PMR Learning as Inference

Probabilistic Modelling and Reasoning

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Outline

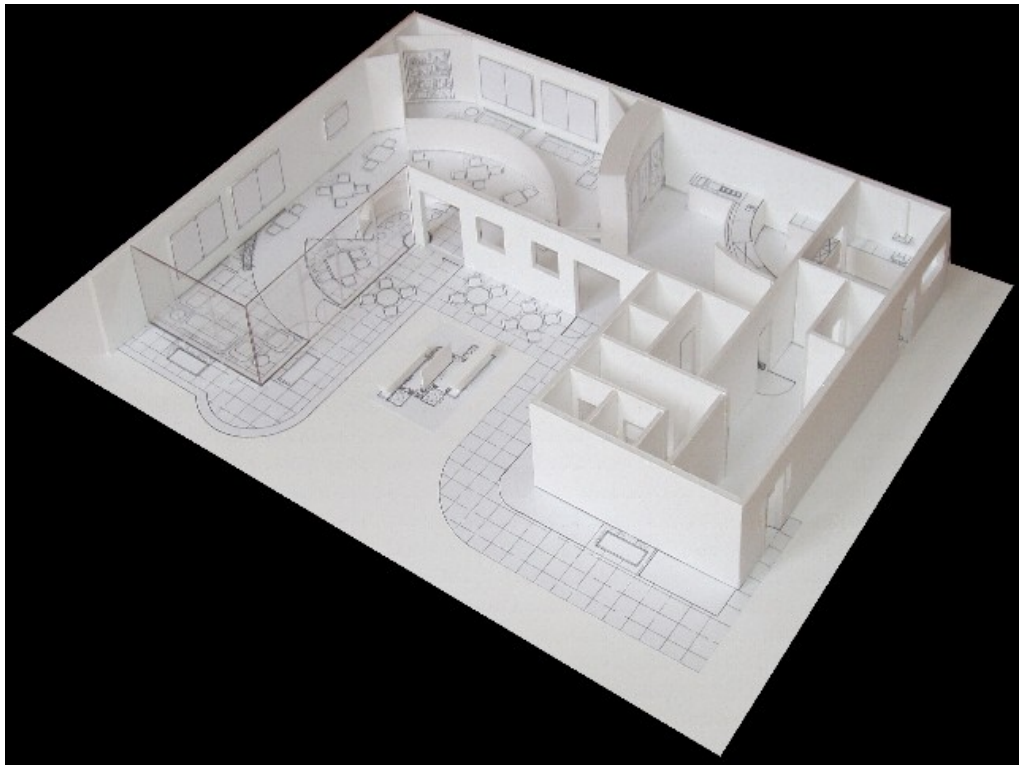
Modelling

Probabilistic Modelling is about building models and using them.

What do we mean by modelling?

Modelling

Modelling



A Generative Model

- Building an idealisation to capture the essential elements of an item.
- Think of a model as a model for future data generation
- Given a model (a distribution) we can sample from that distribution to get artificial data.
- Need to specify enough to do this generation.
- Often make IID (Independent and Identically Distributed) Assumption
- Models are not truth. They try to capture our uncertainties.

The Inverse Problem

- We built a generative model, or a set of generative models on the basis of what we know (prior).
- Can generate artificial data.
- BUT what if we want to *learn* a good distribution for data that we then see? How is goodness measured?

Explaining Data

A particular distribution explains the data better if the data is more probable under that distribution.

- The likelihood approach

Likelihood

- $P(\mathcal{D}|\mathcal{M})$. The probability of the data $\mathcal{D}$ given a distribution (or model) $\mathcal{M}$. This is called the likelihood of the model.
- This is

$$P(\mathcal{D}|\mathcal{M}) = \prod_{n=1}^{N} P(x^n|\mathcal{M})$$

  i.e. the product of the probabilities of generating each data point individually.
- This is a result of the independence assumption (indep $\rightarrow$ product of probabilities by definition).
- Try different $\mathcal{M}$ (different distributions). Pick the $\mathcal{M}$ with the highest likelihood $\rightarrow$ Maximum Likelihood Approach.

Bernoulli model

Example

Data: 1 0 0 1 0 1 0 1 0 0 0 0 0 1 0 1 1 1 0 1.

