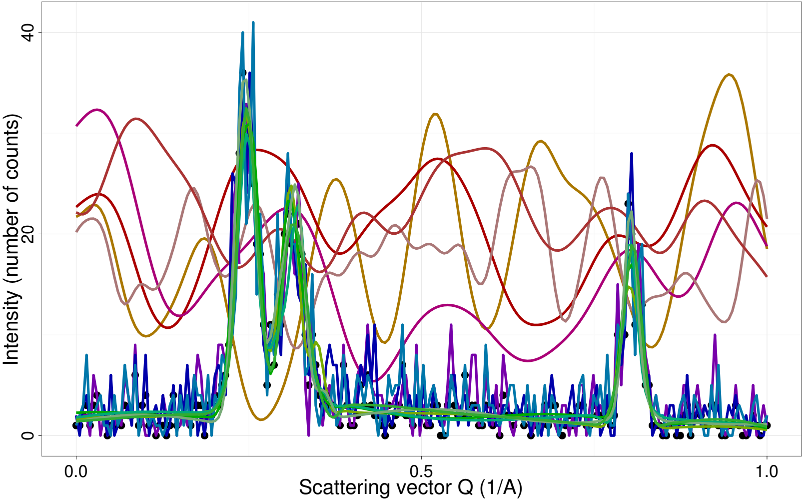
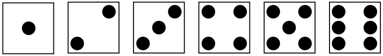


Random variables; Random functions



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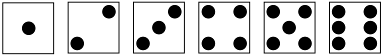

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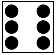
$F =$ ,

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    (roll the die,
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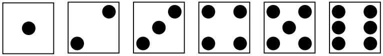

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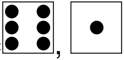
$F =$  ,

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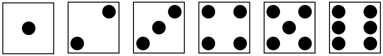

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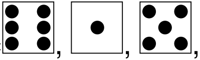
$F =$ 

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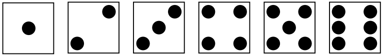

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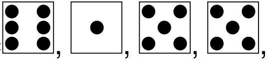
$F =$ 

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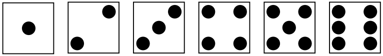

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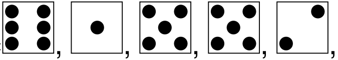
$F =$ 

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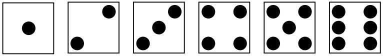

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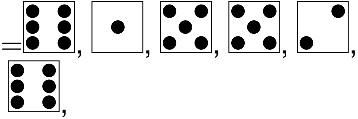

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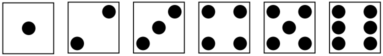

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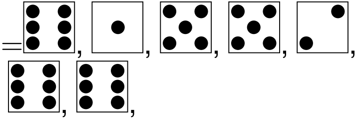

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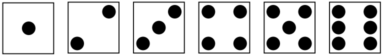

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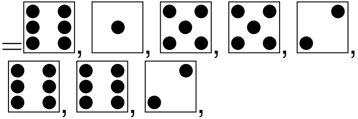

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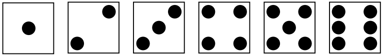

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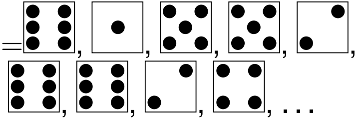

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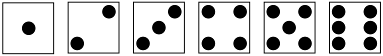

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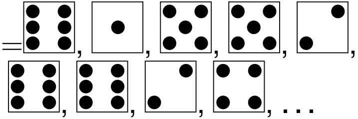
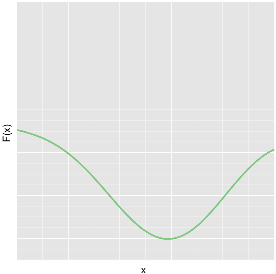
$F =$  , …



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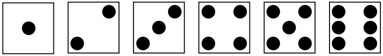

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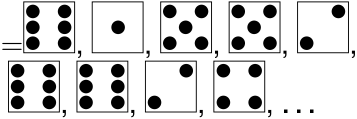
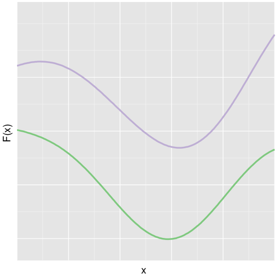
$F =$  ...



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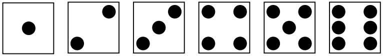

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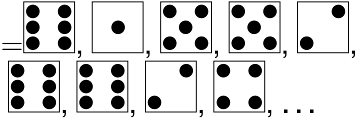
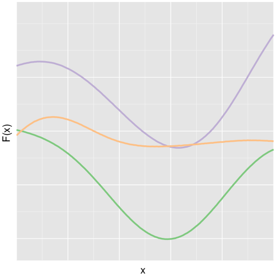
$F =$  , . . .



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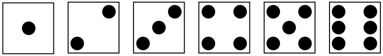

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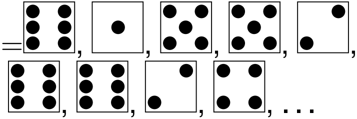

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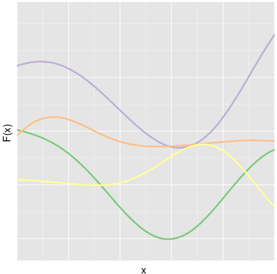

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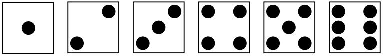

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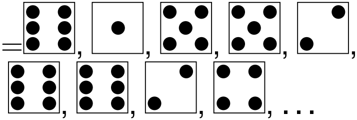

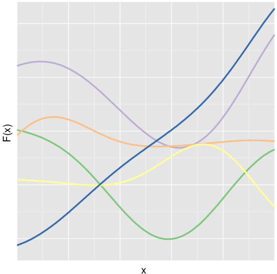

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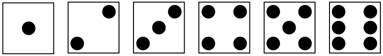

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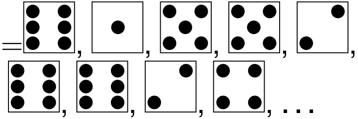

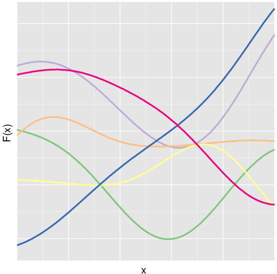

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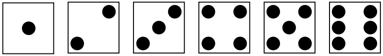

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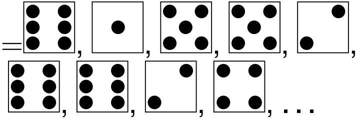

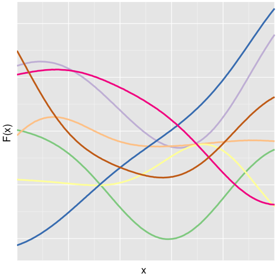

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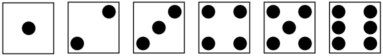

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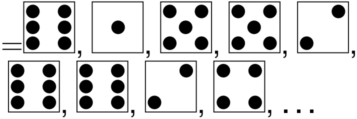
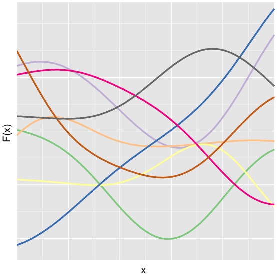
$F =$  , ...



