Statistical model criticism using kernel two sample tests

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- …but reality typically breaks these assumptions…
  - 'A man in daily muddy contact with field experiments could not be expected to have much faith in any direct assumption of independently distributed normal errors' [Box76]
- …and this can lead us to produce false inferences
  - 'We were seeing things that were 25-standard deviation moves, several days in a row'

EXAMPLE: LINEAR REGRESSION

```
Call:
lm(formula = y ~ x)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
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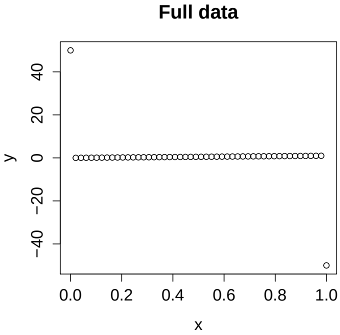

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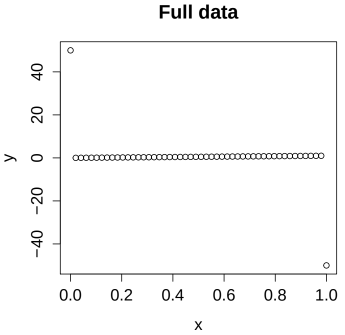
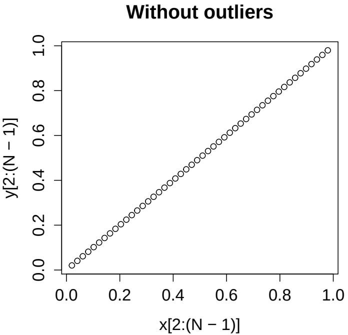
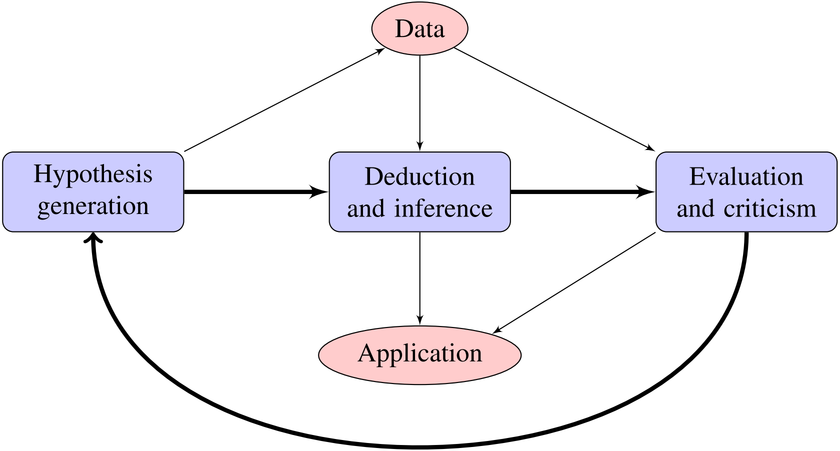
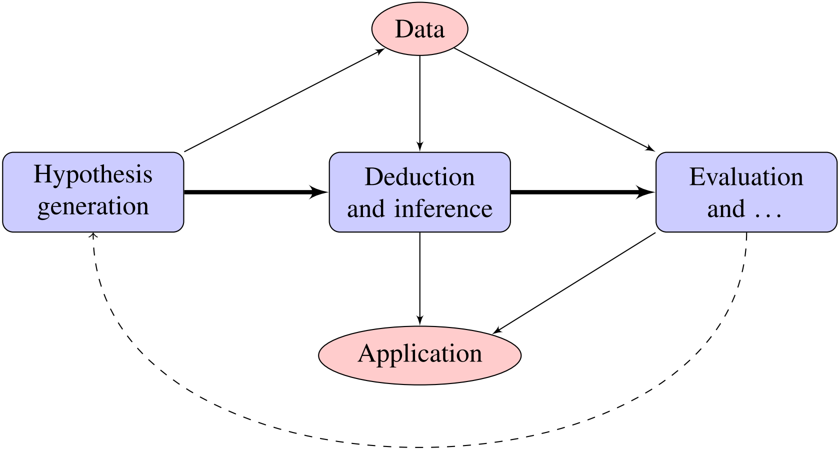




A version of the scientific method



MANY ML PAPERS STOP AT EVALUATION



AGENDA

- Why I became interested in model criticism
- Review of frequentist and Bayesian theory
- A concern about calibration and a potential resolution
- An application of a nonparametric test to model criticism
- Discussion

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- I wanted these model building systems to know when they had produced a model which was 'obviously' wrong
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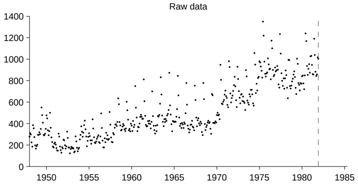
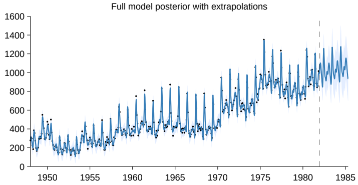
- …and generally very little actionable advice on which method of model criticism to use and when

IS THIS MODEL ‘CORRECT’?





