Advanced Machine Learning

Bayesian Inference

Bayes, Conjugate Priors, Uninformative Priors

Outline

1. **Bayes' Rule**

2. Conjugate Priors

3. Uninformative Priors

Dealing with Uncertainty

- In machine learning we are attempting to make inference under uncertainty

- The natural language for discussing uncertainty is probability

- The natural framework for making inferences is Bayesian statistics

- However, this requires that we encode our prior knowledge of the problem and specify a likelihood

- In consequence, probabilistic methods tend to be bespoke, rather then general purpose black boxes

Revision on Bayes

- Bayes' rule

$$\mathbb{P}(\mathcal{H}_i|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\mathcal{H}_i)\mathbb{P}(\mathcal{H}_i)}{\mathbb{P}(\mathcal{D})}$$

⋆ $\mathbb{P}(\mathcal{H}_i|\mathcal{D})$ is the **posterior** probability of a hypothesis $\mathcal{H}_i$ (i.e. the probability of $\mathcal{H}_i$ **after** we see the data)

⋆ $\mathbb{P}(\mathcal{D}|\mathcal{H}_i)$ is the **likelihood** of the data given the hypothesis. Note, that we calculated this from the forward problem

⋆ $\mathbb{P}(\mathcal{H}_i)$ is the **prior** probability (i.e. the probability of $\mathcal{H}_i$ **before** we see the data)

⋆ $\mathbb{P}(\mathcal{D})$ is the **evidence** or **marginal likelihood**

$$\mathbb{P}(\mathcal{D}) = \sum_{i=1}^{n}\mathbb{P}(\mathcal{H}_i,\mathcal{D}) = \sum_{i=1}^{n}\mathbb{P}(\mathcal{D}|\mathcal{H}_i)\mathbb{P}(\mathcal{H}_i)$$

Solving Inverse Problems

Object $\longrightarrow$ Observation $\longrightarrow$ Data

Inverse Problem
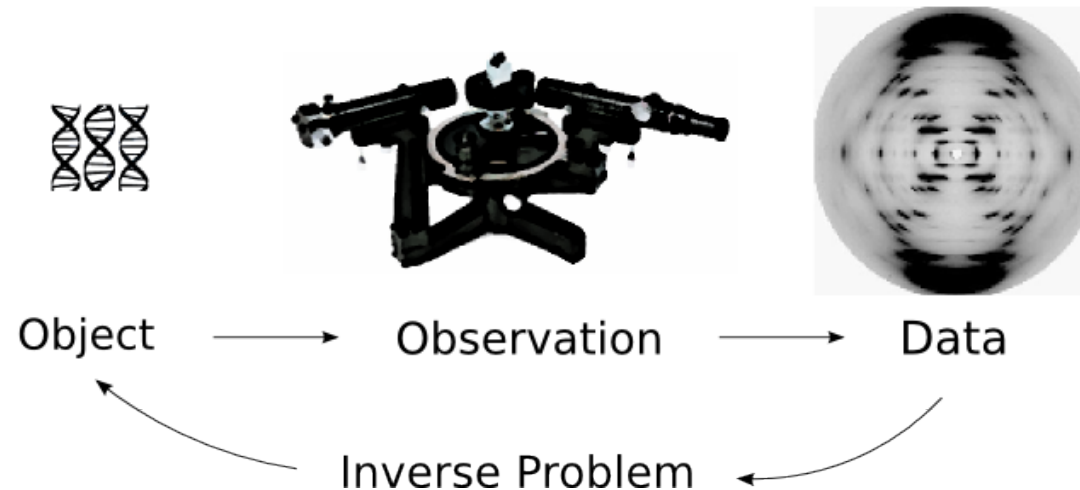
- We want the posterior $\mathbb{P}(\mathcal{H}_i|\mathcal{D})$ (i.e. the probability of what happened given some evidence)

- The Bayesian formalism converts this into the forward problem

$$\mathbb{P}(\mathcal{H}_i|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\mathcal{H}_i)\,\mathbb{P}(\mathcal{H}_i)}{\mathbb{P}(\mathcal{D})}$$

Bayesian Inference

- Bayes' rule says $\mathbb{P}(\mathcal{H}_i|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\mathcal{H}_i)\mathbb{P}(\mathcal{H}_i)}{\mathbb{P}(\mathcal{D})}$

- We calculate the likelihood $\mathbb{P}(\mathcal{D}|\mathcal{H}_i)$ (i.e. assuming the hypothesis, what is the chance of obtaining the data?)