- Continuous range of hypotheses: $\mathcal{M} = p$ - Generated from a Boolean distribution with $P(1|p) = p$.
- Likelihood of data. Let c=number of ones:

$$\prod_{n=1}^{N} P(x^n|p) = p^c(1-p)^{20-c}$$

- Maximum likelihood hypothesis? Differentiate w.r.t. p to find maximum
- In fact usually easier to differentiate $\log P(\mathcal{D}|\mathcal{M})$: $\log$ is monotonic. So argmax $\log(f(x))$ = argmax $f(x)$.

Bernoulli model

Example

Data: 1 0 0 1 0 1 0 1 0 0 0 0 0 1 0 1 1 1 0 1.

- Likelihood of data. Let c=number of ones:

$$\log \prod_{n=1}^{N} P(x^n|p) = c \log p + (20 - c) \log(1 - p)$$

- Set $d/dp \log P(\mathcal{D}|\mathcal{M}) = c/p - (20 - c)/(1 - p)$ to zero to find maximum.
- So $c(1 - p) - (20 - c)p = 0$. This gives $p = c/20$. Maximum likelihood is unsurprising.

Distributions over Parameters

Parameter bias

- Although we are uncertain about the parameter values, often some are more probable than others.
- Uncertainty $\rightarrow$ probability: put *prior* (distribution) on parameters.
- Compute max *posterior* instead of max likelihood
- Bayes Rule:

$$\text{Posterior} \rightarrow P(p|\mathcal{D}) = \frac{P(\mathcal{D}|p)P(p)}{P(\mathcal{D})} \leftarrow \text{Prior}$$

- $P(\mathcal{D}) = \int dp\ P(p|\mathcal{D})P(p)$ does not depend on p.
- argmax $P(\mathcal{D}|p)P(p)$
- argmax $(\log P(\mathcal{D}|p) + \log P(p)) \leftarrow$ penalty term

Maximum Posterior

Example

1 0 0 1 0 1 0 1 0 0 0 0 0 1 0 1 1 1 0 1. $P(p) \propto p(1-p)$

- Let c=number of ones (9). Then $\log P(p|\mathcal{D}) =$

$$c \log p + (20 - c) \log(1 - p) + \log p + \log(1 - p) + \text{const}$$

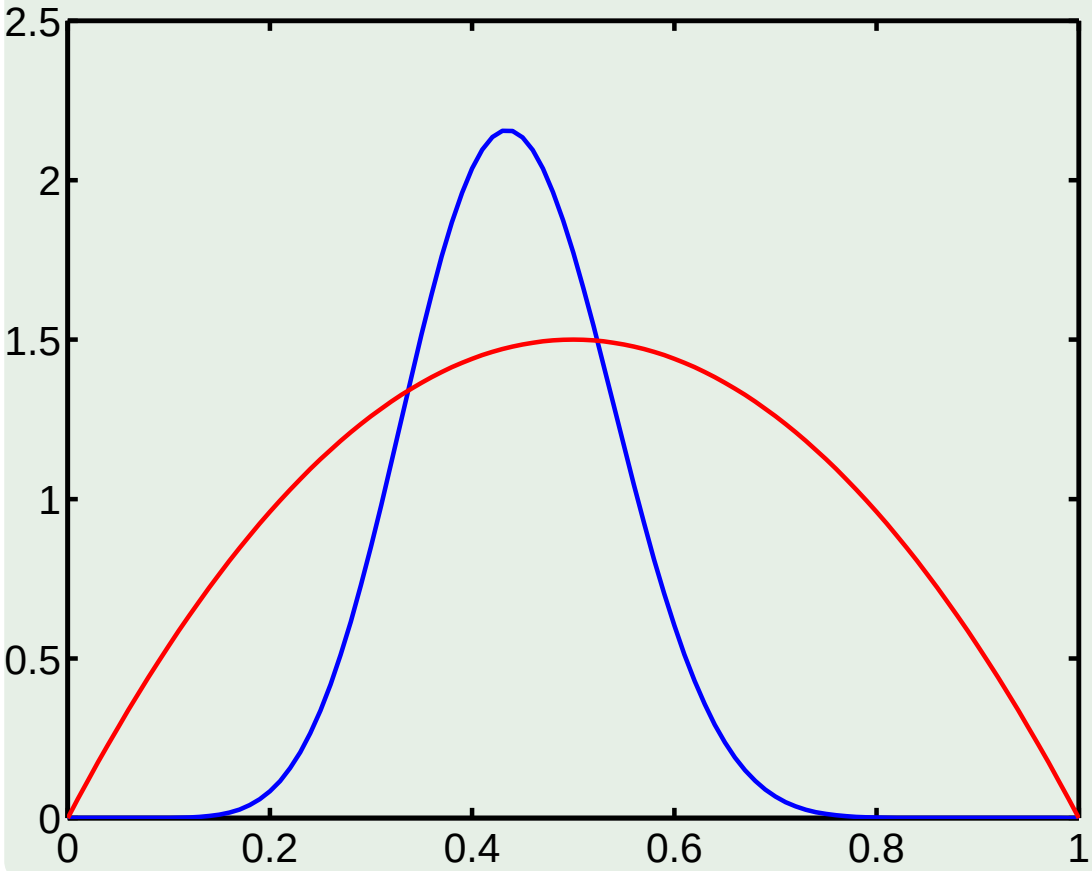
- Set $d/dp \log P(\mathcal{D}|\mathcal{M}) = (c+1)/p - (20 - c + 1)/(1 - p)$ to zero to find maximum.
- So $(c + 1)(1 - p) - (20 - c + 1)p = 0$. This gives $p = (c + 1)/22 = 9/22 \approx 0.41$.
- With this prior, max. posterior prefers p closer to $1/2$.

