COMP 551 - Applied Machine Learning Lecture 22 — Bayesian inference

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(with slides and content from Joelle Pineau and Herke van Hoof)

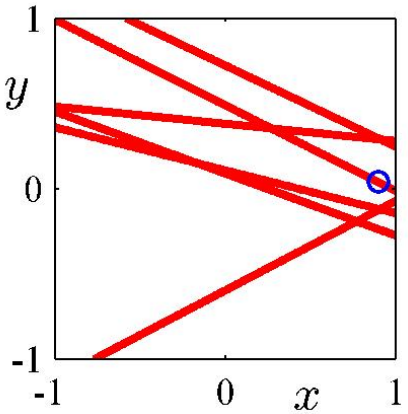
Bayesian probabilities

- An example from regression
- Given few noisy data points, multiple parameter values are possible
- Can we quantify uncertainty over our parameters using probabilities?

- I.e. given a dataset: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

  and some model with weights w, can we find:

$$p(\mathbf{w}|\mathcal{D})$$



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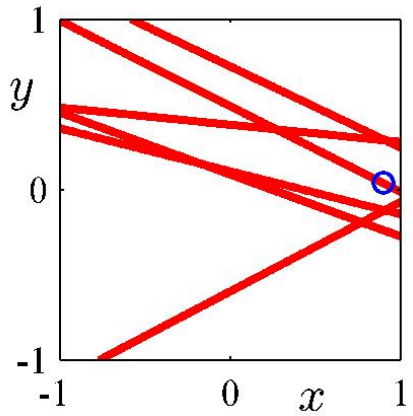
Bayesian probabilities

- Yes we can!!
- **Bayesian view:** probability represents *uncertainty about some value or variable*
- We use Bayesian probabilities to represent uncertainty about the *parameters of our model*



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Bayesian probabilities

- To calculate uncertainty, need to **specify a model**. Two ingredients:
  1. Prior over model parameters: $p(\mathbf{w})$
  2. Likelihood term: $p(\mathcal{D}|\mathbf{w})$

- We are given a dataset:

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$$

- Want to do **inference** using Bayes' theorem:

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

Bayesian terminology

$p(\mathcal{D}|\mathbf{w})$

- Likelihood: our model of the data. Given our weights, how do we assign probabilities to dataset examples?

$p(\mathbf{w})$

- Prior: before we see any data, what do we think about our parameters?

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

- Posterior: our distribution over weights, given the data we've observed and our prior

$p(\mathcal{D})$

- Marginal likelihood: also called the normalization constant. Does not depend on w, so not usually calculated explicitly

Bayesian probabilities

- How do we make predictions if we have a distribution over parameters?

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int_{\mathbb{R}} p(y^*, \mathbf{w}|\mathbf{x}^*, \mathcal{D}) d\mathbf{w}$$

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D}) p(y^*|\mathbf{x}^*, \mathbf{w}) d\mathbf{w}$$

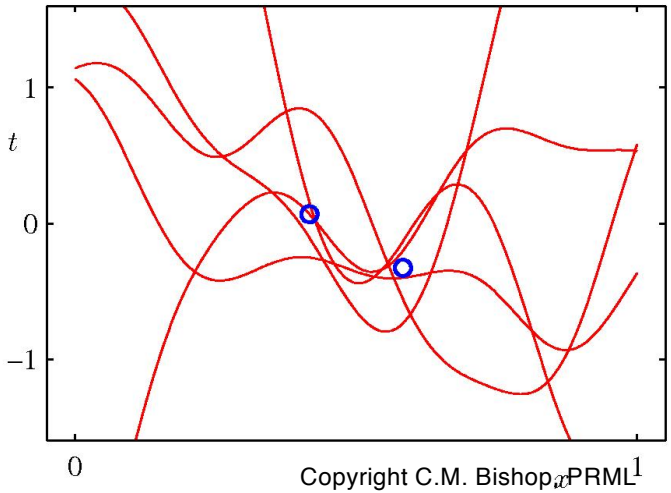
Posterior predictive distribution

- Rather than using a fixed value for parameters, integrate over all possible parameter values!
- (Integration is annoying, we will try to avoid this when possible)

Why Bayesian probabilities?