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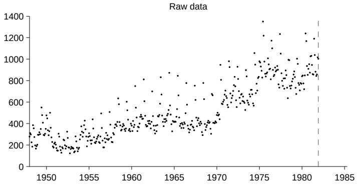

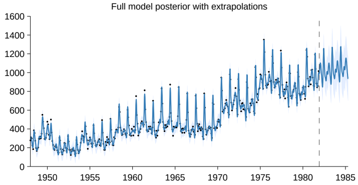

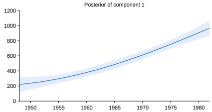

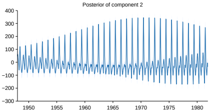

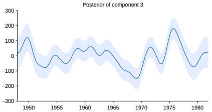

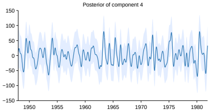

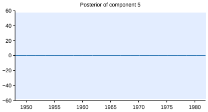

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- A frequentist p-value is a random variable which has a uniform $[0, 1]$ distribution under the null hypothesis

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- When θ is unknown a typical approach is to choose T such that its distribution is independent of θ
  - These are called pivotal quantites
  - Studentised residuals are an example of a pivotal quantity

Maximum likelihood linear regression

- Assume that outputs y are linearly related to inputs X plus independent Gaussian errors or noise ε
  - $y = X\beta + \varepsilon$
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- Many assumptions to be tested before we believe these solutions
  - e.g. X non-random, linearity, constant variance, Gaussianity, independent errors

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- These are the studentised residuals
  - They are pivotal quantities since their distribution does not depend on β or σ.

BAYESIAN MODEL CRITICISM

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- A more relevant null hypothesis for a Bayesian is that the data was generated from the prior predictive distribution
  - Prior predictive just means the prior over data (as opposed to parameters)

- We could therefore compute prior predictive p-values
  - $p_{\text{prior}}(x_{\text{obs}}) = \mathbb{P}_{f(x \mid \theta)\pi(\theta)}(T(X) > T(x_{\text{obs}}))$
  - [Box80]

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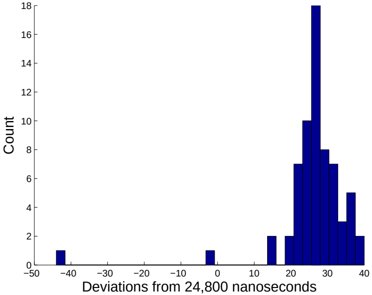
- Vague priors can lead to vague tests
  - Probably best used when one really has a subjective prior or the model is not vague about the test statistic

EXAMPLE: SPEED OF LIGHT DATA



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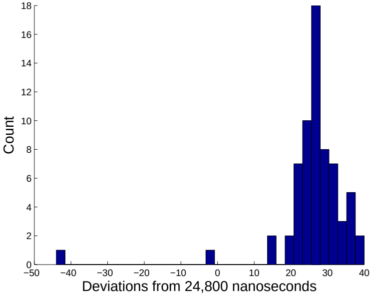