Uncertainty of Parameters

- Maximizing the posterior gets us one value for the parameter.
- Is it right?
- No it is an estimate. But how good an estimate? There is some uncertainty. How much?
- Uncertainty $\rightarrow$ probability.
- Find posterior *distribution* over parameters, not just maximum.

Posterior Distribution

Example



Prior in Red,
Posterior in Blue

Inference and Marginalisation

Example

1 0 0 1 0 1 0 1 0 0 0 0 0 1 0 1 1 1 0 1. $P(p) \propto p(1-p)$

- What is probability of next item x^* being 1? Predict.
- Could take maximum posterior parameter and compute probability of next item? (≈ 0.41)
- But: lots of possible posterior parameters. Some more possible than others.
- Instead marginalise:

$$\int dp \; P(x_* = 1|p)P(p|\mathcal{D})$$

- This gives approximately 0.46.

Test

- We considered choosing between model, where each model defined a precise distribution.
- But what if each model defines a whole *type* of distribution.
- We might not know the precise *parameters* of the distribution.
- Compute the *evidence* or *marginal likelihood*:
- Marginalise out the unknown parameters to get likelihood of model.

Learning as inference

- Its just as if the parameters were nodes in our graphical model.
- In fact that is exactly what they are.
- Latent variables - intrinsic - separate variables for each data item.
- Parameters - extrinsic - shared across all data items.

Summary of Bayesian Computation

- Define prior model $P(\mathcal{D})$, usually by using

$$P(\mathcal{D}) = \int d\boldsymbol{\theta}\ P(\mathcal{D}|\boldsymbol{\theta})P(\boldsymbol{\theta})$$

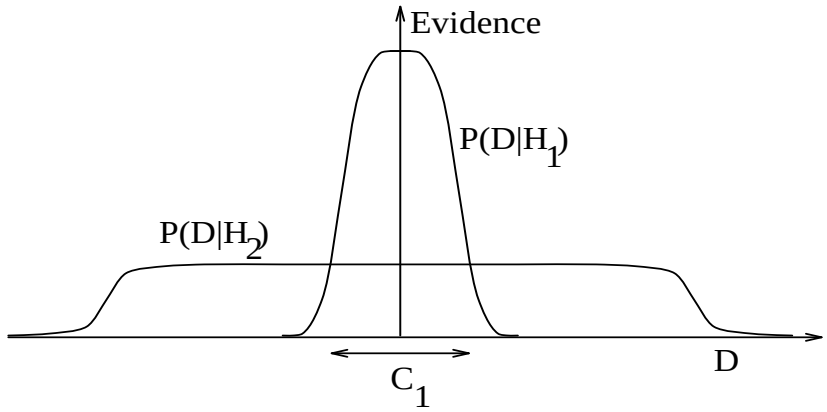
  and defining:
  - The likelihood $P(\mathcal{D}|\boldsymbol{\theta})$ with parameters $\boldsymbol{\theta}$.
  - The *prior distribution* (over parameters) $P(\boldsymbol{\theta}|\boldsymbol{\alpha})$ which might also be parameterized by hyper-parameters $\boldsymbol{\alpha}$.
- Conditioning on data to get the *posterior distribution* over parameters $P(\boldsymbol{\theta}|\mathcal{D})$.
- Using the posterior distribution for prediction (inference)