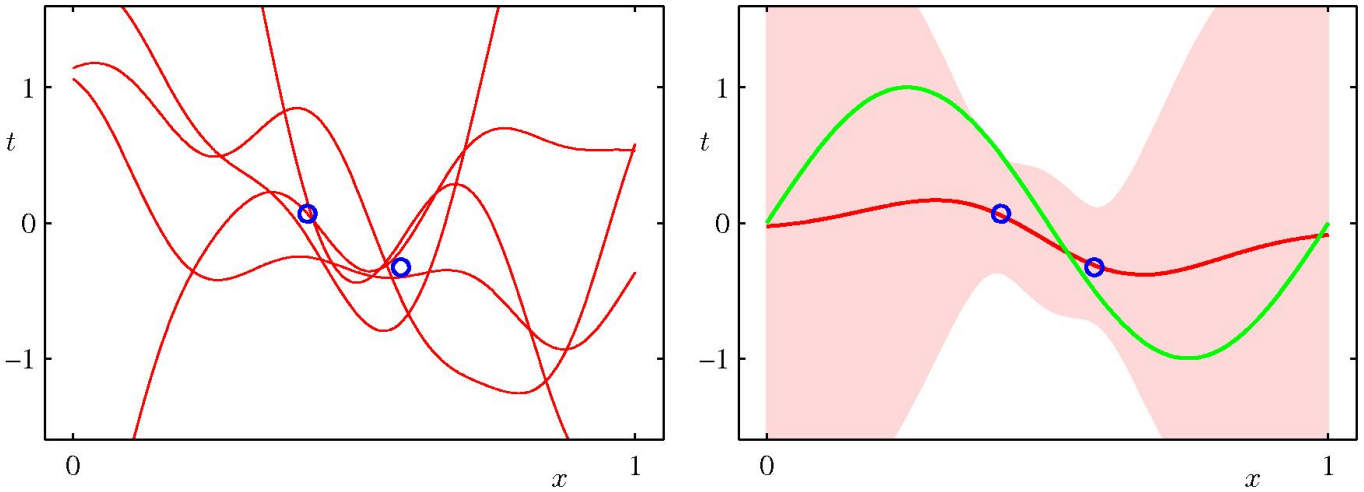
- Maximum likelihood estimates can have **large variance**
- We might desire or need an estimate of uncertainty
- Have small dataset, unreliable data, or small batches of data
- Use prior knowledge in a principled fashion

Why do we need uncertainty?



- Regression with (extremely) small and noisy dataset
- Many functions are compatible with data

Why do we need uncertainty?



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- Quantify the uncertainty using probabilities (e.g. Gaussian mean and variance for every input $\mathbf{x}$)