- We consider the process of how the data is generated

- This uses the data we have (doesn't care about missing data)

- But we also need to know the prior $\mathbb{P}(\mathcal{H}_i)$

- Also, this can get difficult when we have many hypotheses

Evidence

- The normalisation term

$$\mathbb{P}(\mathcal{D}) = \sum_{i=1}^{n} \mathbb{P}(\mathcal{H}_i, \mathcal{D}) = \sum_{i=1}^{n} \mathbb{P}(\mathcal{D}|\mathcal{H}_i)\,\mathbb{P}(\mathcal{H}_i)$$

  tells you how likely the data is (given the prior and likelihood function)█

- It is called the **marginal likelihood**█ or **evidence**█

- If we have two models M_1 and M_2 we can do **model selection** by choosing the model with the largest evidence $\mathbb{P}(\mathcal{D} \mid M_1)$ or $\mathbb{P}(\mathcal{D} \mid M_2)$█

- This also allows us to select hyperparameters for a model█

Probability Density

- When we are working with continuous variables it is more natural to work with probability densities

$$f_X(x) = \lim_{\delta x \to 0} \frac{\mathbb{P}(x \leq X < x + \delta x)}{\delta x}$$

- Note that densities are non-negative, but can be greater than 1 (they are not probabilities)

- However

$$\mathbb{P}(a \leq X \leq b) = \int_a^b f_X(x)\,\mathrm{d}x$$

is a probability and is less than or equal to 1

Densities and Bayes

- Bayes' rule also applies to densities

$$\mathbb{P}(x \leq X < x + \delta x | Y) = \frac{\mathbb{P}(Y|x)\,\mathbb{P}(x \leq X < x + \delta x)}{\mathbb{P}(Y)}$$

- Dividing by δx and taking the limit $\delta x \to 0$

$$f_{X|Y}(x|Y) = \frac{\mathbb{P}(Y|x)\,f_X(x)}{\mathbb{P}(Y)}$$

- Similarly if X is discrete and Y continuous

$$\mathbb{P}(X|y) = \frac{f_{Y|X}(y|X)\,\mathbb{P}(X)}{f_Y(y)}$$

- If both X and Y are continuous

$$f_{X|Y}(x|y) = \frac{f_{Y|X}(y|x)\,f_X(x)}{f_Y(y)}$$

Practical Bayesian Inference

- Often consider learning parameters $\boldsymbol{\theta}$

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})\,p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

- This can be hard for large data sets as the posterior, $p(\boldsymbol{\theta}|\mathcal{D})$, is often a mess

- If we are lucky and have a simple likelihood then if we choose the right prior we end up with a posterior of the same form as the prior

- This occurs in some classic probabilistic inference problems, but as we will see soon it is also true for Gaussian Processes

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2. **Conjugate Priors**

3. Uninformative Priors

Learning a Probability

- Suppose we have a coin and we want to establish the probability of a head▮

- We want to learn this from a series of independent trials▮

- (Independent trials with two possible outcomes are known in probability theory as Bernoulli trials)▮

- Let X_i equal 1 if the ith trial is a head and 0 otherwise▮

- If the probability of a head is p then the **likelihood** of a X_i is

$$\mathbb{P}(X_i|p) = p^{X_i}(1-p)^{1-X_i}▮ = \begin{cases} p & \text{if } X_i = 1 \\ (1-p) & \text{if } X_i = 0 \end{cases}$$

Prior

- We may have a prior belief (e.g. we have made a few trials or we see the coin looks like a normal penny)

- We will suppose we can model our prior belief in terms of a **Beta distribution**

$$f(p) = \text{Beta}(p|a,b) = \frac{p^{a-1}(1-p)^{b-1}}{B(a,b)}$$

- $B(a,b)$ is just a normalisation constant

$$B(a,b) = \int_0^1 p^{a-1}(1-p)^{b-1}\mathrm{d}p = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

- This is a useful function for modelling the distribution of a random variable in the range 0 to 1

Uninformative Prior

- Suppose we have no idea about p what should we do?

