# Introduction to Bayesian learning <br> Lecture 2: Bayesian methods for (un)supervised problems 

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1. Supervised learning example : Naive Bayes Classification
2. Bayesian linear regression

Regression : reminders
Bayesian linear regression
3. Bayesian model choice

Bayesian model averaging
Bayesian model selection
Automatic complexity penalty
Laplace approximation and BIC criterion
Empirical Bayes

## Setting

Not purely Bayesian framework : the training step is not necessarily Bayesian, only the prediction step is.

- Sample space $\mathcal{X}=\mathcal{X}_{1} \times \cdots \times \mathcal{X}_{d}$ ( $d$ features)
- some features may be categorical, some discrete, some continuous
- data $X_{i}=\left(X_{i, 1}, \ldots X_{i, d}\right), i=1, \ldots, n$.
- Classification problem : $X_{i}$ may come from anyone of $K$ classes $\left(\mathcal{C}_{1}, \ldots, \mathcal{C}_{K}\right)$.
- Example $\begin{cases}X_{i, 1} \in \mathbb{R}^{p \times p}: & \text { X-ray image from patient } i \\ X_{i, 2} \in\{0,1\}: & \text { result of a blood test from patient } i\end{cases}$
- classes : \{ill, healthy, healthy carrier\}.
- Goal predict the class $c \in\{1, \ldots, K\}$ of a new patient.


## Naive Bayes assumption

Conditionally to the class $c(i) \in\{1, \ldots, K\}$ of observation $i$, the features $\left(X_{i, 1}, \ldots, X_{i, d}\right)$ are independent.

- Looks like a strong (and erroneous) assumption!
- In practice : produces reasonable prediction (even though the posterior probabilities of each class are not to be taken too seriously)


## 1. Training step

- Training set $\left\{\left(x_{i, j}, c(i)\right), i \in\{1, \ldots, n\}, j \in\{1, \ldots, d\}\right\}$, $c(i) \in\{1, \ldots, K\}$.
- for $k \in\{1, \ldots, K\}$ :
- Retain observations of class $k \rightarrow i \in I_{k}$.
- For $j \in\{1, \ldots, d\}$ estimate the class distribution, with density

$$
p_{j, k}\left(x_{j}\right)=p\left(x_{i, j} \mid c(i)=k\right),
$$

using data $\left(x_{i, j}\right)_{i \in l_{k}}$, usually in a parametric model with parameter $\theta_{j, k}: \rightarrow$ estimated density $p_{j, k, \widehat{\theta}_{j, k}}(\cdot)$

- output : the conditional distribution of $X$ given $C=k$,

$$
p_{k}(x)=\prod_{j=1}^{k} p_{j, k, \widehat{\theta}_{j, k}}\left(x_{j}\right)
$$

## 2. computing the predictive class probabilities

input:

- new data point $x=\left(x_{1}, \ldots, x_{d}\right)$
- From step 1: conditional distributions of $X$ given $C=k$ : $p_{k}(\cdot)=\prod p_{j, k, \widehat{\theta}_{j, k}}$ (plug-in method, neglect estimation error of $\widehat{\theta}_{j, k}$ ).
(a) Assign a prior probability to each class : $\pi=\left(\pi_{1}, \ldots, \pi_{K}\right)$, $\pi_{k}=\mathbb{P}_{\pi}(C=k)$. step $1 \rightarrow$ joint density of $(X, C): q(x, k)=\pi_{k} p_{k}(x)$.
(b) Apply the discrete Bayes formula :

$$
\pi(k \mid x)=\frac{\pi_{k} p_{k}(x)}{\sum_{c=1}^{K} \pi_{c} p_{c}(x)}=\frac{\pi_{k} \prod_{j=1}^{d} p_{j, k, \widehat{\theta}_{j, k}}\left(x_{j}\right)}{\sum_{c=1}^{K} \pi_{c} \prod_{j=1}^{d} p_{j, c, \widehat{\theta}_{j, c}}\left(x_{j}\right)}
$$

Easy to implement! $O(k d N)$ for $N$ testing data.