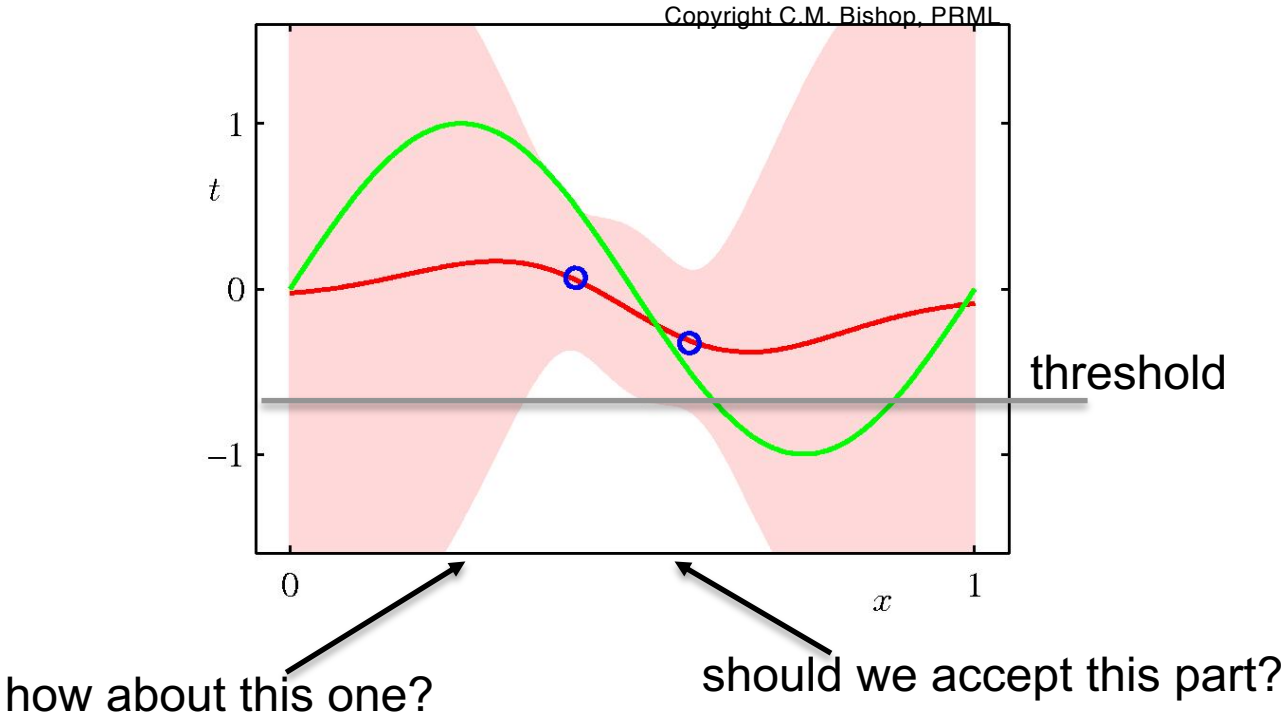
Why do we need uncertainty?

- Knowing uncertainty of output is *helpful in decision making*

- Consider inspecting task.
  - $\mathbf{x}$: some measurement
  - y: predicted breaking strength

- Parts which are too weak (breaking strength < t) are rejected
  - Falsely rejecting a part incurs a small cost (*c=1*)
  - Falsely accepting a part can cause more damage down the line (expected cost *c=100*)

Decision making under uncertainty



Algorithms for Bayesian inference

- Given a dataset $\mathcal{D}$, how do we make predictions for a new input?

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$$

Algorithms for Bayesian inference

- Given a dataset $\mathcal{D}$, how do we make predictions for a new input?

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- Step 1: Define a model that represents your data (the **likelihood**): $p(\mathcal{D}|\mathbf{w})$
- Step 2: Define a **prior** over model parameters: $p(\mathbf{w})$
- Step 3: Calculate **posterior** using Bayes' rule: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$
- Step 4: Make **prediction** by integrating over model parameters:

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D})p(y^*|\mathbf{x}^*, \mathbf{w})d\mathbf{w}$$

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- When can we do step 4) in closed form?

Conjugate priors

- Posterior for some dataset:

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

- Posterior for old data can act like a prior for new data:

$$p(\mathbf{w}|\mathcal{D}_1, \mathcal{D}_2) = \frac{p(\mathcal{D}_2|\mathbf{w})p(\mathbf{w}|\mathcal{D}_1)}{p(\mathcal{D}_2)}$$

- Desirable that posterior and prior have same family!
  - Otherwise posterior would get more complex with each step

- Such priors are called conjugate priors to a likelihood function

Algorithms for Bayesian inference

- Not all likelihood functions have conjugate priors
- However, so-called **exponential family** distributions do
  - Normal
  - Exponential
  - Beta
  - Bernoulli
  - Categorical
  - …