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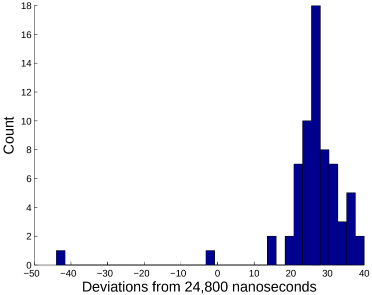

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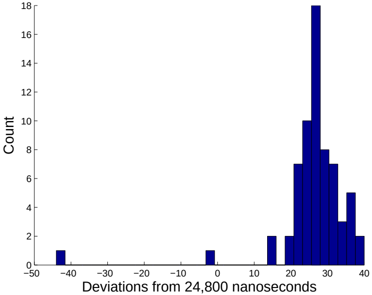

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  - Skewness = -4.5; *p*-value = tiny

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- One may be concerned about using the data twice
  - The common retort is that the posterior predictive p-value is a well defined subjective probability statement and should be interpreted as such

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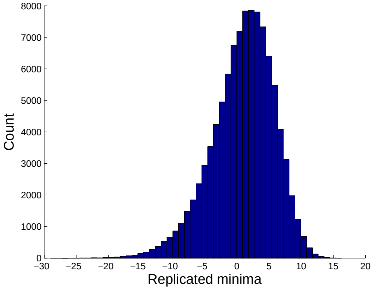

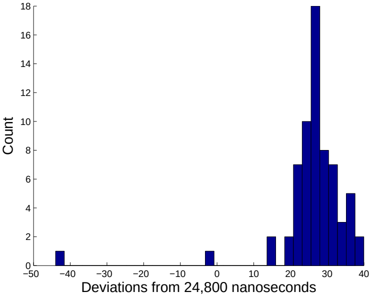

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A problem of calibration

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- Alternatives were proposed by [BB99] and were shown to be asymptotically frequentist p-values by [RvdVV00]
- But maybe this isn't a problem — perhaps we are confusing the use of the word 'model'
  - *"If our goal is to check the model $f(x;\theta)$ rather than the prior $\pi(\theta)$, our procedures should perform adequately whatever the prior, including point-mass priors"* — James Robins discussion of [BB99]

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Different tests for different goals

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- Can also use held out data to test posterior distributions

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- Can we instead define a statistic in high level terms, and then compute the statistic which most demonstrates any discrepancy?
  - And will we be able to interpret this statistic?

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- Substituting and squaring:
  - $\text{MMD}^2(\mathcal{F}, p, q) = \mathbb{E}_{x,x' \sim p}[k(x, x')] + 2\mathbb{E}_{x \sim p, y \sim q}[k(x, y)] + \mathbb{E}_{y,y' \sim q}[k(y, y')]$

EMPIRICAL ESTIMATION

- We can estimate these expectations from finite samples
  - $\mathrm{MMD}_b^2(\mathcal{F}, X, Y) = \frac{1}{m^2}\sum_{i,j=1}^{m} k(x_i, x_j) - \frac{2}{mn}\sum_{i,j=1}^{m,n} k(x_i, y_j) + \frac{1}{n^2}\sum_{i,j=1}^{n} k(y_i, y_j)$