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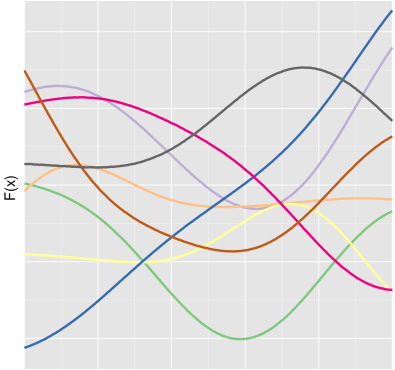

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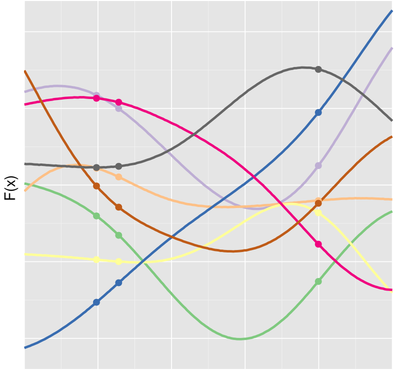

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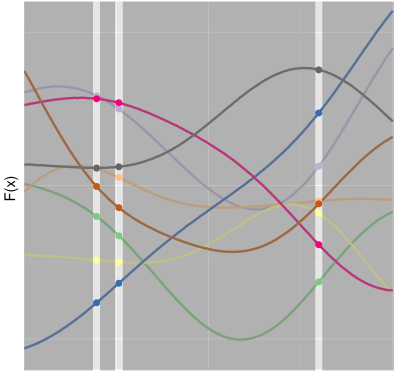

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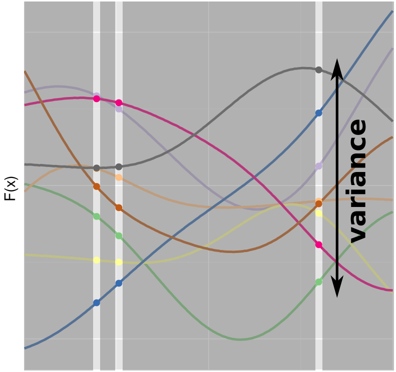

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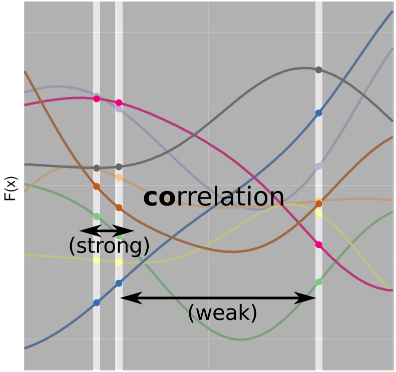

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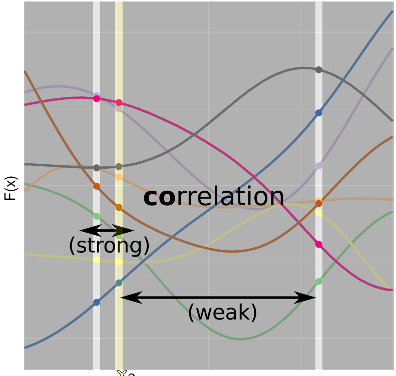

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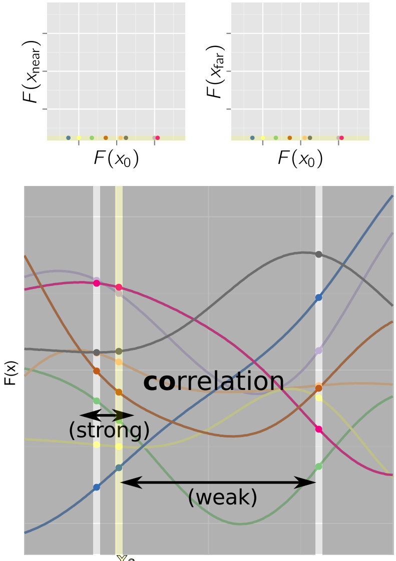

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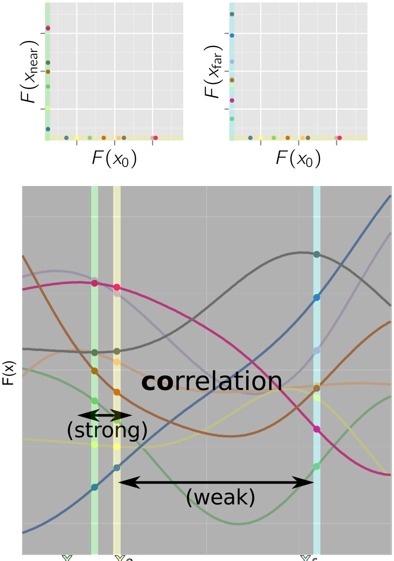

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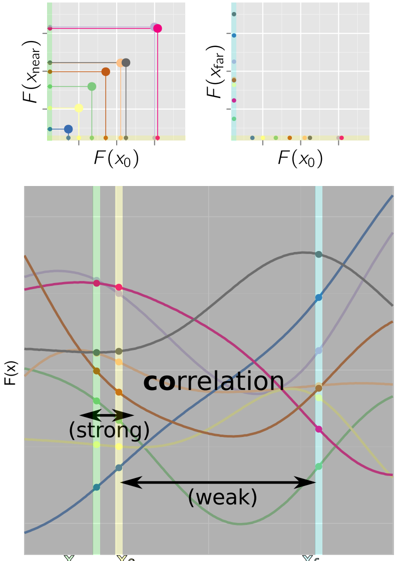

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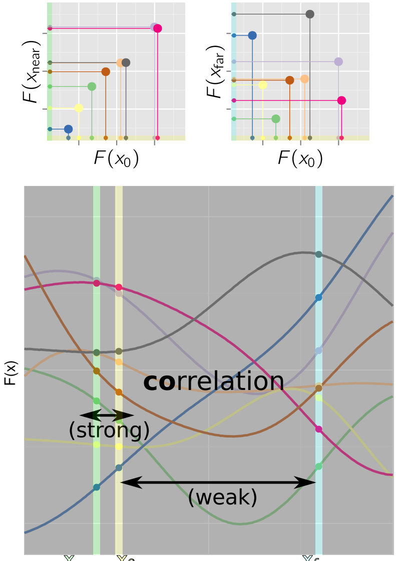

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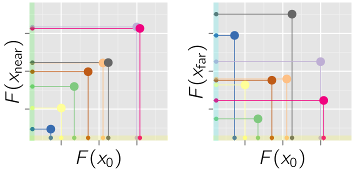

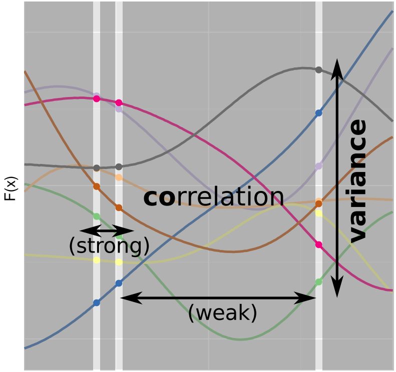

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- **correlation** $\times$ **variance**: ***covariance***