Examples

- We will look into supervised learning problems later
- Start with a simple problem, learning a single parameter with no inputs (i.e. no *x*): **a coin toss**
- Dataset consists of outcomes:

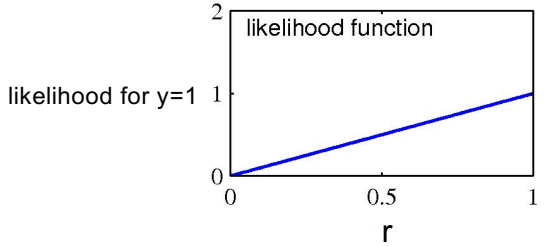
$$D = \{heads, heads, tails, heads, tails, \ldots\}$$

Simple example: coin toss

- Flip (possibly unfair) coin N times — get h heads and t tails
- Probability of 'heads' unknown value r
- How do we calculate the probability of the next flip being 'heads' (i.e., value of r) in a Bayesian way?

Simple example: coin toss

- Step 1: define model (distribution for likelihood) $\text{Bern}(y|r) = r^y(1-r)^{1-y}$
- Likelihood for a single flip:
  - y is one ('heads') or zero ('tails')
  - r is unknown parameter, between 0 and 1



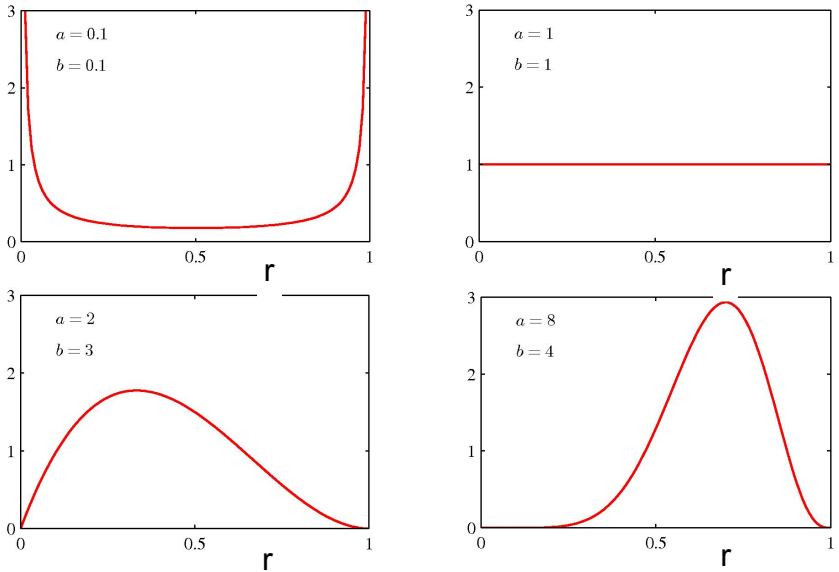
- Likelihood for N flips proportional to Binomial:

$$p(h|r,N) = r^h(1-r)^{N-h} \propto \text{Bin}(h|r,N)$$

Simple example: coin toss

- Step 2: Define (conjugate) prior $p(r)$:

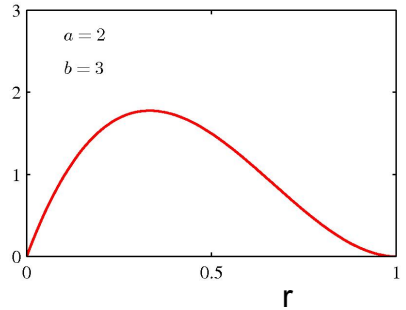
$$\text{Beta}(r|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} r^{a-1}(1-r)^{b-1}$$