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  - $\hat{f}(x) = \frac{1}{m}\sum_{i=1}^{m} k(x, x_i) - \frac{1}{n}\sum_{i=1}^{n} k(x, y_i)$
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- We can estimate the null distribution of the MMD statistic by a bootstrap procedure
  - It is an example of a permutation test

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Application to model checking

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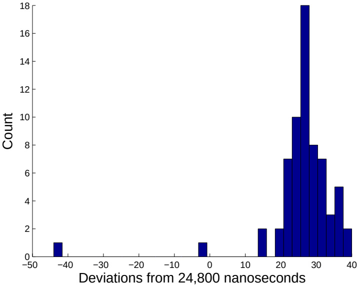
  - Data y are generated $i.i.d.$ from some distribution q
  - We make a point estimate of q which we denote p
- The hypothesis that $p = q$ is now the hypothesis that the model is correct
- We can generate samples from p and then perform a two sample test

EXAMPLE: SPEED OF LIGHT DATA AGAIN (AGAIN)



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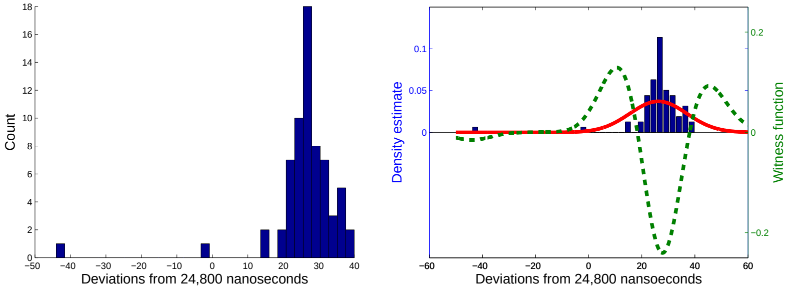

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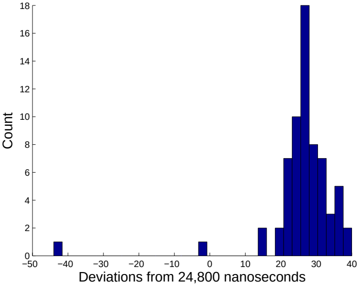

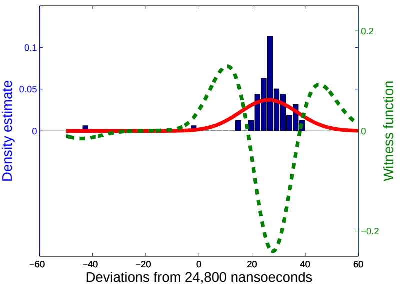

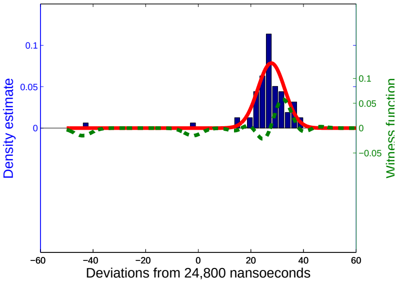

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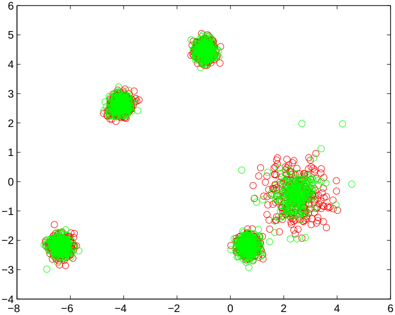
- Interpretability of test comes from interpretation of witness function as difference of kernel density estimates
- Kernel density estimation is high variance in high dimensions and will likely be uninterpretable
- Potential solution: Include dimensionality reduction as part of the test statistic
  - $\frac{1}{m^2}\sum_{i,j=1}^{m} k(x_i^{\text{PCA}}, x_j^{\text{PCA}}) - \frac{2}{mn}\sum_{i,j=1}^{m,n} k(x_i^{\text{PCA}}, y_j^{\text{PCA}}) + \frac{1}{n^2}\sum_{i,j=1}^{n} k(y_i^{\text{PCA}}, y_j^{\text{PCA}})$

WHAT HAPPENS IN HIGH DIMENSIONS?



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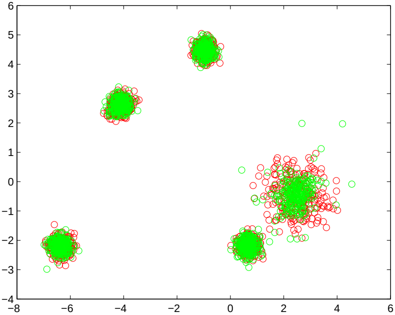

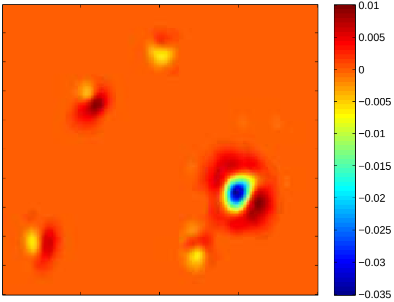

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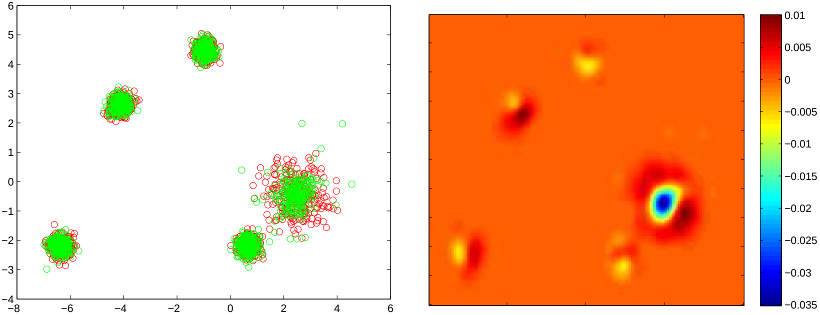


- Estimated p-value of 0.05

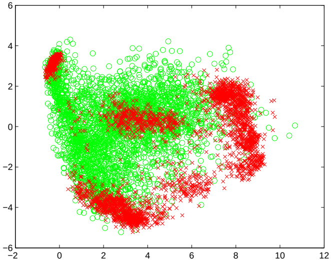
WHAT DO NEURAL NETWORKS DREAM ABOUT?