$$P(\mathbf{x}^*|\mathcal{D}) = \int d\boldsymbol{\theta}\ P(\mathbf{x}^*|\boldsymbol{\theta})P(\boldsymbol{\theta}|\mathcal{D})$$

Why not maximize?

We have described learning as an inference procedure. But why not maximize.

- Why be Bayesian? Why not compute best parameters and compare?
- More parameters=better fit to data. ML: bigger is better.
- But might be overfitting: only these parameters work. Many others don't.



- Prefer models that are unlikely to 'accidentally' explain the data.
- That said, maximum posterior parameters are often good

Recap

- For Bernoulli likelihood with Beta prior, could do Bayesian computation analytically.
- For Binomial likelihood and Beta prior, could do Bayesian computation analytically.
- For Multinomial likelihood and Dirichlet prior, could do Bayesian computation analytically.
- Question: are there other distributions for which we can do analytical Bayesian computations?
- Is this a good thing? Discuss.

Analytical methods

- Yes: conjugate exponential models.
- Good thing: easy to do the sums.
- Bad thing: prior distribution should match beliefs. Does a Beta distribution match your beliefs? Is it good enough?
- Certainly not always.

The exponential family

- Any distribution over some $\mathbf{x}$ that can be written as

$$P(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left(\boldsymbol{\eta}^T\mathbf{u}(\mathbf{x})\right)$$

  with h and g known, is in the *exponential family* of distributions.
- Many of the distributions we have seen are in the exponential family. A notable exception is the t-distribution.
- The $\boldsymbol{\eta}$ are called the *natural parameters* of the distribution.

Wait - I didn't get that!

$$P(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left(\boldsymbol{\eta}^T\mathbf{u}(\mathbf{x})\right)$$

- More simply....
- Any distribution that can be written such that the interaction term (between parameters and variables) is log linear in the parameters is in the *exponential family*.
- i.e.

$$\log P(\mathbf{x}|\boldsymbol{\eta}) = \sum_i \eta_i u_i(\mathbf{x}) + (\text{other stuff that only contains } \mathbf{x} \text{ or } \boldsymbol{\eta})$$

- A distribution may usually be parameterized in a way that is different from the exponential family form.
- So sometimes useful to convert to exponential family representation and find the 'natural' parameters.

The exponential family

- Multinomial Distribution

$$P(\mathbf{x}|\{\log p_k\}) \propto \exp\left(\sum_k x_k \log p_k\right)$$

The Gaussian Distribution

- Need to intro the Gaussian first.

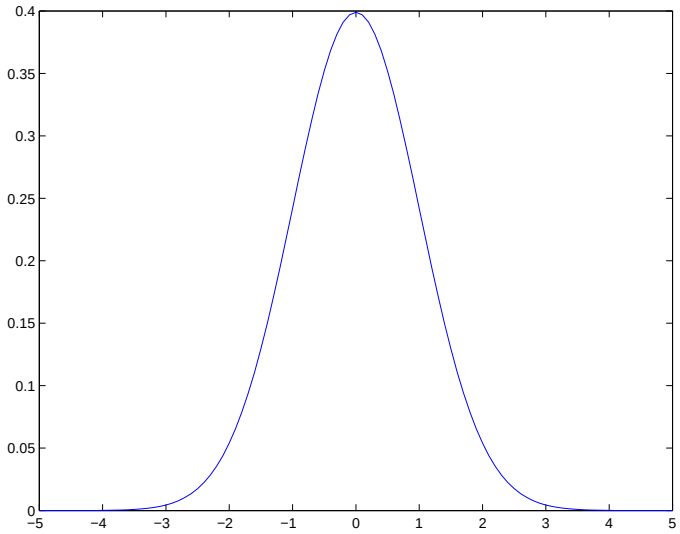
Definition

- The one dimensional Gaussian distribution is given by

$$P(x|\mu,\sigma^2) = N(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{(x-\mu)^2}{2\sigma^2}$$

- μ is the *mean* of the Gaussian and σ^2 is the *variance*.
- If $\mu = 0$ and $\sigma^2 = 1$ then $N(x;\mu,\sigma^2)$ is called a *standard* Gaussian.