## 3. final step : class prediction

- Classification task : output $=$ a predicted class $\widehat{x}$
- Naive Bayes prediction for a new point $x$

$$
\widehat{c}=\underset{k \in\{1, \ldots, k}{\operatorname{argmax}} \pi(k \mid x) .
$$

(a maximum a posteriori)

## Example : text documents classification

- 2 classes: $\{1=$ spam, $2=$ non spam $\}$
- vocabulary $\mathcal{V}=\left\{w_{1}, \ldots, w_{V}\right\}$.
- dataset : documents (email) $T_{i}=\left(T_{i, j}, j=1, \ldots, N_{i}\right), i \leq n$ with
- $N_{i}$ : number of words in $T_{i}$
- $t_{i, j} \in \mathcal{V}: j^{t h}$ word in $T_{i}$


## Conditional model (text documents)

- Naive Bayes assumption : in document $T_{i}$, conditionally to the class, words are drawn independently from each other in the vocabulary $\mathcal{V}$
- $T_{i}$ can be summarized by a 'bag of words' $X_{i}=\left(X_{i, 1}, \ldots, X_{i, v}\right)$ :

$$
X_{i, j}: \text { number of occurrences of word } j \text { in } T_{i} .
$$

- Conditional model for $X_{i}$ given its class $k \in\{1,2\}$ :

$$
\begin{gathered}
\mathcal{L}\left(X_{i} \mid C=k\right)=\operatorname{Multi}\left(\theta_{k}=\left(\theta_{1, k}, \ldots, \theta_{V, k}\right), N_{i}\right), \quad \text { i.e. } \\
p_{k, \theta_{k}}(x)=\frac{N_{i}!}{\prod_{j=1}^{V} x_{i, j}!} \prod_{j=1}^{v} \theta_{j, k}^{x_{i, j}}
\end{gathered}
$$

## 1. training step (text documents)

Fit separately 2 Multinomial models on spam and non-spam

- Here : the Dirichlet prior $\operatorname{Diri}\left(a_{1} \ldots, a_{v}\right), a_{j}>0$ is conjugate for the Multinomial model, with density

$$
\operatorname{diri}\left(\theta \mid a_{1}, \ldots, a_{V}\right)=\frac{\Gamma\left(\sum_{j=1}^{V} a_{j}\right)}{\prod_{j=1}^{V} \Gamma\left(a_{j}\right)} \prod_{j=1}^{V} \theta_{j}^{a_{j}-1}
$$

on $\mathcal{S}_{V}=\left\{\theta \in \mathbb{R}_{+}^{V}: \sum_{j=1}^{V} \theta_{j}=1\right\}$ the $V$ - 1-simplex.

- Mean of $\boldsymbol{\theta}$ under $\boldsymbol{\pi}=\mathcal{D i r i}\left(a_{1}, \ldots, a_{V}\right)$ :

$$
\mathbb{E}_{\boldsymbol{\pi}}(\boldsymbol{\theta})=\left(\frac{a_{1}}{\sum_{j} a_{j}}, \ldots, \frac{a_{V}}{\sum_{j} a_{j}}\right)
$$

- The posterior for $x_{1: n}=\left(x_{i, 1}, \ldots, x_{i, V}\right)_{i \in\{1, \ldots, n\}}$ is

$$
\mathcal{D i r i}\left(\left(a_{1}+\sum_{i=1}^{n} x_{i, 1}\right), \ldots,\left(a_{V}+\sum_{i=1}^{n} x_{i, v}\right)\right)
$$

## 1. training step (text documents) Cont'd

- Concatenate documents of each class separately

$$
\rightarrow \quad x^{(k)}=\left(x_{j}^{(k)}\right)_{j=1, \ldots, V}, \quad k=1,2
$$

with $x_{k, j}=$ total \# occurrences of word $j$ in documents of class $k$.

- $\theta_{k}=\left(\theta_{k, 1}, \ldots, \theta_{k, v}\right)$ multinomial parameter for class $k$.
- Flat priors on $\boldsymbol{\theta}_{k}: \boldsymbol{\pi}_{1}=\boldsymbol{\pi}_{2}=\operatorname{Diri}(1, \ldots, 1)$
- Posterior mean estimates

$$
\widehat{\theta}_{k}=\mathbb{E}_{\boldsymbol{\pi}_{k}}\left[\boldsymbol{\theta} \mid x^{(k)}\right]=\left(\frac{x_{1}^{(k)}+1}{V+\sum_{j=1}^{V} x_{j}^{(k)}}, \ldots, \frac{x_{V}^{(k)}+1}{V+\sum_{j=1}^{V} x_{j}^{(k)}}\right)
$$

(the prior acts as regularizer : ' +1 ' term avoids 0 probabilities.