- Various versions of deep belief networks have been trained to produce generative models of MNIST handwritten digits

What do neural networks dream about?

- Various versions of deep belief networks have been trained to produce generative models of MNIST handwritten digits
- Samples from these models certainly look like digits, but what aspects of the distribution over handwritten digits do these models not capture?

AN RBM TRAINED ON MNIST



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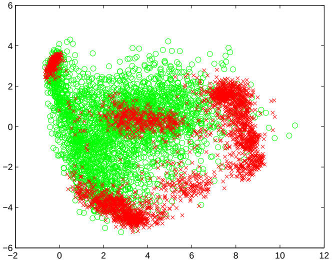

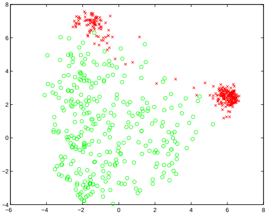

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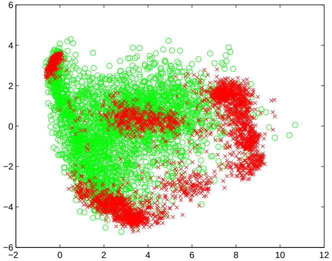
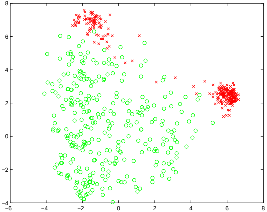
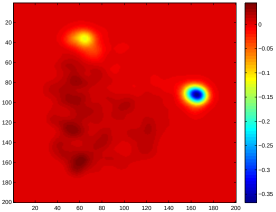
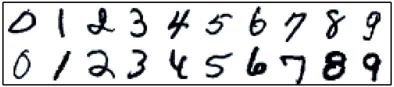






What do neural networks dream about?

Real digits



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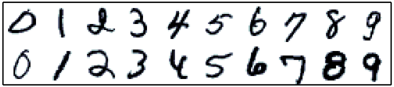
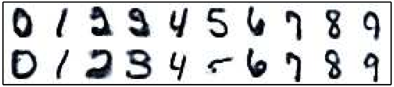


Witness fn troughs : RBM



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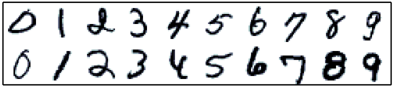

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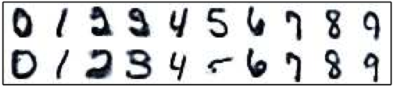

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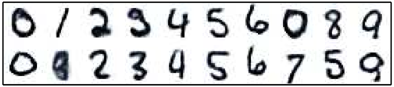

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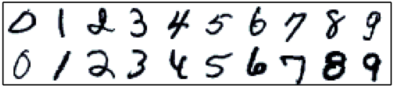

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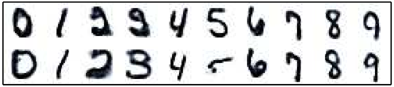

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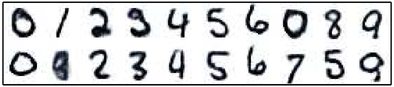
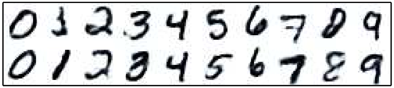


Witness fn troughs : DBN



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Why have I not mentioned power?

- Quantification of power requires specification of an explicit alternative model or hypothesis
- "Model criticism ... is intended as an open-minded phase of investigation to identify any problems with the model. Formulation of explicit alternatives comes after the model criticism phase has identified some problems." [O'H03]
- I'm not sure anymore that alternative free hypothesis tests are the correct way to think about model criticism
  - Some effort should be made to characterise the alternative hypotheses for which certain tests have high power

FUTURE WORK

- Can we usefully characterise the types of alternative models for which MMD tests have high power?