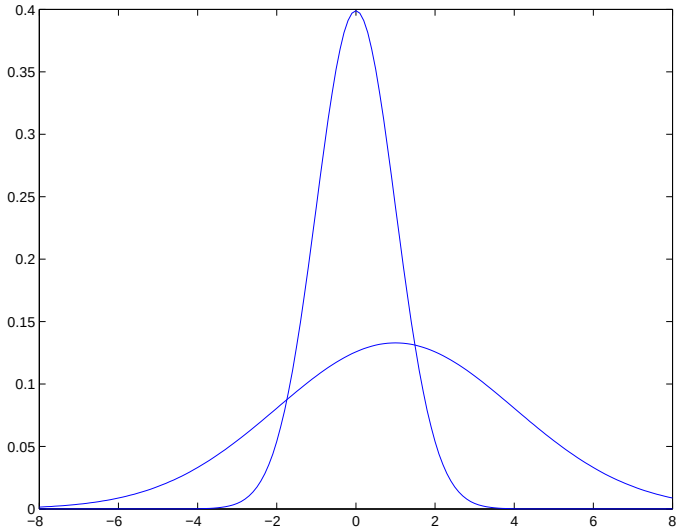
Plot



- This is a standard one dimensional Gaussian distribution.
- All Gaussians have the same shape subject to scaling and displacement.
- If x is distributed $N(x; \mu, \sigma^2)$, then $y = (x - \mu)/\sigma$ is distributed $N(y; 0, 1)$.

Normalisation

- Remember all distributions must integrate to one. The $\sqrt{2\pi\sigma^2}$ is called a normalisation constant - it ensures this is the case.
- Hence tighter Gaussians have higher peaks:



Central Limit Theorems

- X_i mean 0, variance Σ, not necessarily Gaussian.
- X_i subject to various conditions (e.g. IID, light tails).

$$\frac{1}{\sqrt{N}} \sum_{i=1}^{N} X_i \sim N(0, \Sigma)$$

asymptotically as $N \to \infty$.