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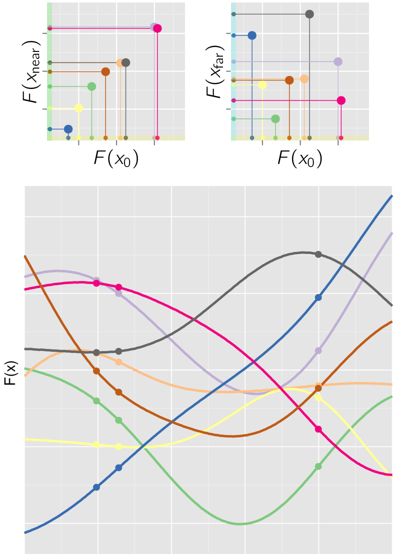

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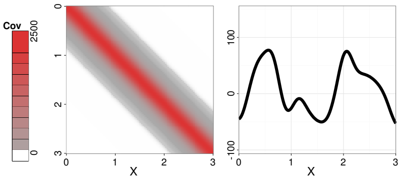
  - **correlation** × **variance**: ***covariance***
- **Gaussian Process:**
  - Every point is a Random Variable
  - Any (finite) subset has *Gaussian* joint distribution

How to read a Covariance Matrix



- How to read the matrix?

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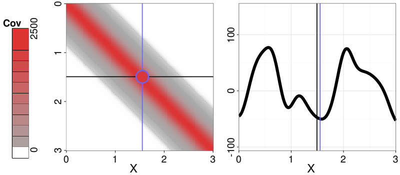

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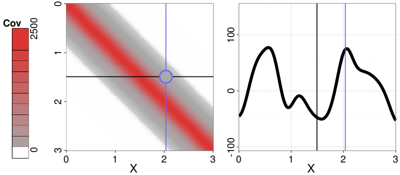

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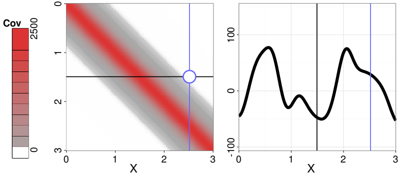

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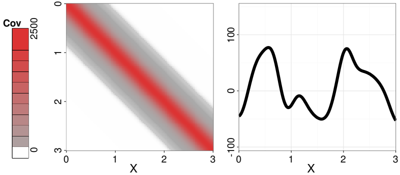
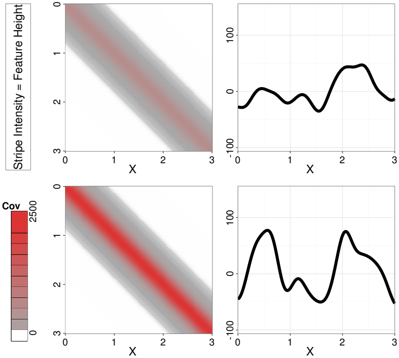


- How to read the matrix?
    1. By individual entries
    2. As a whole
       (central stripe)
        - **Intensity:**
          height of features
        - **Width:**
          width of features

How to read a Covariance Matrix



- How to read the matrix?
  1. By individual entries
  2. As a whole (central stripe)
     - **Intensity:** *height* of features
     - **Width:** *width* of features

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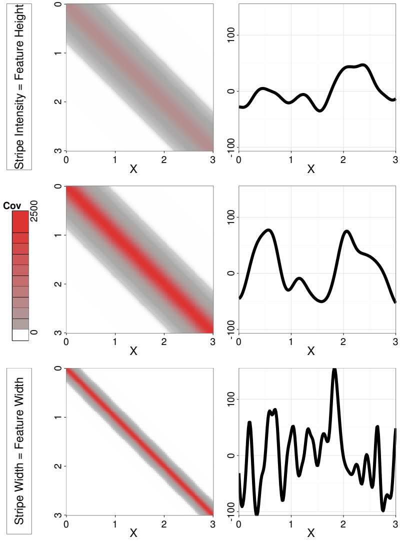

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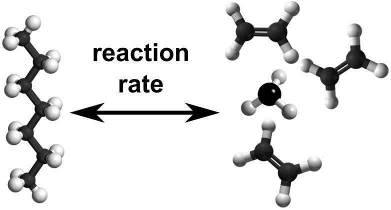
Example 1: Hydrocarbon combustion

(Dave Sheen and Wing Tsang, NIST, Div. 632)



Hydrocarbon burning simulations

- Need (many!) reaction rate constants
  - Measured individually
  - Predictions are precise, quantitative

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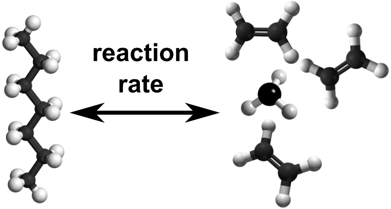
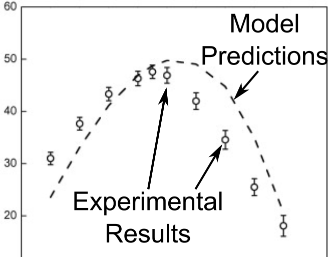


Fig. 6 of: Ji et al. Combustion and Flame, 2011 (in press)



Hydrocarbon burning simulations

- Need (many!) reaction rate constants
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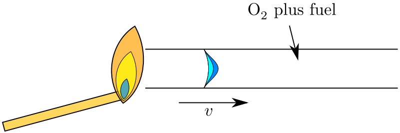
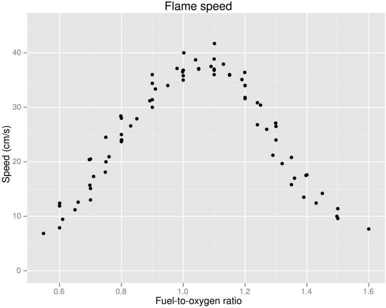
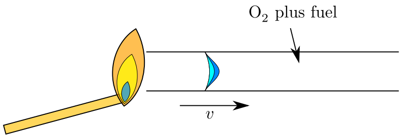
Hydrocarbon combustion: flame speed experiments

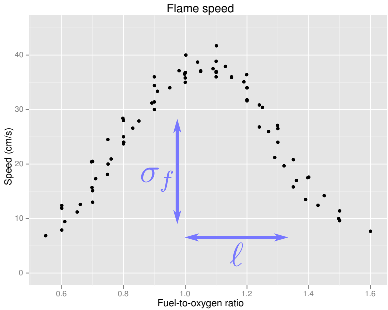




- Datapoints (from several experiments)

Hydrocarbon combustion: flame speed experiments





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- **Model**: lengthscales ℓ and σ_f

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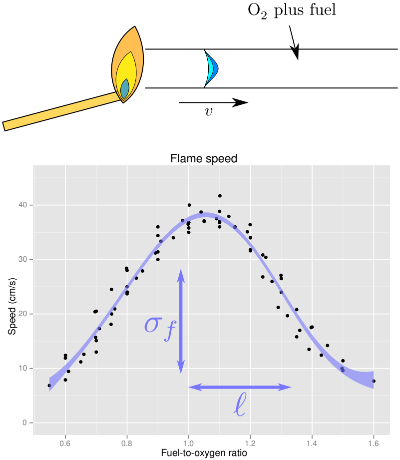