- Laplace (one of the first Bayesian's) suggested giving equal weighting to all values of p

- This corresponds to a beta distribution with $a = b = 1$

- (Surprisingly other arguments suggest using $a = b = 0$ which provides a strong bias towards $p = 0$ and $p = 1$)

- Given enough data the prior is not so important and we will stick with Laplace for now

Independent Trials

- Using Bayes' rule

$$f(p|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|p)\,f(p)}{\mathbb{P}(\mathcal{D})}$$

- Assuming the trials are independent (a reasonably fair assumption for tossing coins) then the likelihood factorises

$$\mathbb{P}(\mathcal{D}|p) = \prod_{i=1}^{n} p^{X_i}(1-p)^{1-X_i}$$

$$= p^{X_1}(1-p)^{1-X_1} p^{X_2}(1-p)^{1-X_2} \cdots p^{X_n}(1-p)^{1-X_n}$$

$$= p^{\sum_i X_i}(1-p)^{\sum_i (1-X_i)} = p^{s}(1-p)^{n-s}$$

$s = \sum_i X_i$ (number of successes/heads)

Posterior

- Plugging in a prior $f(p) = \text{Beta}(p|a_0, b_0)$

$$f(p|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|p)\,f(p)}{\mathbb{P}(\mathcal{D})} = \frac{p^s(1-p)^{n-s} \times p^{a_0-1}(1-p)^{b_0-1}}{\mathbb{P}(\mathcal{D})\,B(a_0, b_0)}$$

- The denominator is a normalising factor

$$\mathbb{P}(\mathcal{D}) = \int_0^1 \mathbb{P}(\mathcal{D}|p)\,f(p)\,\mathrm{d}p = \int_0^1 \frac{p^{s+a_0-1}(1-p)^{n-s+b_0-1}}{B(a_0, b_0)}\mathrm{d}p$$

$$= \frac{B(s+a_0, n-s+b_0)}{B(a_0, b_0)}$$

Conjugate Priors

- The posterior distribution is Beta distribution

$$f(p|\mathcal{D}) = \frac{p^{s+a_0-1}(1-p)^{n-s+b_0-1}}{B(s+a_0, n-s+b_0)} = \text{Beta}(p|s+a_0, n-s+b_0)▮$$

- Something rather nice happened▮

- Starting with a beta distributed prior $f(p) = \text{Beta}(p|a_0, b_0)$ for a set of Bernoulli trials we obtain a beta distributed posterior $f(p|\mathcal{D}) = \text{Beta}(p|a_0 + s, b_0 + n - s)▮$

- This is not always the case (often the posterior will be very complicated) but it happens for a few likelihoods and priors▮

- When the posterior is the same as the prior then the likelihood and prior distributions are said to be **conjugate**▮

Incremental Updating

- For independent data we can update incrementally
  $\mathcal{D} = (X_1, X_2, \ldots, X_n)$