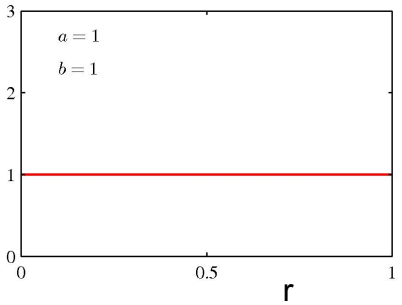
Simple example: coin toss

- Conjugate prior: $$\text{Beta}(r|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} r^{a-1}(1-r)^{b-1}$$

- Prior denotes *a priori* belief over the value r
- r is a value between 0 and 1 (denotes prob. of heads or tails)
- a, b are 'hyperparameters'



coin probably more likely to give 'tails'



no idea about the fairness

Simple example: coin toss

- Side note: why is the Beta distribution the conjugate prior for a Binomial likelihood? ($N = \#flips, h = \#heads$)

$$
\begin{aligned}
p(r|\mathcal{D}) &= p(r|N,h) \\
&= p(h|r,N) \cdot p(r) \\
&= \mathrm{Bin}(h|r,N) \cdot \mathrm{Beta}(r|a,b) \\
&= r^h(1-r)^{N-h} \cdot \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} r^{a-1}(1-r)^{b-1} \\
&= z^{-1} r^{h+a-1}(1-r)^{N-h+b-1} \\
&= \mathrm{Beta}(r|h+a, N-h+b)
\end{aligned}
$$

N, *h* describe dataset completely

posterior = prior x likelihood

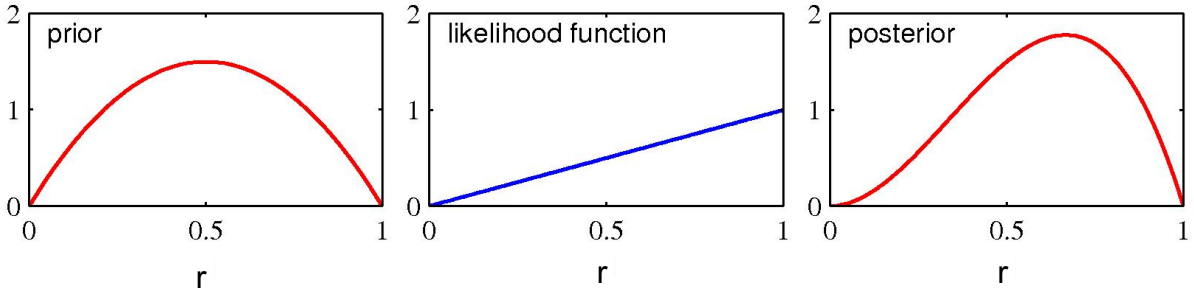
normalization factor

$$z^{-1} = \frac{\Gamma(h+a)\Gamma(N-h+b)}{\Gamma(a+b+N)}$$

Same distribution family (Beta) as prior!!!

Simple example: coin toss

- Posterior: $p(r|\mathcal{D}) = z^{-1} r^{h+a-1}(1-r)^{N-h+b-1}$



- We observe more ‘heads’ -> suspect more strongly coin is biased

- Note that *a, b* get added to the actual outcome: ‘pseudo-observations’

Simple example: coin toss

- Model:
  - Likelihood:
  - Conjugate prior:
  - Posterior:

Simple example: coin toss

- Model:
  - Likelihood: $\text{Bern}(y|r) = r^y(1-r)^{1-y}$
  - Conjugate prior:
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Simple example: coin toss

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$$= z^{-1} r^{h+a-1}(1-r)^{N-h+b-1}$$

Simple example: coin toss

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$$= z^{-1} r^{h+a-1}(1-r)^{N-h+b-1}$$

  - Step 4: Make prediction!