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- Can we usefully characterise the types of alternative models for which MMD tests have high power?
  - Using different kernels will identify different types of discrepancy
  - This characterisation probably already in the literature
- Could these alternatives be usefully understood as specific nonparametric models by exploiting the connections between RKHSs and Gaussian processes?

DISCUSSION

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  - Probabilistic version of falsification

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- Box advocated for model criticism to be part of the loop of the scientific process…
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- …but should we just be estimating the utility of a model?
- Perhaps we should be using model criticism to estimate the utility of expanding a model?
  - They are often much cheaper to compute (thinking and computing time) than performing inference in an expanded model class
- What are other forms of model criticism that are widely applicable and can help identify the nature of discrepancies between model and data in highly complicated systems

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Appendix

Is cross validation enough?

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- So we're fine, right?

IS CROSS VALIDATION ENOUGH?

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- So outliers again?

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5 nearest neighbours	0.1 (0.01)

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- When I said outliers I actually meant non-linearity

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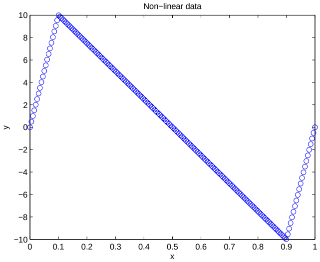

Is being Bayesian enough?

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Is being Bayesian enough?

- Why not just do all inference in a super model that contains everything we could ever possibly believe?
  - And then e.g. estimate the utility of smaller models for certain tasks
- How long did you spend coding your last inference scheme?
  - Or have you ever got probabilistic programming to work in a non-trivial model?
- Model criticism / checking gives us tools to explore potential inadequacies of a method…
  - …without having to implement inference for every expanded method we can think of

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DISCREPANCY p-VALUES

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- $p_{\text{dis}}(x_{\text{obs}}) = \mathbb{P}(d(X, \theta) \geq d(x_{\text{obs}}, \theta) \,|\, x_{\text{obs}})$

- Can be estimated using samples of the joint posterior distribution of (X, θ) e.g. from MCMC

Example: Forecasting U.S. elections

- Copied without permission from Gelman, A. et al. Bayesian Data Analysis, Third Edition. (Taylor & Francis, 2013)

- Fitting a linear model to proportion of votes for Democrats by state for 11 presidential elections

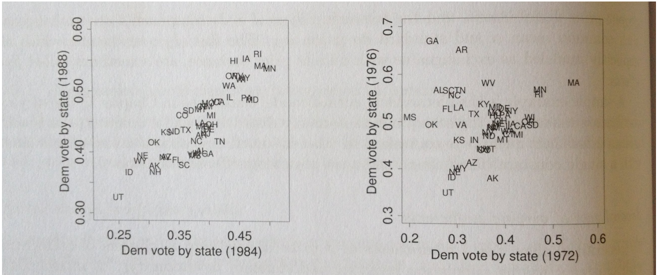

Figure 15.1 *(a) Democratic share of the two-party vote for president, for each state, in 1984 and 1988. (b) Democratic share of the two-party vote for president, for each state, in 1972 and 1976.*

EXAMPLE: FORECASTING U.S. ELECTIONS

Description of variable	Sample quantiles min	median	max
Nationwide variables:			
Support for Dem. candidate in Sept. poll	0.37	0.46	0.69
(Presidential approval in July poll) × Inc	−0.69	−0.47	0.74