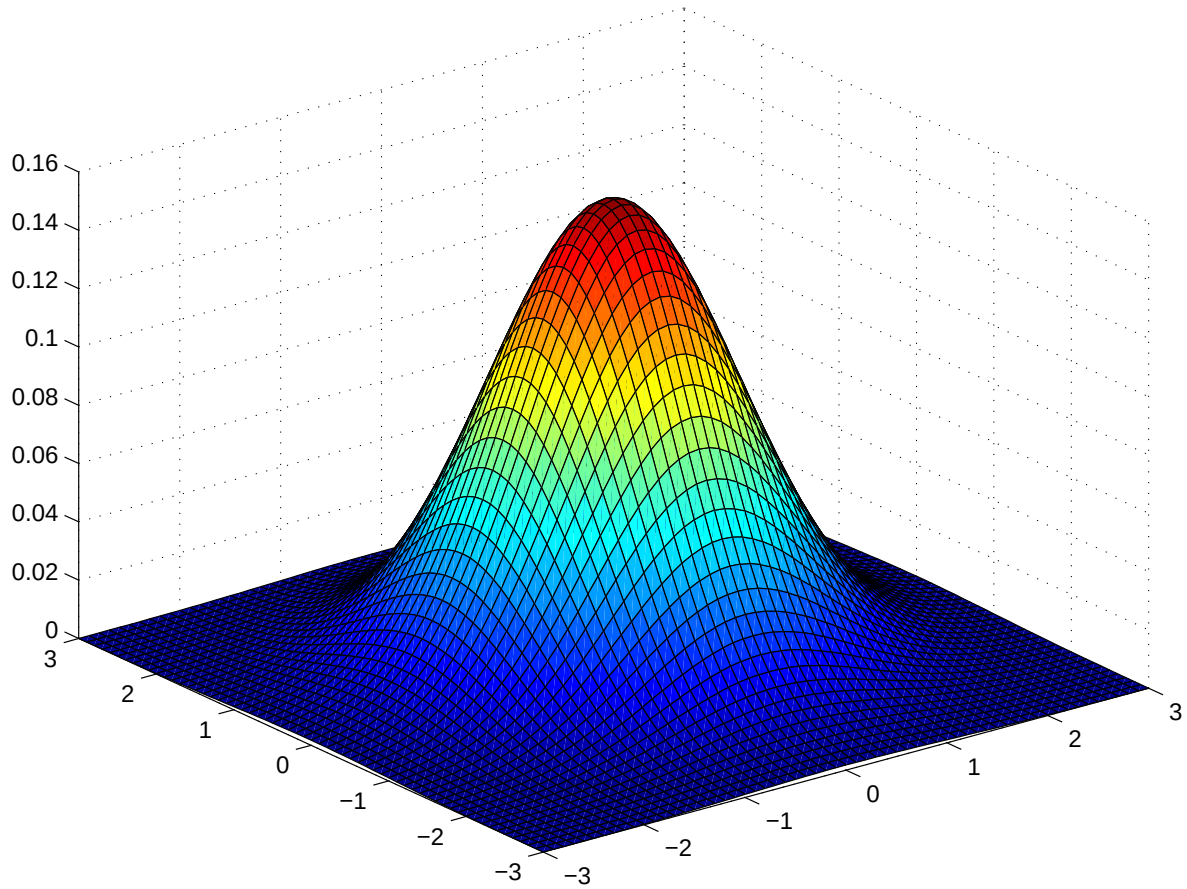
Multivariate Gaussian

- The vector $\mathbf{x}$ is multivariate Gaussian if for mean μ and covariance matrix Σ, it is distributed according to

$$P(\mathbf{x}|\mu,\Sigma) = \frac{1}{|(2\pi)\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\right)$$

- The univariate Gaussian is a special case of this.
- Σ is called a covariance matrix. It says how much attributes co-vary. More later.

Multivariate Gaussian: Picture



The exponential family

- Gaussian Distribution

$$P(\mathbf{x}|\boldsymbol{\eta}) \propto \exp\left(\sum_k \eta_k x_k - \frac{1}{2}\sum_{ij} \Sigma_{ij}^{-1} x_i x_j)\right)$$

- $\eta = \Sigma^{-1}\mu$.

Pause

Conjugate exponential models

- If the prior takes the same functional form as the posterior for a given likelihood, a prior is said to be *conjugate* for that likelihood.
- There is a conjugate prior for any exponential family distribution.
- If the prior and likelihood are conjugate and exponential, then the the model is said to be *conjugate exponential*
- In conjugate exponential models, the Bayesian integrals can be done analytically.

Conjugacy

- In high dimensional spaces it is hard to accurately estimate the parameters using maximum likelihood. Can utilise Bayesian methods.
- Conjugate distribution for the Gaussian with mean parameter is another Gaussian.
- Conjugate distribution for the Gaussian with precision (inverse variance) parameter is the Gamma distribution.
- Conjugate distribution for the Gaussian with precision matrix (inverse covariance is the Wishart distirbution.
- Conjugate distribution for the Gaussian with both mean and precision matrix is the Gaussian-Wishart distribution.
- Wishart distribution is distribution over matrices!

Conjugacy

- Remember - for conjugate distribution posterior is of the same form.
- So given the data, we just need to update the hyperparameters of the prior distribution to get the posterior.

Example

- Gaussian $N(\mu, \Lambda^{-1})$. Fixed precision Λ, but μ distributed $N(\mu_0, \Lambda_0^{-1})$
- Posterior mean $(\Lambda_0 + n\Lambda)^{-1}(\Lambda_0\mu_0 + n\Lambda\bar{x})$
- Posterior precision $(\Lambda_0 + n\Lambda)$.