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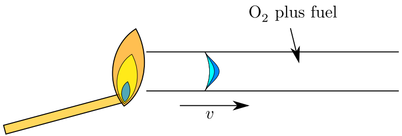
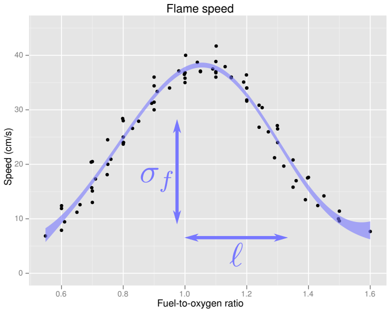
Hydrocarbon combustion: flame speed experiments





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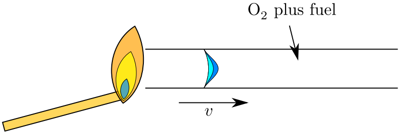
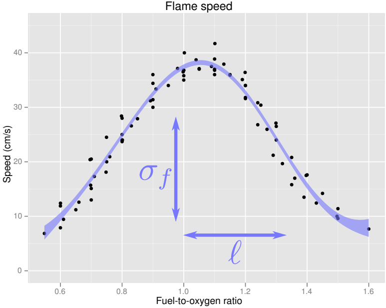
Hydrocarbon combustion: flame speed experiments





- Datapoints (from several experiments)
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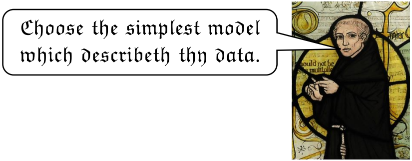
- See also: individual curves
- But where did this model come from. . . ?

Occam's razor, intro

- William of Occam
  c. 1288 - c. 1348
- Gave us **Occam's Razor**

Occam's razor, intro



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Occam's razor, intro

Choose the simplest model
which describeth thy data.

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- *Claim:* use **probability**, get this **automatically**
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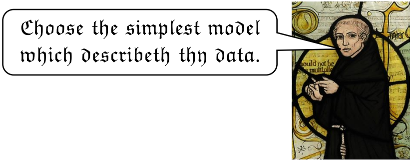
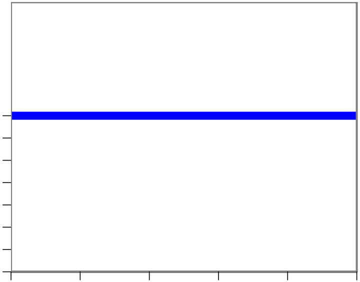


MODEL 1:
flat



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- Example: 3 models. . .

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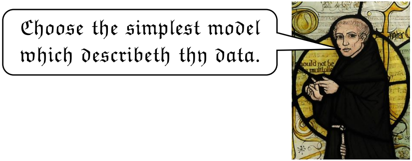
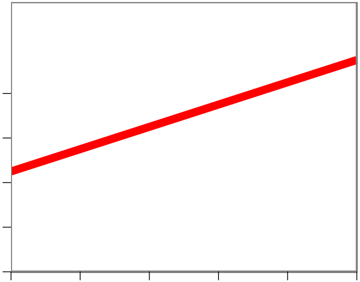


MODEL 2:
flat + line



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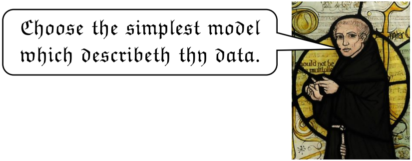
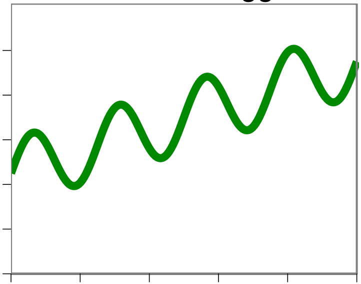


MODEL 3:
flat + line + wiggle



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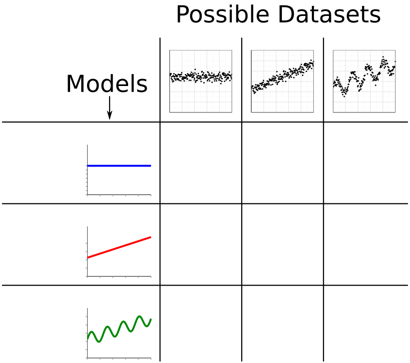
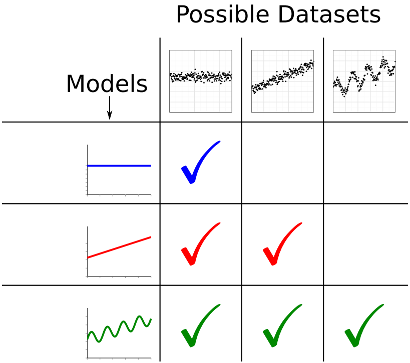
Occam's razor in action



- Some models can explain more datasets

Occam's razor in action



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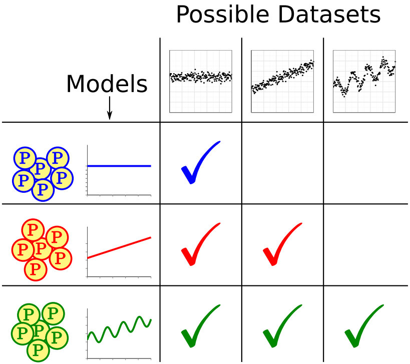

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  - Same total **probability** to **distribute**

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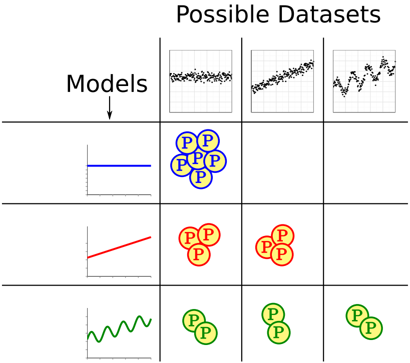

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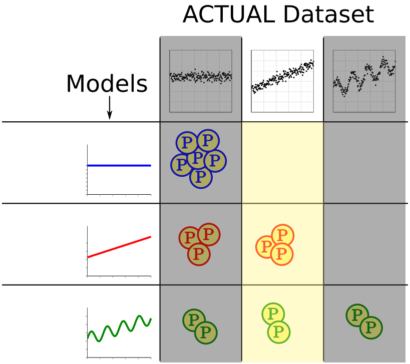

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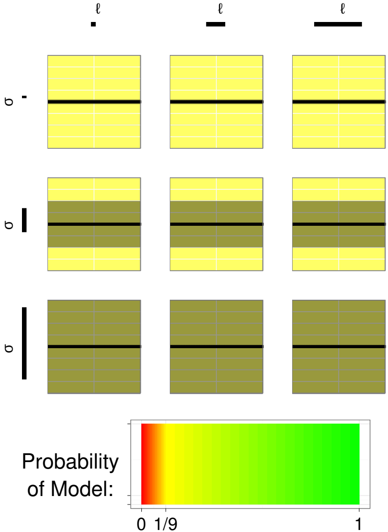
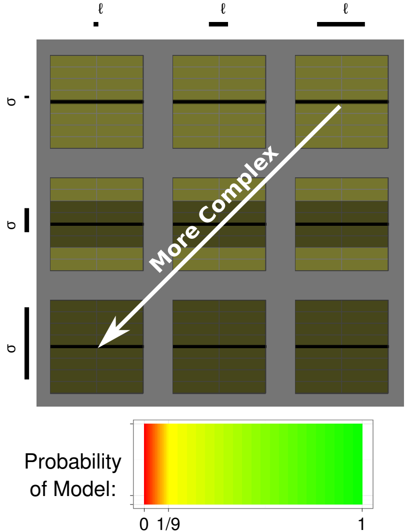
- Which data *actually observed?*