## 2. Prediction step

- For a new document $x^{\text {new }}$ the predictive probabilities of each class are :

$$
\pi\left(C=k \mid x^{\text {new }}\right)=\frac{p\left(x^{n e w} \mid C=k\right) \pi_{1}}{p\left(x^{n e w} \mid C=k\right) \pi_{1}+p\left(x^{\text {new }} \mid C=2\right) \pi_{2}}
$$

with

$$
p\left(x^{n e w} \mid C=k\right) \propto \prod_{j=1}^{V}{\widehat{\theta_{k, j}}}^{x_{j}^{n e w}}
$$

- The class prediction is

$$
k^{*}\left(x^{\text {new }}\right)=\underset{k=1,2}{\operatorname{argmax}} p\left(x^{\text {new }} \mid C=k\right)
$$

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## The regression problem

- Supervised learning : training dataset $\left(x_{i}, Y_{i}\right), i \leq n$, with
- $x_{i} \in \mathcal{X}$ the features for observation $i$ (considered non random)
- $Y_{i} \in \mathbb{R}$ the label (random variable).
- goal : for a new observation with features $x_{\text {new }}$, predict $Y_{\text {new }}$, i.e. construct a regression function $h \in \mathcal{H}$, so that $h(x)$ is our best prediction of $Y$ at point $x$.
- $h$ should
- be simple (avoid over-fitting) $\rightarrow$ simple class $\mathcal{H}$.
- fit the data well : measured through a loss function $L(x, y, h)$. example : squared error loss $L(x, y, h)=(y-h(x))^{2}$.


## Multiple classical strategies

- Statistical learning approach : empirical risk minimization

$$
\begin{aligned}
R_{n}\left(x_{1: n}, y_{1: n}, h\right)= & \frac{1}{n} \sum_{1}^{n} L\left(x_{i}, y_{i}, h\right) \\
\rightarrow \underset{h \in \mathcal{H}}{\operatorname{minimize}} \quad & R_{n}\left(x_{1: n}, y_{1: n}, h\right)
\end{aligned}
$$

- Probabilistic modeling approach (likelihood based) : assume e.g.

$$
Y_{i}=h_{0}\left(x_{i}\right)+\epsilon_{i},
$$

$\epsilon_{i} \sim P_{\epsilon}$ independent noises, e.g. $P_{\epsilon}=\mathcal{N}\left(0, \sigma^{2}\right), \sigma^{2}$ known or not.
$\rightarrow$ likelihood of $h, p_{h}\left(x_{1: n}, y_{1: n}\right)=\prod_{i=1}^{n} p_{\epsilon}\left(y_{i}-h\left(x_{i}\right)\right)$.

$$
\rightarrow \underset{h \in \mathcal{H}}{\operatorname{minimize}}-\sum_{i=1}^{n} \log p_{\epsilon}\left(y_{i}-h\left(x_{i}\right)\right)
$$

- With Gaussian noises, both strategies coincide.


## Linear regression

- $h$ : a linear combination of basis functions $\phi_{j}: \mathcal{X} \mapsto \mathbb{R}$ (feature maps), $j \in\{1, \ldots, p\}$

$$
\begin{array}{r}
h(x)=\sum_{j=1}^{p} \theta_{j} \phi_{j}(x), \quad \theta_{j} \text { unknown, } \quad \phi_{j} \text { known, } \quad \text { i.e. } \\
\mathcal{H}=\left\{\sum_{j=1}^{p} \theta_{j} \phi_{j}: \quad \theta=\left(\theta_{1}, \ldots, \theta_{p}\right) \in \mathbb{R}^{p}\right\}
\end{array}
$$

- Examples
- $\mathcal{X}=\mathbb{R}^{p}, \quad \phi_{j}(x)=x_{j}:$ canonical feature map
- $\mathcal{X}=\mathbb{R}, \quad \phi_{j}(x)=x^{j-1}:$
polynomial basis function
- $\mathcal{X}=\mathbb{R}^{d}, \quad \phi_{j}(x)=\frac{1}{(2 \pi)^{d / 2} \operatorname{det} \Sigma_{j}} \exp -\frac{1}{2}\left(x-\mu_{j}\right)^{\top} \Sigma_{j}^{-1}\left(x-\mu_{j}\right)$,

Gaussian basis function

## Empirical risk minimization for linear regression

- Empirical risk :

$$
R_{n}\left(x_{1: n}, y_{1: n}, \theta\right)=\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-\left\langle\theta, \phi\left(x_{i}\right)\right\rangle\right)^{2}=\frac{1}{2}\left\|y_{1: n}-\Phi \theta\right\|^{2}
$$

with $\Phi \in \mathbb{R}^{n \times p}:$ design matrix, $\Phi_{i, j}=\phi_{j}\left(x_{i}\right)$.