$$f(p|X_1) = \frac{\mathbb{P}(X_1|p)\, f(p)}{\mathbb{P}(X_1)}$$

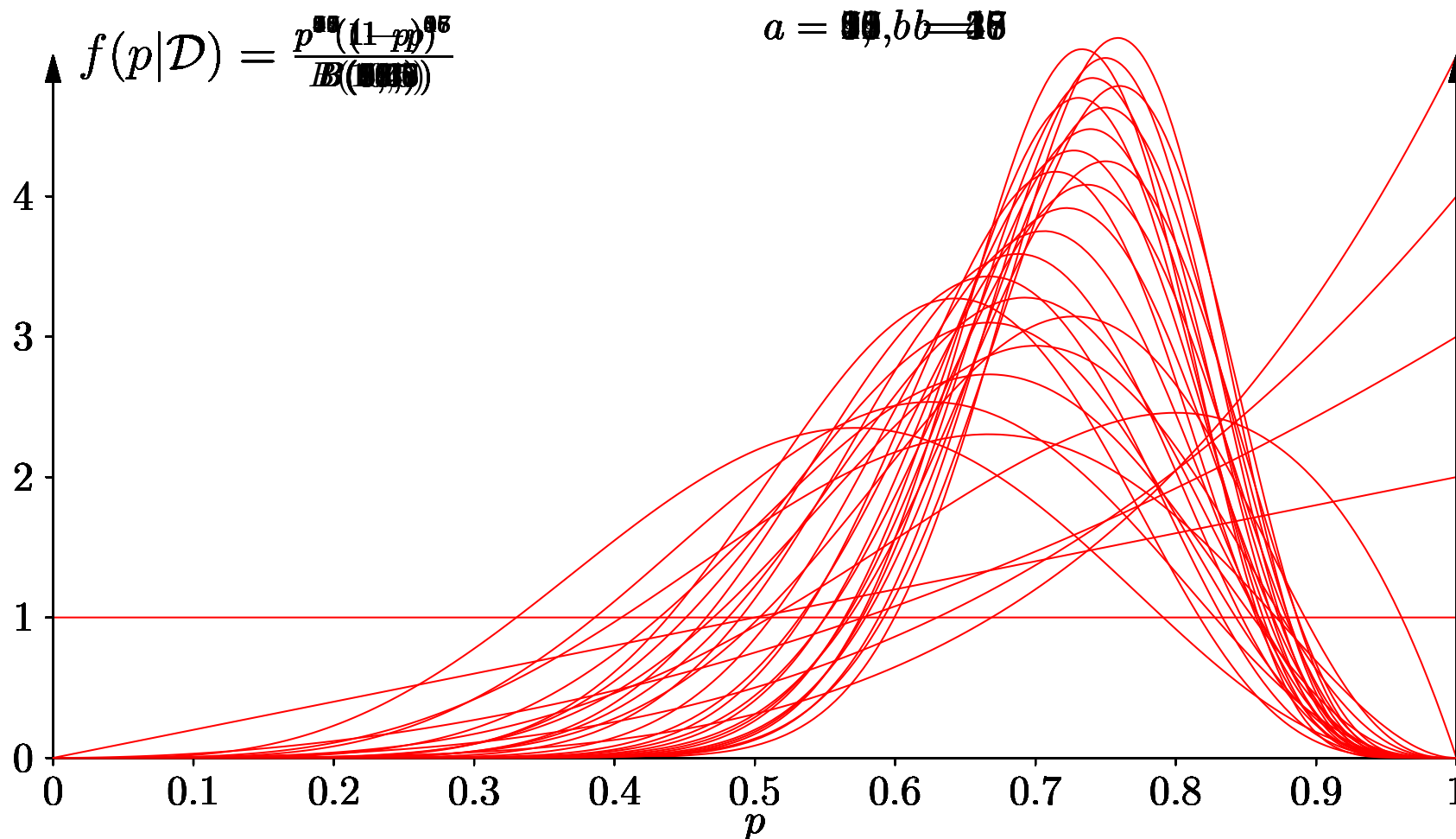$$f(p|X_1, X_2) = \frac{\mathbb{P}(X_2|p)\, f(p|X_1)}{\mathbb{P}(X_2)}$$

$$\vdots \quad = \quad \vdots$$

$$f(p|X_1, X_2, \ldots, X_n) = \frac{\mathbb{P}(X_n|p)\, f(p|X_1, \ldots, X_{n-1})}{\mathbb{P}(X_n)}$$

- The posterior becomes the prior for the next piece of data

- For our problem the posterior is always Beta distributed

Example (p=0.7)

$$\mathcal{D} = \{H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,T,H,H,H,H,T,H,H,H,T\}$$

Estimating Prediction Errors

- A full Bayesian treatment gives a prediction of its own error

- Assuming $f(p|\mathcal{D}) = \text{Beta}(p|a,b)$

- The expected value of p is given by $a/(a+b) = 23/32 = 0.719$

- The standard deviation is

$$\sqrt{\frac{ab}{(a+b)^2(a+b+1)}} = 0.078$$

Poisson Likelihoods

- Let's look at a second example of conjugate priors

- Suppose we want to find the rate of traffic along a road between 1:00pm and 2:00pm