Occam's razor and Gaussian Processes



- 9 models, varying complexity

Occam's razor and Gaussian Processes



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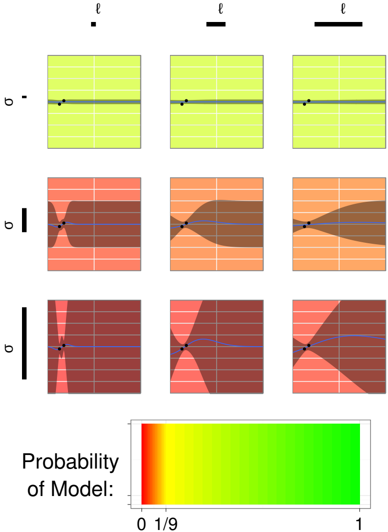

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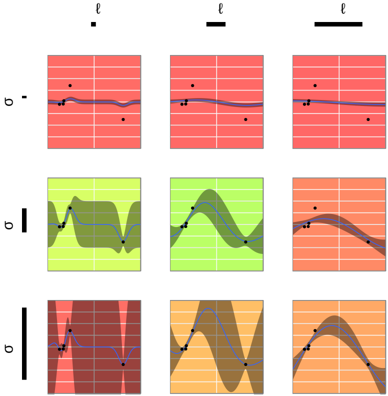

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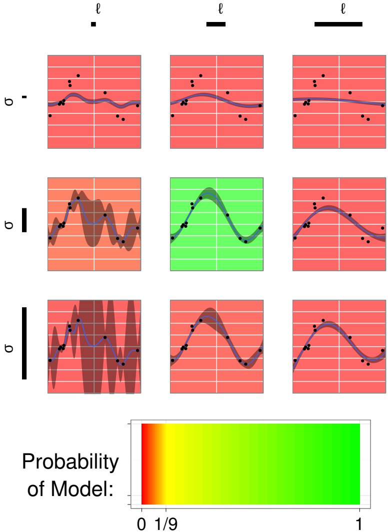

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  - Three tiers
    1. Fit too poor
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    3. Just right

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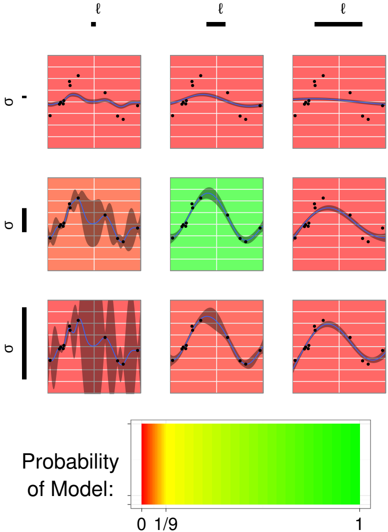

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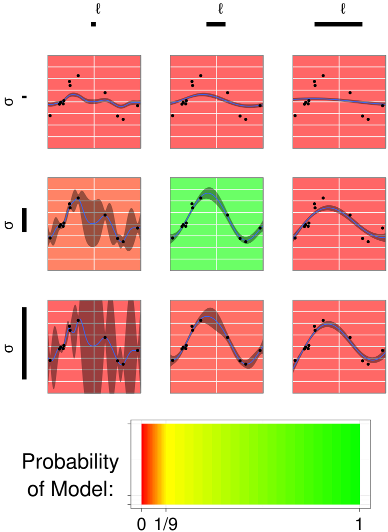

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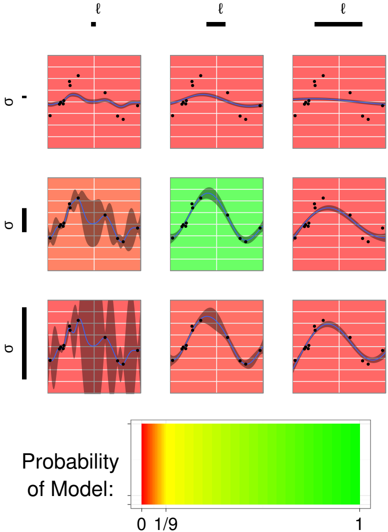

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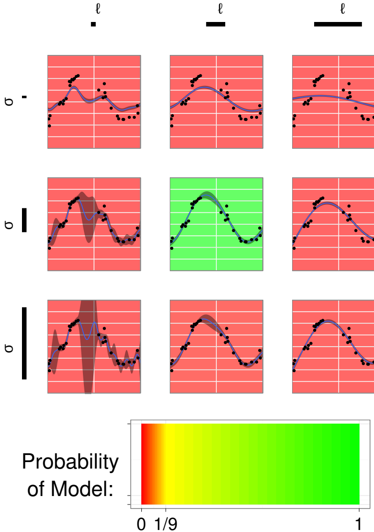

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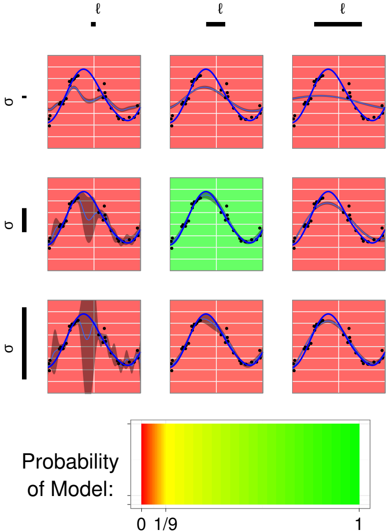

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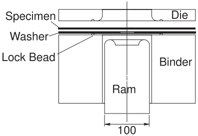
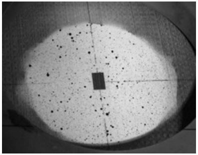
Example 2: Metal Strain

(Adam Creuziger and Mark Iadicola, NIST, Div. 655)





(Figures courtesy of Mark Iadicola)

- Testing stress/strain of steels (auto parts, etc.)
- Clamp flat plate; push upwards on middle
- Measure:
  1. **Stress:** X-ray diffraction
  2. **Strain:** Digital imaging of spray-paint pattern

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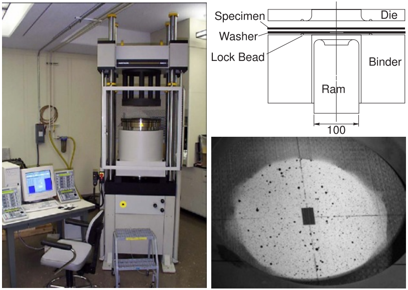

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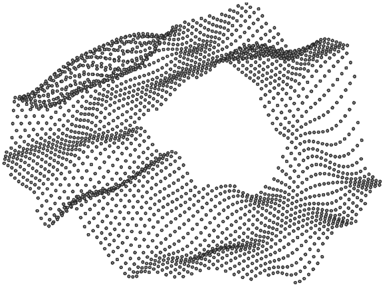
- Clamp flat plate; push upwards on middle
- Measure:
  1. **Stress:** X-ray diffraction
  2. **Strain:** Digital imaging of spray-paint pattern
     - Can't paint everywhere!