- Minimizer of $R_{n}$ : the least squares estimator
- explicit solution when $\Phi^{\top} \Phi$ is of rank $p$ (invertible)

$$
\widehat{\theta}=\left(\Phi^{\top} \Phi\right)^{-1} \Phi^{\top} y_{1: n}
$$

## Regularization

- goals : prevent
- over-fitting
- numerical instabilities (inversion of $\left(\Phi^{\top} \Phi\right)$.
- Add a complexity penalty (function of $\theta$ ) to the empirical risk
- penalty $: \lambda\|\theta\|_{2}^{2} \rightarrow$ ridge regression
- penalty : $\lambda\|\theta\|_{1} \rightarrow$ Lasso regression
- e.g. with $L_{2}$ penalty, the optimization problem becomes

$$
\begin{aligned}
& \hat{\theta}=\underset{\theta}{\operatorname{argmin}}\left\|y_{1: n}-\Phi \theta\right\|^{2}+\lambda\|\theta\|_{2}^{2} \quad \text { for some } \lambda>0 . \\
& \rightarrow \text { solution } \widehat{\theta}=\left[\Phi^{\top} \Phi+\lambda I_{p}\right]^{-1} \Phi^{\top} y_{1: n} .
\end{aligned}
$$

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## Bayesian linear model

- Again, $Y_{i}=\left\langle\theta, \Phi\left(x_{i}\right)\right\rangle+\epsilon_{i}$
- Assume $\epsilon_{i} \sim \mathcal{N}\left(0, \beta^{-1}\right), \beta>0$ noise precision viewed as a constant (known or not)
- Prior distribution on $\boldsymbol{\theta} \in \mathbb{R}^{p}: \boldsymbol{\pi}=\mathcal{N}\left(m_{0}, S_{0}\right)$.
- independence assumption : $\epsilon_{1} \Perp \epsilon_{2} \Perp \cdots \Perp \boldsymbol{\theta}$.
- $Y=Y_{1: n}=\Phi \theta+\epsilon_{1: n}$, with $\Phi \in \mathbb{R}^{n \times p}, \Phi_{i, j}=\phi_{j}\left(x_{i}\right)$.


## Bayesian model

$$
\left\{\begin{array}{l}
\boldsymbol{\theta} \sim \boldsymbol{\pi}=\mathcal{N}\left(m_{0}, S_{0}\right) \\
\mathcal{L}[Y \mid \theta]=\mathcal{N}\left(\Phi \theta, \frac{1}{\beta} I_{n}\right)
\end{array}\right.
$$

- Natural Bayesian estimator : $\widehat{\theta}=\mathbb{E}_{\boldsymbol{\pi}}\left(\boldsymbol{\theta} \mid Y_{1: n}\right)$.
$\rightarrow$ posterior distribution?


## Conditioning and augmenting Gaussian vectors

## Lemma

Let

$$
\left\{\begin{aligned}
W & \sim \mathcal{N}\left(\mu, \Lambda^{-1}\right) \\
\mathcal{L}[Y \mid w] & =\mathcal{N}\left(A w+b, L^{-1}\right)
\end{aligned}\right.
$$

i.e. $Y=A W+b+\epsilon$ with $\epsilon \sim \mathcal{N}\left(0, L^{-1}\right) \Perp W$.

Then $\mathcal{L}[W \mid y]=\mathcal{N}\left(m_{y}, S\right)$ with

$$
\begin{aligned}
S & =\left(\Lambda+A^{\top} L A\right)^{-1} \\
m_{y} & =S\left[A^{\top} L(y-b)+\Lambda \mu .\right]
\end{aligned}
$$

proof : homework (see exercises sheet online)