- We assume the number of cars is given by a Poisson distribution

$$\mathbb{P}(N) = \mathrm{Pois}(N|\mu) = \frac{\mu^N}{N!}\mathrm{e}^{-\mu}$$

- μ is the rate of traffic per hour which we want to infer from observation taken on different days

Using Bayes

- Let us assume a Gamma distributed prior

$$p(\mu) = \Gamma(\mu|a_0, b_0) = \frac{b_0^{a_0} \mu^{a_0-1} e^{-b_0\mu}}{\Gamma(a)}$$

- We will assume that we know nothing. The uninformative prior is $a_0 = b_0 = 0$

- The data is $\mathcal{D} = \{N_1, N_2, \ldots, N_n\}$

- The likelihood is $\mathrm{Pois}(N_i|\mu)$

Posterior

- The posterior after seeing the first piece of data is

$$p(\mu|N_1) \propto \mathbb{P}(N_1|\mu)\,p(\mu)$$

$$\propto \frac{\mu^{N_1}}{N_1!}\mathrm{e}^{-\mu}\mu^{a_0-1}\mathrm{e}^{-b_0\mu}$$

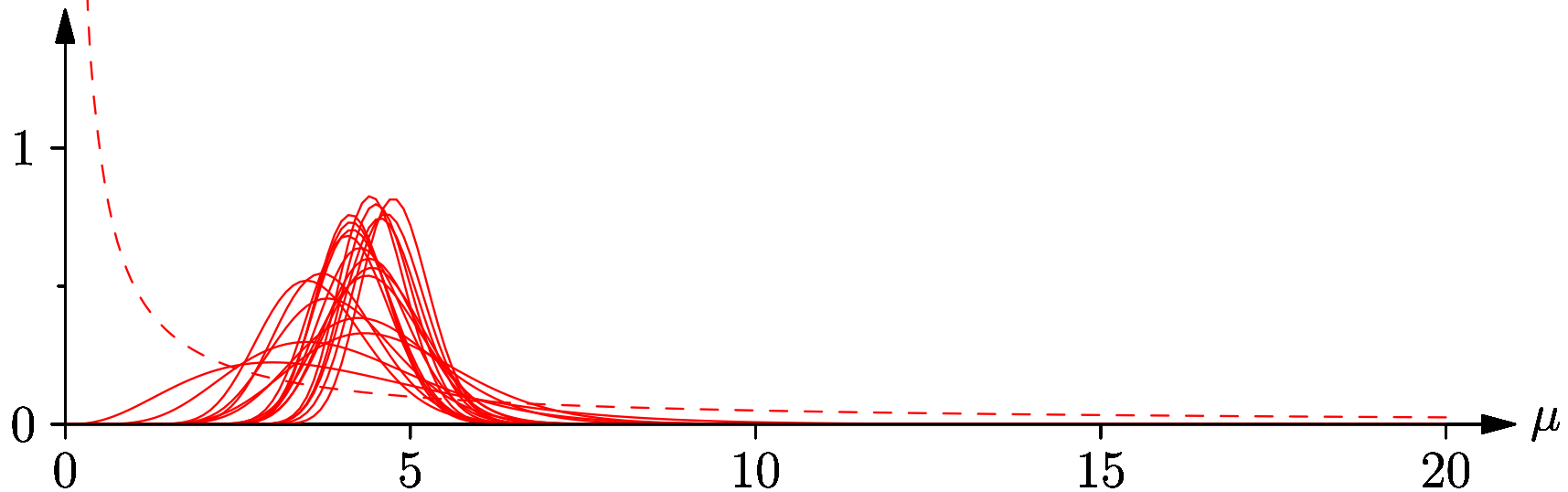$$\propto \mu^{N_1+a_0-1}\mathrm{e}^{-(b_0+1)\mu}$$

- The posterior is also a Gamma distribution $\Gamma(\mu|a_1,b_1)$ with $a_1 = a_0 + N_1$, $b_1 = b_0 + 1$

Example ($\mu = 5$)

$$\mathcal{D} = \{4,4,6,4,2,2,5,9,5,4,3,2,5,4,4,11,6,2,3,11\}$$

$p(\mu \mid \mathcal{D})$ (overlapping equation)

$a = 96, b = 20$ (overlapping values)

$$\mathbb{E}[\mu] = \frac{a}{b} = \frac{96}{20} = 4.8 \qquad \sqrt{\mathbb{V}\mathrm{ar}(\mu)} = \sqrt{\frac{a}{b^2}} = 0.49$$

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Uninformative Priors

- What if we have no prior knowledge, what should we do?