Simple example: coin toss

- Step 4: Make prediction!

likelihood

posterior

$$p(x=1|\mathcal{D}) = \int_0^1 p(x=1|r)p(r|\mathcal{D})dr$$

$$= \int_0^1 r \cdot \text{Beta}(r|h+a, N-h+b)dr$$

$$= \mathbb{E}[\text{Beta}(r|h+a, N-h+b)]$$

mean of the Beta distribution

$$= \frac{h+a}{N+a+b} = \frac{\#\text{heads}+a}{\#\text{heads}+\#\text{tails}+a+b}$$

- Instead of taking one parameter value, average over all of them
- a, b, again interpretable as effective # observations
- Consider the difference if **a=b=1, #heads=1, #tails=0**
- Note that as #flips increases, prior starts to matter less

Takeaways

- Instead of predicting using one parameter value, average over all of them
  - True for all Bayesian models

- Hyperparameters interpretable as effective # observations
  - True for many Bayesian models
    (depends on parametrization)

- As amount of data increases, prior starts to matter less
  - True for all Bayesian models

Example 2: mean of a 1d Gaussian

- Try to learn the **mean** μ of a Gaussian distribution that generated some real number. e.g. $\mathrm{D} = \{0.3427\}$

- Note: still no x, only y
- Model:
  - Step 1: Likelihood $p(y) = \mathcal{N}(\mu, \sigma^2)$
  - Step 2: Conjugate prior $p(\mu) = \mathcal{N}(0, \alpha^{-1})$

- Assume **variances of the distributions are known** (σ, α)
- Prior: we know the mean is close to zero but not its exact value

Example 2: inference for Gaussian

- Calculation is slightly easier to carry out in log space
  - log likelihood: $\text{const} - \frac{1}{2}\frac{(y-\mu)^2}{\sigma^2}$
  - log conjugate prior: $\text{const} - \frac{1}{2}\mu^2\alpha$
- **Step 3:** calculate posterior distribution (in log space) $\log p(\mu|\mathcal{D})$

Inference for Gaussian

Step 3: calculate posterior distribution (in log space)

$$\log p(\mu|\mathcal{D}) = \log p(\mathcal{D}|\mu) + \log p(\mu) + \text{const}$$

$$= -\frac{1}{2}\frac{y-\mu^2}{\sigma^2} - \frac{1}{2}\mu^2\alpha + \text{constant}$$

$$= \frac{1}{2}\frac{\left(\frac{\sigma^{-2}}{\alpha+\sigma^{-2}}y - \mu\right)^2}{(\alpha+\sigma^{-2})^{-1}}$$

Inference for Gaussian

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mean of posterior distribution is between MLE (y) and prior (0)

Inference for Gaussian

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mean of posterior distribution is between MLE (y) and prior (0)

covariance of posterior: smaller than either covariance of likelihood or prior

Inference for Gaussian

Step 3: calculate posterior distribution (in log space)

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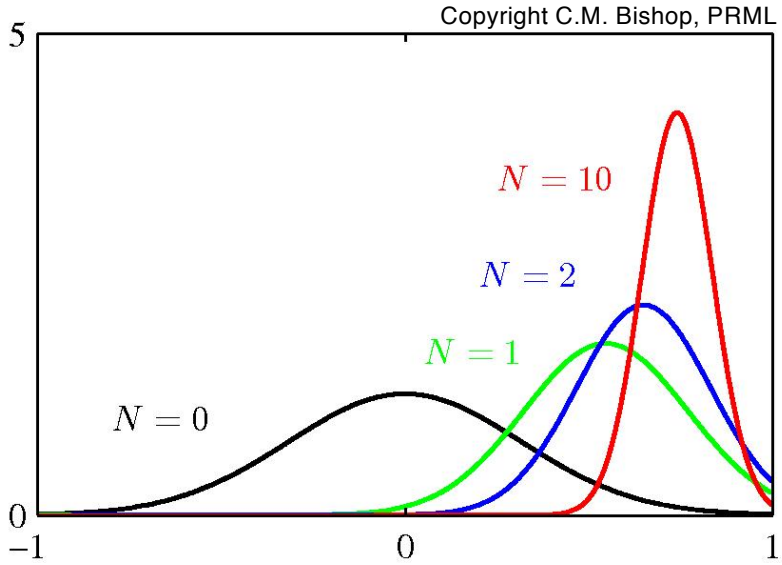
$$= \frac{1}{2}\frac{\left(\frac{\sigma^{-2}}{\alpha+\sigma^{-2}}y - \mu\right)^2}{(\alpha+\sigma^{-2})^{-1}}$$