(Presidential approval in July poll) × Presinc	−0.69	0	0.74
(2nd quarter GNP growth) × Inc	−0.024	−0.005	0.018
Statewide variables:			
Dem. share of state vote in last election	−0.23	−0.02	0.41
Dem. share of state vote two elections ago	−0.48	−0.02	0.41
Home states of presidential candidates	−1	0	1
Home states of vice-presidential candidates	−1	0	1
Democratic majority in the state legislature	−0.49	0.07	0.50
(State economic growth in past year) × Inc	−0.22	−0.00	0.26
Measure of state ideology	−0.78	−0.02	0.69
Ideological compatibility with candidates	−0.32	−0.05	0.32
Proportion Catholic in 1960 (compared to U.S. avg.)	−0.21	0	0.38
Regional/subregional variables:			
South	0	0	1
(South in 1964) × (−1)	−1	0	0
(Deep South in 1964) × (−1)	−1	0	0
New England in 1964	0	0	1
North Central in 1972	0	0	1
(West in 1976) × (−1)	−1	0	0

Example: Forecasting U.S. elections

- Linear model assumes that each (input, output) tuple is exchangeable

EXAMPLE: FORECASTING U.S. ELECTIONS

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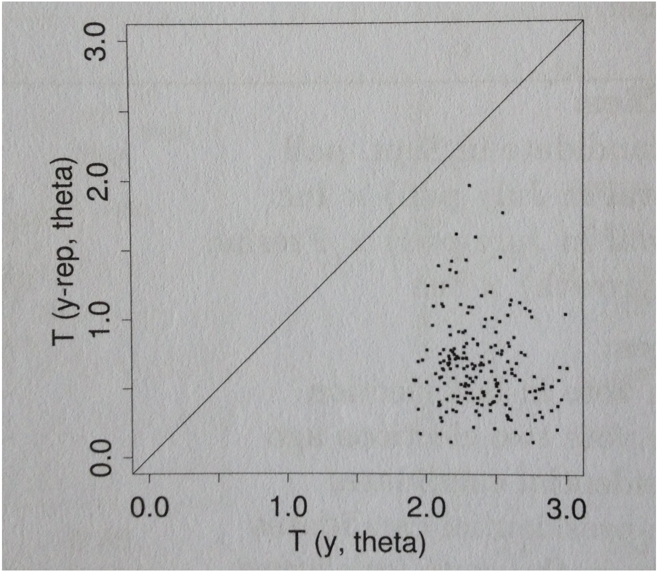
Example: Forecasting U.S. elections

- Linear model assumes that each (input, output) tuple is exchangeable
- This ignores any correlation between states in a particular year due to nationwide swings in voting
- We can construct a test staistic that can test for this correlation
  - For each year compute the average error of the prediction in each state
  - Compute the root mean square of these averageerrors over the 11 years

EXAMPLE: FORECASTING U.S. ELECTIONS



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EXAMPLE: FORECASTING U.S. ELECTIONS

- The posterior distribution underestimates the test statistic
- The practical consequence of this is that the model will give overly precise predictions of national election results
- The model can be improved by adding indicator variables for each year
  - Can also include year $\times$ region features to capture regional voting swings

Model criticism for Gaussian processes

- Suppose that $y_i \sim f(x_i) + \varepsilon_i$ where
  - $f \sim \mathcal{GP}(0, k)$
  - $\varepsilon \sim_{\text{iid}} \mathcal{N}(0, \sigma^2)$

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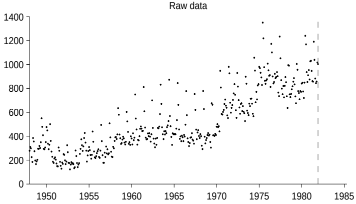
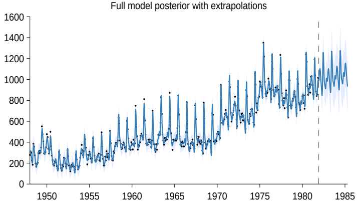
- Similarly, we could construct discrepancies based on $y_i - \varepsilon_i$
  - This amounts to comparing the prior and posterior of f

Example: Is this model 'correct'?





- A very smooth monotonically increasing function.
- An approximately periodic function with a period of 1.0 years.
- A smooth function.
- A smooth function.
- Uncorrelated noise.

DIFFERENT STATISTICS FOR EACH COMPONENT

- p-values of several statistics for each model component
- Mea culpa these p-values are unadjusted for multiple comparisons, but they are also uncalibrated (they are conservative)

	ACF		Periodogram		QQ	
#	min	min loc	max	max loc	max	min
1	0.502	0.582	0.341	0.413	0.341	0.679
2	0.802	0.199	0.558	0.630	0.049	0.785
3	0.251	0.475	0.799	0.447	0.534	0.769
4	0.527	0.503	0.504	0.481	0.430	0.616
5	0.493	0.477	0.503	0.487	0.518	0.381

Example: Identifying outliers

The following discrepancies between the prior and posterior distributions for this component have been detected.

- The qq plot has an unexpectedly large positive deviation from equality ($x = y$). This discrepancy has an estimated p-value of 0.049.