Metal Strain: Preliminary Results



- Spheres represent datapoints

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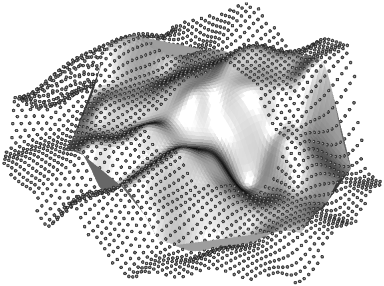

- Spheres represent datapoints
- Continuous surface

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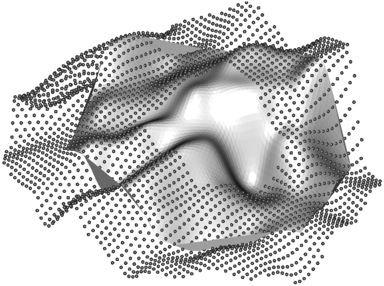

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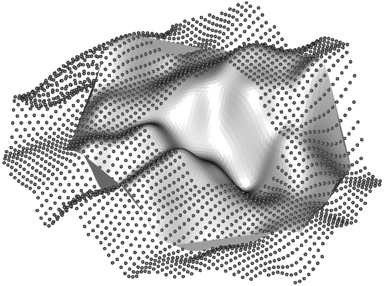

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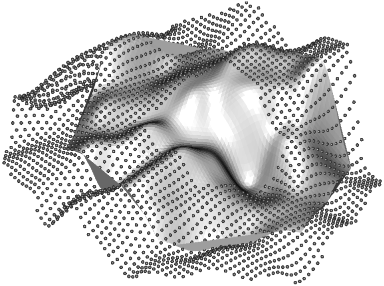

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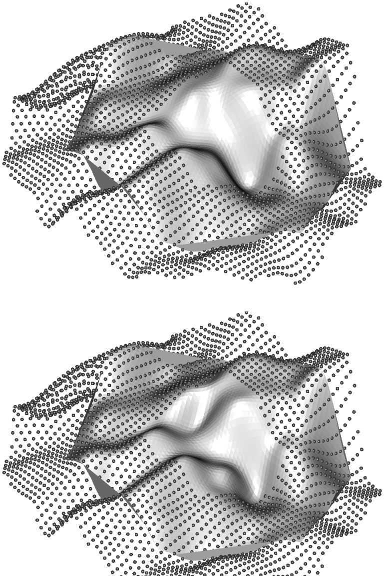

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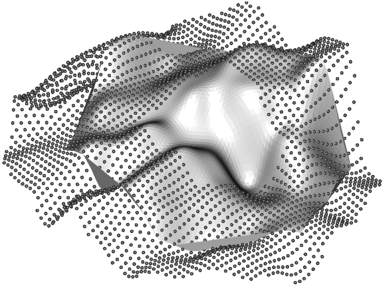

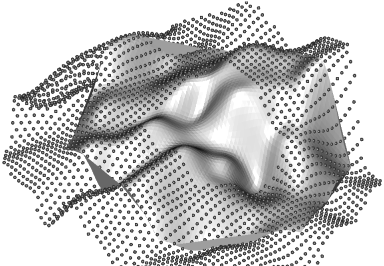

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  - $\Delta \log(\mathrm{ML}) = +183.4$

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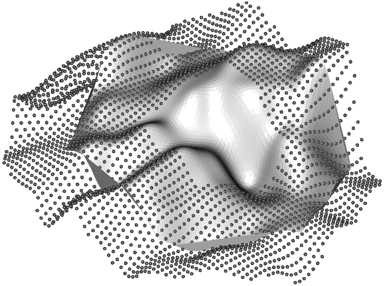

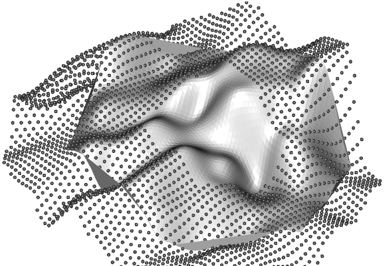

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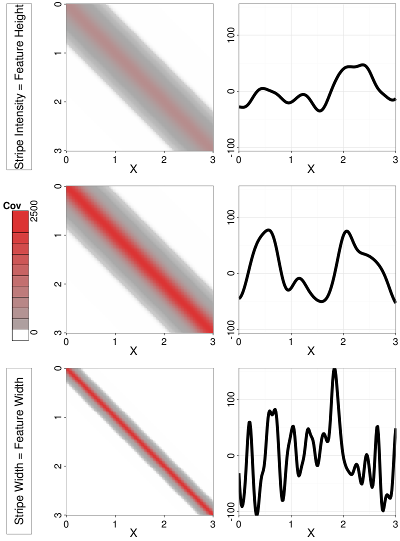
- Suggestions for experimental design

Need to extend the model



- Recall: how to read covariance matrices "as a whole"
    - **Intensity:** *height* of features
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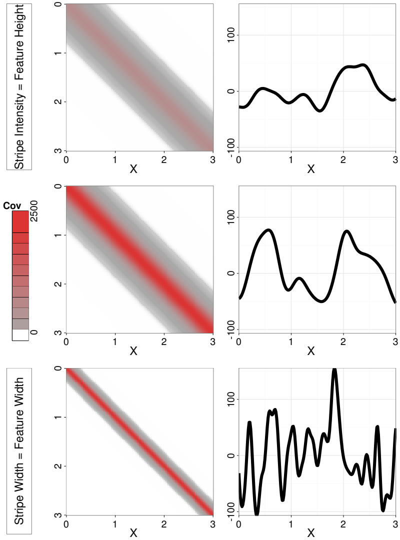
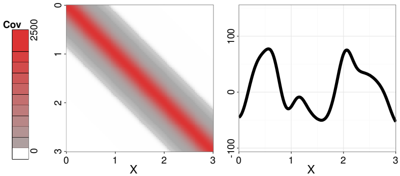


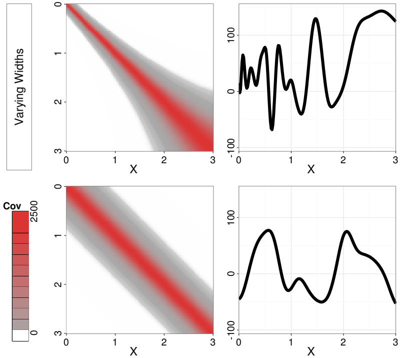
- Recall: how to read covariance matrices "as a whole"
  - **Intensity:** *height* of features
  - **Width:** *width* of features
- ***Not*** *flexible enough for* ***real*** *data!*

Two extensions



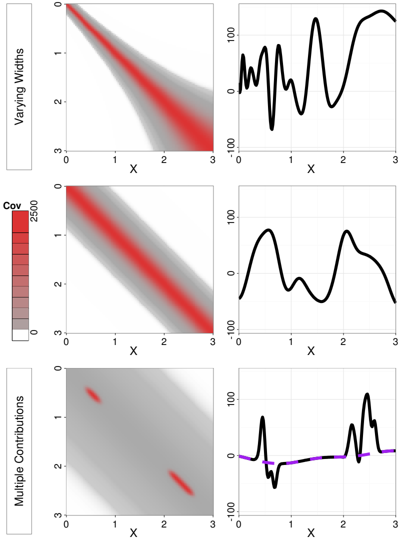
- Two main extensions. . .