Important thing: The posterior is another Guassian distribution.

$$\mathcal{N}\left(\frac{\sigma^2}{\alpha+\sigma^{-2}}y, (\alpha+\sigma^{-2})^{-1}\right)$$

Inference for Gaussian



Prediction for Gaussian

- Step 4: make prediction

$$
\begin{aligned}
p(y^*|\mathcal{D}) &= \int_{-\infty}^{\infty} p(y^*, \mu|\mathcal{D}) d\mu \\
&= \int_{-\infty}^{\infty} p(y^*|\mu) p(\mu|\mathcal{D}) d\mu \\
&= \int_{-\infty}^{\infty} \mathcal{N}(y^*|\mu, \sigma^2) \mathcal{N}\left(\mu \left| \frac{\sigma^{-2}}{\alpha + \sigma^{-2}} y_{\text{train}}, \frac{1}{\alpha + \sigma^{-2}} \right.\right) d\mu
\end{aligned}
$$

- Convolution of Gaussians, can be solved in closed form

$$
p(y^*|\mathcal{D}) = \mathcal{N}\left(y^* \left| \frac{\sigma^{-2}}{\alpha + \sigma^{-2}} y_{\text{train}}, \sigma^2 + \frac{1}{\alpha + \sigma^{-2}} \right.\right)
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Prediction for Gaussian

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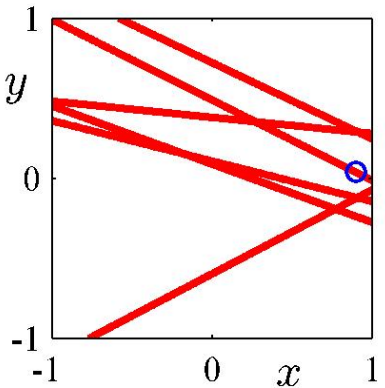
$$

noise + parameter uncertainty

Bayesian vs. frequentist

- Can we quantify uncertainty over models using probabilities?
- Classical / frequentist statistics: no
  - Probability represents *frequency of repeatable event*
  - There is only one true model
  - Do not consider 'prior knowledge'