Conjugacy: Evidence

Example

- Gaussian likelihood $N(\mathbf{x}; \boldsymbol{\mu}, \Sigma)$, Gaussian prior $N(\boldsymbol{\mu}; \boldsymbol{\mu}_0, \Sigma_0)$. Simple case: $\boldsymbol{\mu}_0 = 0$, Σ known.
- Marginal likelihood (Evidence)? We know Marginal Likelihood is Gaussian. So using $\mathbf{x} = \boldsymbol{\mu} + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}$ mean 0, covariance Σ, compute mean $\mathbf{m}$ and covariance C of marginal likelihood

$$\mathbf{m} = \langle \mathbf{x} \rangle = \langle \boldsymbol{\mu} \rangle + 0 = 0$$

$$C = \langle \mathbf{x}\mathbf{x}^T \rangle = \langle \boldsymbol{\mu}\boldsymbol{\mu}^T \rangle + \langle \boldsymbol{\epsilon}\boldsymbol{\epsilon}^T \rangle + 0 = \Sigma + \Sigma_0$$

Give me more...

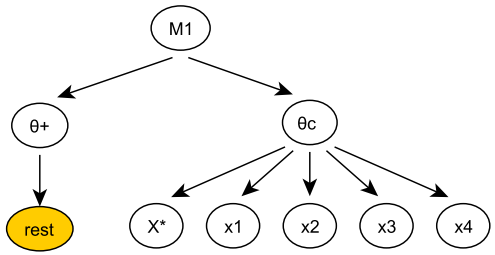
- Red Orange Yellow Aquamarine
- Haggis Mountains Loch Celtic Castle
- Trees, Forests, Pruning, Parent, Machine Learning, Bayesian.
- Google Sets

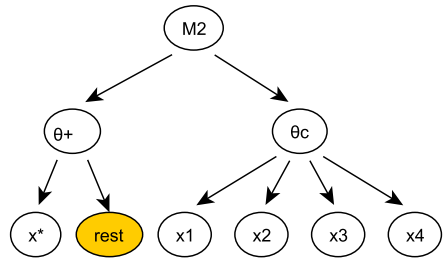
Different features

- Have a large database of objects, each described by $\mathcal{D}^+$ (e.g. Web)
- Have a small number of examples from the dataset, each with various (binary) features, which we collect into $\mathcal{D}_c$.
- Want to pick things from $\mathcal{D}^+$ that 'belong to the same set' as those in $\mathcal{D}_c$
- How should we do it?

Model

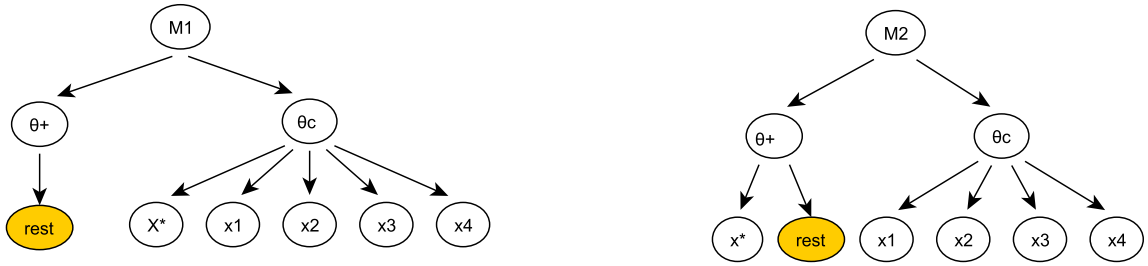
- Data consists of $\mathcal{D}_c$ and query point $\mathbf{x}^*$. Denote by $\mathcal{D}$.
- Two models: $\mathcal{M}_1$: $\mathcal{D}$ all from same subset C, or $\mathcal{M}_2$: $\mathcal{D}_c$ from the same subset C, but $\mathbf{x}$ from the general distribution over all data $\mathcal{D}^+$





- Parameter vector is vector of (Boolean) probabilities, one for each feature.
- $\mathcal{D}^+$ is vast, and so presume maximum likelihood estimate good enough for $\mathcal{M}1$: have vector θ^+ for this.

Score



- Parameter vector θ_c for subset C is not known. So put a conjugate prior on the parameters: a Beta distribution for each component i of the feature vector, with hyper-parameters a_i and b_i.
- Compute $P(\mathcal{D}|\mathcal{M}_1)/P(\mathcal{D}|\mathcal{M}_2)$ (called the Bayes Factor).
- The larger this ratio is, the more this favours $\mathbf{x}^*$ being included in the set.
- Bayesian Model Comparison: parameters integrated out:

$$P(\mathcal{D}|\mathcal{M}_2) = \int P(\mathcal{D}|\theta)P(\theta|\alpha)d\theta$$