- OK usually we know whether we should make a measurement using a micrometer, ruler or car mileage, but we might still know almost nothing

- This led to Bayesian statistics being labelled as *subjective*

- However Ed. Jaynes (the greatest proponent of Bayesian methods) argued that we could answer this using symmetry arguments

Uninformative Priors for Scale Parameter

- Why did we choose $a_0 = b_0 = 0$ implying a prior $p(\mu) = 1/\mu$?

$$\mathbb{P}\left(\tfrac{A}{c} \leq \mu \leq \tfrac{B}{c}\right) = \mathbb{P}(A \leq \mu \leq B)$$
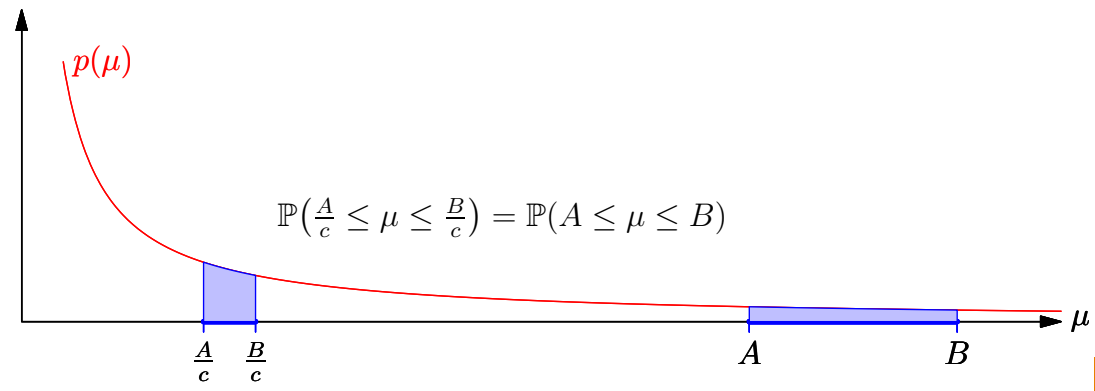
- That is, we have no idea on what scale to measure μ

$$\int_A^B p(\mu)\mathrm{d}\mu = \int_{A/c}^{B/c} p(\mu)\mathrm{d}\mu = \int_A^B \frac{1}{c}p(\frac{\nu}{c})\mathrm{d}\nu = \int_A^B \frac{1}{c}p(\frac{\mu}{c})\mathrm{d}\mu$$

making a change of variables $\mu = \nu/c$

- Or $p(\mu) = \frac{1}{c}p(\frac{\mu}{c})$ implying $p(\mu) \propto \frac{1}{\mu}$

Benford's Law

- Numbers occurring in life (physical constants, amounts of money) should not depend on the units (scale) measuring them

- They should then be distributed as $p(x) \propto 1/x$

- A curious consequence of this is that the significant figure has a distribution

$$\mathbb{P}(\text{most s.f. of } x = n) = \frac{\int_n^{n+1} \frac{1}{x}\mathrm{d}x}{\int_1^{10} \frac{1}{x}\mathrm{d}x} = \frac{\int_{10n}^{10n+10} \frac{1}{x}\mathrm{d}x}{\int_{10}^{100} \frac{1}{x}\mathrm{d}x}$$