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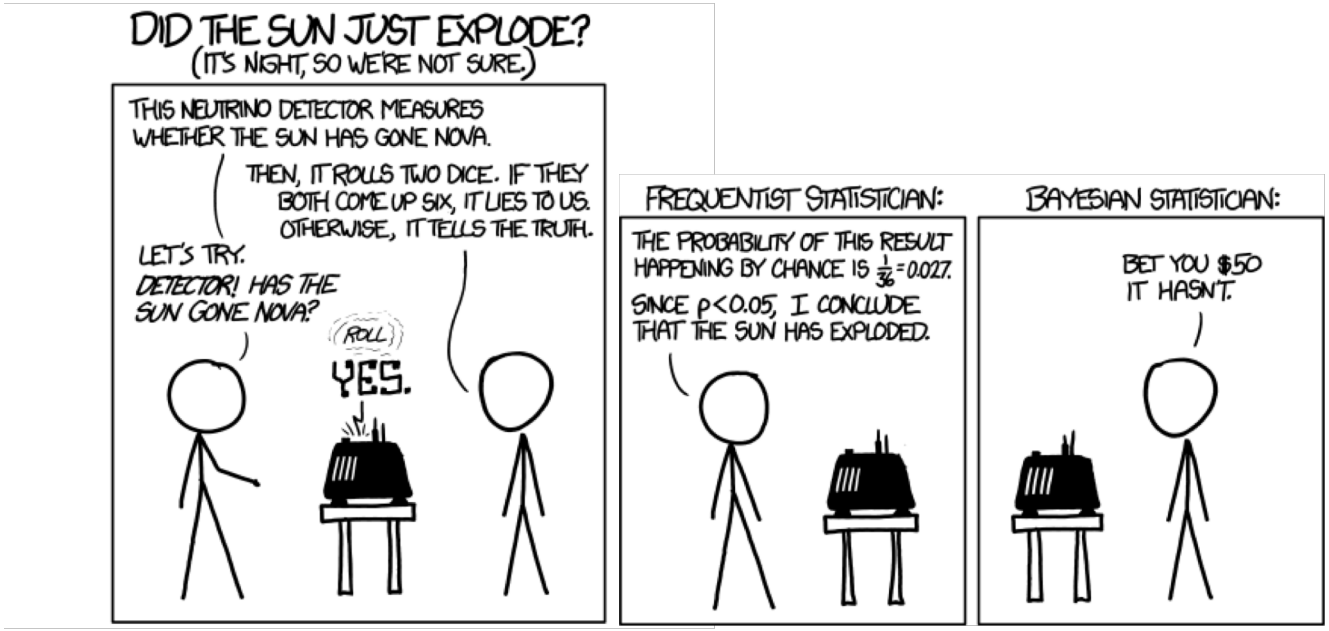
Bayesian probabilities

- Note: that Bayes' theorem is used does not mean a method uses a Bayesian view on probabilities!

- Many frequentist methods refer to Bayes' theorem (naive Bayes, Bayesian networks)

- Bayesian view on probability: Can represent uncertainty (in parameters) using probability

Bayesian probabilities



Randall Munroe / xkcd.com

Inference vs. Learning

- In *traditional machine learning*:
  - Learning: adjusting the parameters of your model to fit the data (by optimization of some cost function)
  - Inference: given your model + parameters and some data, make some prediction (e.g. the class of an input image)

- In *Bayesian statistics*, inference is to say something about the process that generated some data **(includes parameter estimation)**

- Take-away: in an ML problem, we can find a good value of parameters by optimization (*learning*) or calculate a distribution over parameters (*inference*)

Why Bayesian probabilities?

- Maximum likelihood estimates can have large variance
  - Overfitting in e.g. linear regression models
  - MLE of coin flip probabilities with three sequential ‘heads’

Why Bayesian probabilities?

- Maximum likelihood estimates can have large variance

- We might desire or need an estimate of uncertainty
  - Use uncertainty in decision making
    Knowing uncertainty important for many loss functions
  - Use uncertainty to decide which data to acquire
    (active learning, experimental design)

Why Bayesian probabilities?

- Maximum likelihood estimates can have large variance
- We might desire or need an estimate of uncertainty
- Have small dataset, unreliable data, or small batches of data
  - Account for reliability of different pieces of evidence
  - Possible to update posterior incrementally with new data
  - Variance problem especially bad with small data sets

Why Bayesian probabilities?

- Maximum likelihood estimates can have large variance
- We might desire or need an estimate of uncertainty
- Have small dataset, unreliable data, or small batches of data
-
- Use prior knowledge in a principled fashion

Why not Bayesian probabilities?

- Prior induces bias
- Misspecified priors: if prior is wrong, posterior can be far off
- Prior often chosen for mathematical convenience, not actually knowledge of the problem
- In contrast to frequentist probability, uncertainty is subjective, different between different people / agents

What you should know

- What is the Bayesian view of probability?
- Why can the Bayesian view be beneficial?
- What are the general inference and prediction steps?
- Role of the following distributions: Likelihood, prior, posterior, posterior predictive
- How can posterior and posterior predictive distribution be used?