Two extensions



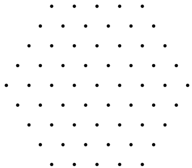
- Two main extensions. . .
  1. Varying Feature widths
     - $\ell \to \ell(X)$

Two extensions



- Two main extensions…
  1. Varying Feature widths
     - $\ell \to \ell(X)$
  2. Multiple contributions
     - Background everywhere
     - *Localized* "peak" regions

Simulated XRD from 2 nm Au nanoparticles



- Core/shell structure
  - Shell atoms vibrate more
  - *Correlated* thermal motion (Signature: hi-Q oscillations)

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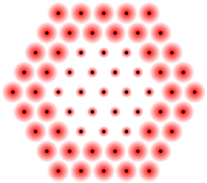

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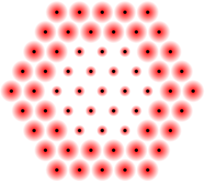

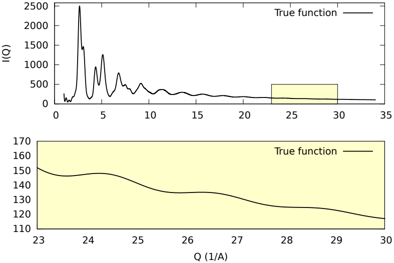

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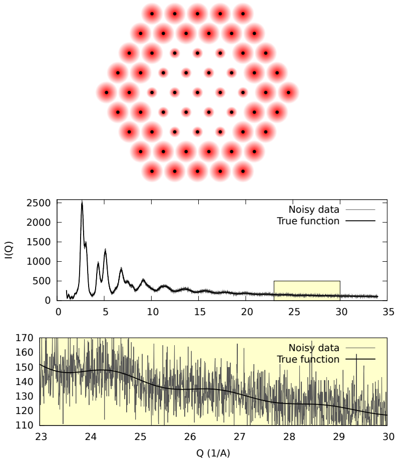

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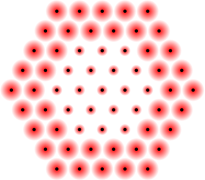

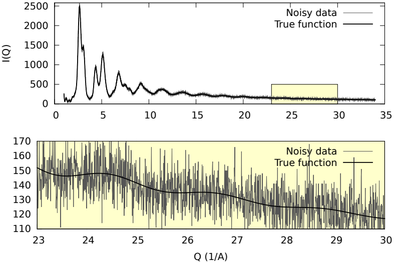

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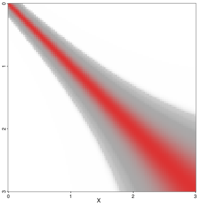
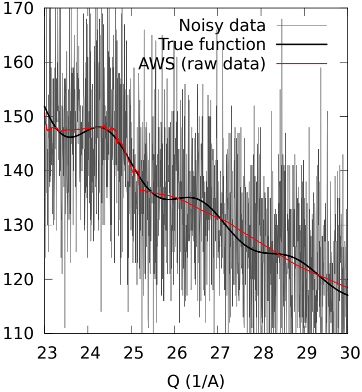
  - Shell atoms vibrate more
  - *Correlated* thermal motion (Signature: hi-Q oscillations)
- Problem: Poisson noise swamps these oscillations!
- Changing feature widths: use $\ell(Q)$



Denoising results



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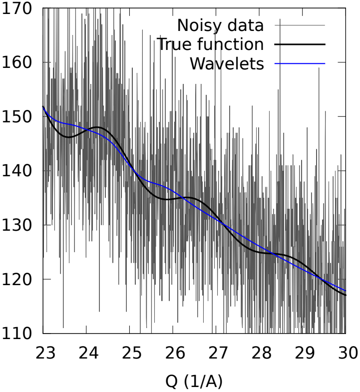

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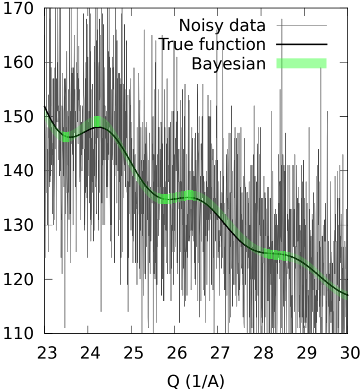

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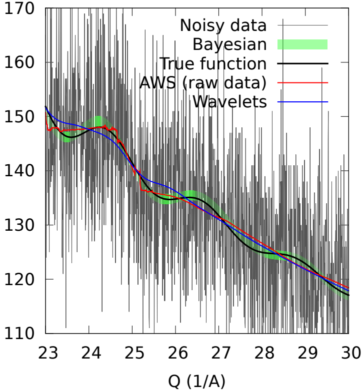

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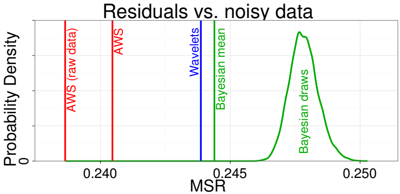
Residuals

- Need: global fidelity measure

Residuals



- Need: global fidelity measure
- Mean square residuals . . .
  1. vs. *noisy data*
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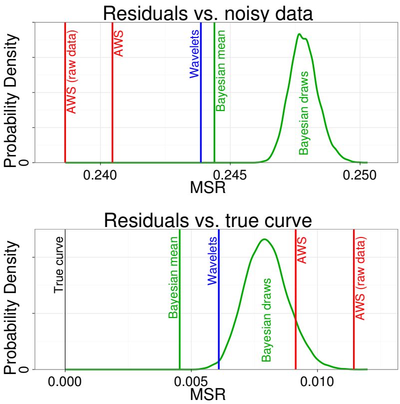
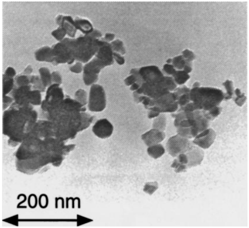
Residuals



- Need: global fidelity measure
- Mean square residuals . . .
  1. vs. *noisy data*
     - AWS looks best
  2. vs. *true curve*
     - Bayes is best
     - AWS “good” score: was overfitting noise!

TiO_2 nanoparticles

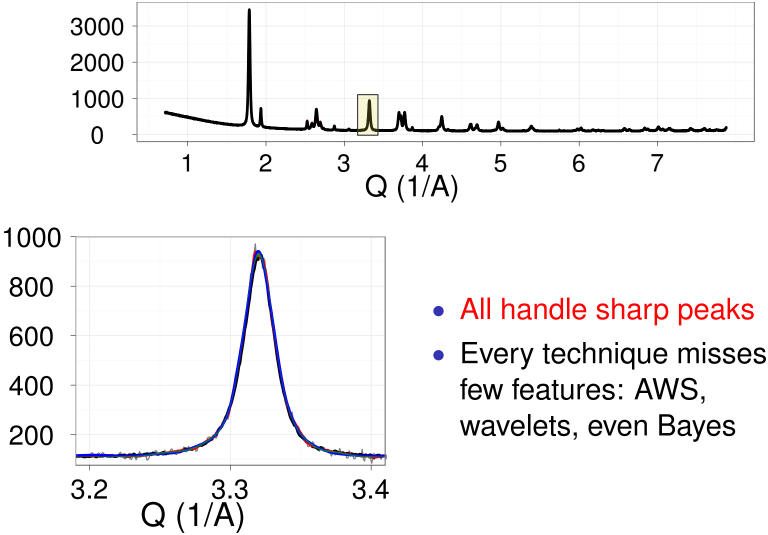
NIST SRM 1898:



(Ohno et al., *J. Catalysis*, 2011)

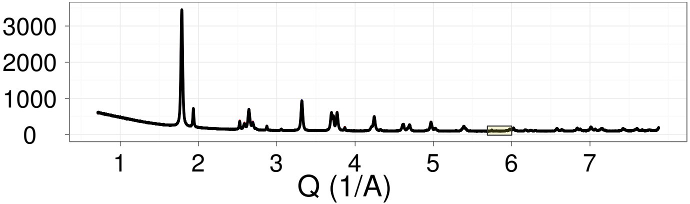
- X-ray powder diffraction from 20 nm TiO_2 nanoparticles
- Motivations:
  1. **Real-world** example (Violates our assumptions)
  2. **More difficult** data (contains feature-free background regions)

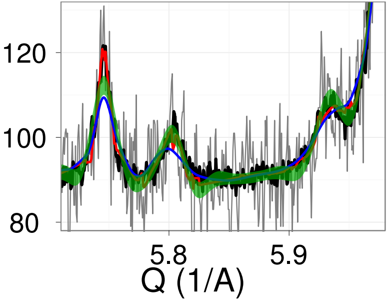
Comparing the fits



- All handle sharp peaks
- Every technique misses a few features: AWS, wavelets, even Bayes

Comparing the fits





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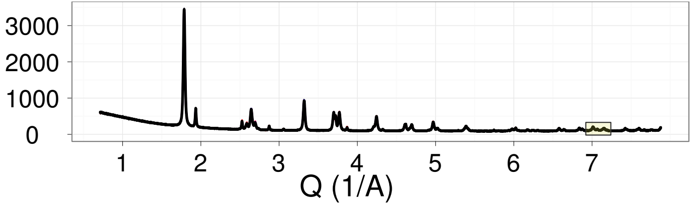

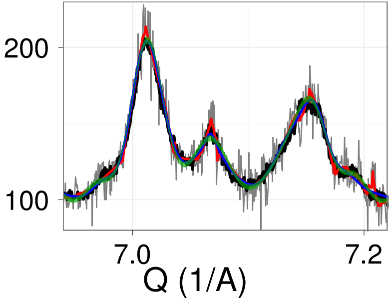

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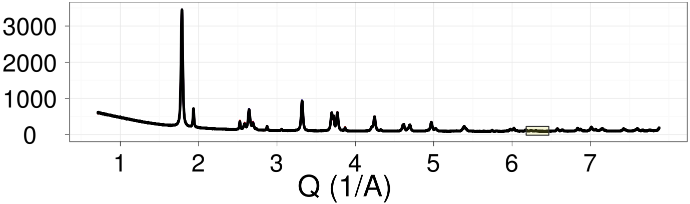

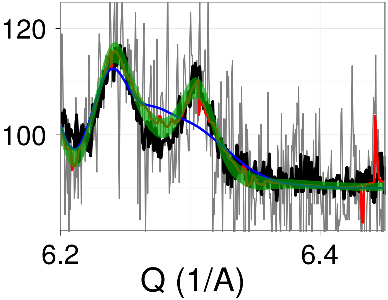

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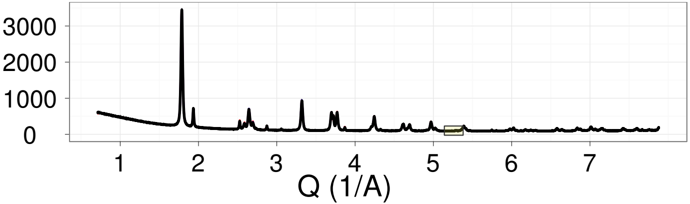

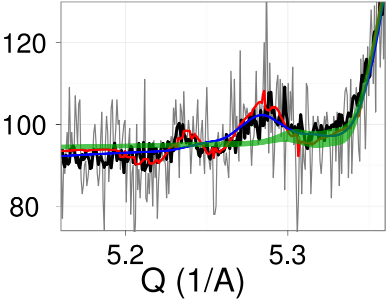

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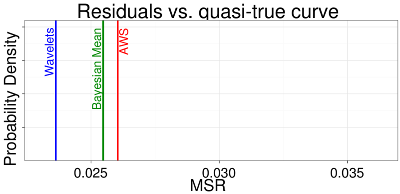

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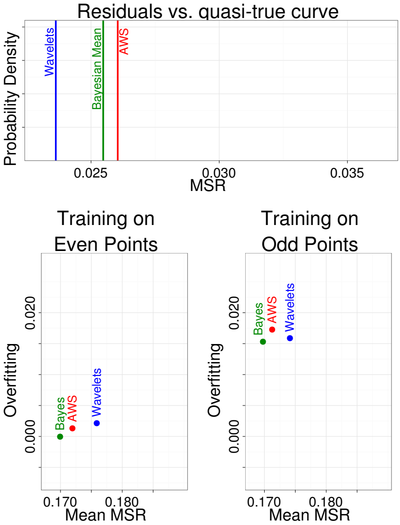
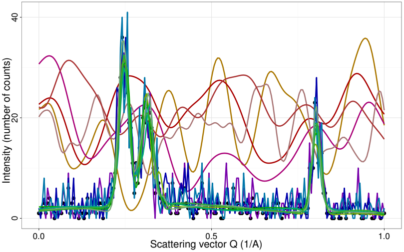
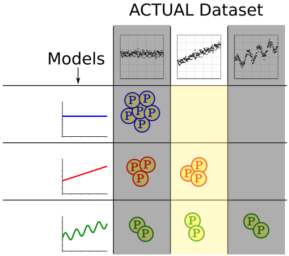
Residuals



- Bayes single-curve comparable to benchmarks
- Cross-validation: (Checking for overfitting) *Bayes is best...*
  1. In *both* categories
  2. For *both* training sets

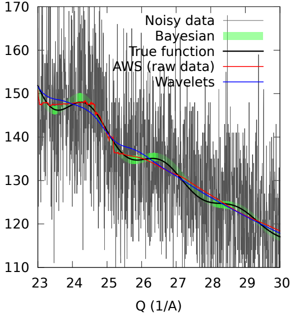
Recap: Bayesian Concepts

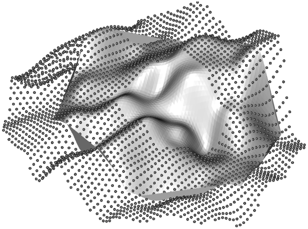




- <u>**Bayesian analysis**</u>: using **probabilities** to describe **uncertainty**
  - choose answers with both **plausibility** and **data fit**
  - a natural framework for **model selection** concepts (Occam's razor)

Recap: Uncertainty in continuous functions





- Gaussian Processes: can stipulate smoothness, without worrying about functional form
- Open-source software package
- Very flexible: can help a variety of projects

Acknowledgements

- **Team members**: Igor Levin, Kate Mullen
- **Collaborators**:
  - *Flame speed*: Dave Sheen, Wing Tsang
  - *Metal Strain*: Adam Creuziger, Mark Iadicola
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- **Statistical guidance**: Antonio Possolo, Blaza Toman