$$= \frac{\log(n+1) - \log(n)}{\log(10)} = \log_{10}\left(\frac{n+1}{n}\right)$$

Population Size of 238 Countries
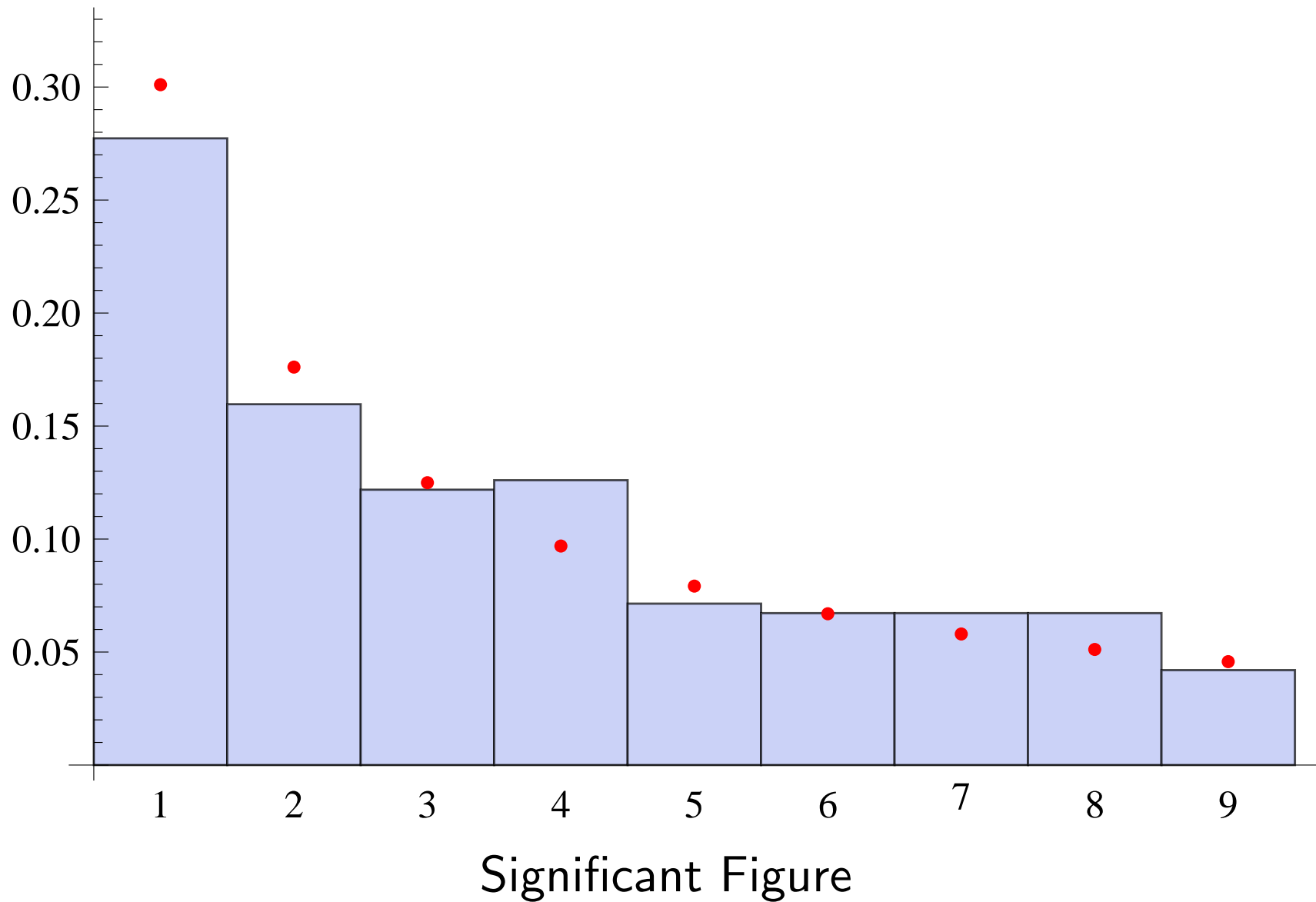
Conclusion

- Bayesian inference provides a coherent framework which we can use for machine learning

- However, it requires a model of what is happening

- In practice Bayesian methods are easy if the data is generated from a likelihood with a conjugate prior distribution—we have to be clever to choose the right prior

- We will see in the next lecture that much more frequently we will have likelihoods with no conjugate prior and we have to work much harder

- When we have no knowledge there are consistent ways to express our ignorance