## Application to posterior computation

Using the lemma with

$$
A=\Phi, \quad b=0, \quad W=\theta, \quad \Lambda=S_{0}^{-1}, \quad \mu=m_{0}, \quad L=\beta I_{p}
$$

we obtain immediately the posterior distribution

$$
\boldsymbol{\pi}\left(\cdot \mid Y_{1: n}\right)=\mathcal{L}\left[\boldsymbol{\theta} \mid y_{1: n}\right]=\mathcal{N}\left(m_{n}, S_{n}\right)
$$

with

$$
\left\{\begin{align*}
S_{n} & =\left(S_{0}^{-1}+\beta \Phi^{\top} \Phi\right)^{-1}  \tag{1}\\
m_{n} & =S_{n}\left(\beta \Phi^{\top} y_{1: n}+S_{0}^{-1} m_{0}\right)
\end{align*}\right.
$$

Posterior mean estimate

$$
\widehat{\theta}=\mathbb{E}_{\boldsymbol{\pi}}\left[\boldsymbol{\theta} \mid y_{1: n}\right]=m_{n}
$$

## Special case : diagonal, centered prior

- choose $m_{0}=0, S_{0}=\alpha^{-1} I_{p}$, with $\alpha$ : prior precision (it makes sense!)
- Then (1) becomes

$$
\left\{\begin{align*}
S_{n}=\left(\alpha I_{p}+\beta \Phi^{\top} \Phi\right)^{-1} & =\beta^{-1}\left(\frac{\alpha}{\beta}+\Phi^{\top} \Phi\right)^{-1}  \tag{2}\\
m_{n}=S_{n}\left(\beta \Phi^{\top} y_{1: n}\right) & =\underbrace{\left(\frac{\alpha}{\beta}+\Phi^{\top} \Phi\right)^{-1} \Phi^{\top} y_{1: n}}_{\text {penalized least squares solution }}
\end{align*}\right.
$$

Adding a prior $\mathcal{N}\left(0, \alpha^{-1} I_{p}\right)$
$\Longleftrightarrow$
Adding a $L_{2}$ regularization with parameter $\lambda=\alpha / \beta$.
remark : Narrow prior $\Longleftrightarrow$ large $\alpha \Longleftrightarrow$ large penalty

## Predictive distribution

New data point $\left(x_{\text {new }}, Y_{\text {new }}\right)$, with $Y_{\text {new }}$ not observed and $x_{\text {new }}$ known:

- goal : obtain the posterior distribution of $Y_{\text {new }}$ (mean and variance $\rightarrow$ credible intervals).
- We still have $Y_{\text {new }}=\left\langle\boldsymbol{\theta}, \phi\left(x_{\text {new }}\right)\right\rangle+\epsilon, \quad \epsilon \sim \mathcal{N}\left(0, \beta^{-1}\right)$ and $\epsilon \Perp \boldsymbol{\theta}$.
- Now (after training step) $\boldsymbol{\theta} \sim \boldsymbol{\pi}\left(\cdot \mid y_{1: n}\right)=\mathcal{N}\left(m_{n}, S_{n}\right)$
- Thus $Y_{\text {new }} \stackrel{\text { d }}{=}$ linear transform of Gaussian vector $(\epsilon, \boldsymbol{\theta})$

$$
\mathcal{L}\left[Y_{\text {new }} \mid y_{1: n}\right]=\mathcal{N}\left(\phi\left(x_{\text {new }}\right)^{\top} m_{n}, \quad \phi\left(x_{\text {new }}\right)^{\top} S_{n} \phi\left(x_{\text {new }}\right)+\beta^{-1}\right)
$$

## Example : polynomial basis functions

- True regression functions : $h_{0}(x)=\sin (x)$
- Polynomial basis functions : $\phi(x)=\left(1, x, x^{2}, x^{3}, x^{4}\right)(p=5)$.



## Estimated regression function

- $\widehat{h}(x)=\langle\widehat{\theta}, \Phi(x)\rangle=\widehat{\theta}_{1}+\sum_{j=2}^{5} \widehat{\theta}_{j} x^{j-1}$
- With the previous dataset



## Predictive distribution

- $\widehat{h}(x)$ : the mean of $\mathcal{L}\left(Y_{\text {new }} \mid y_{1: n}\right)$ for $x_{\text {new }}=x$
- Remind $\mathcal{L}\left(Y_{\text {new }} \mid y_{1: n}\right)=\mathcal{N}\left(\widehat{h}(x), \sigma_{\text {new }}^{2}=\phi(x)^{\top} S_{n} \phi(x)+\beta^{-1}\right)$
- $\rightarrow$ posterior credible interval for $Y$,

$$
I_{x}=\left[\widehat{h}(x)-1 / 96 \sqrt{\sigma_{\text {new }}^{2}}, \widehat{h}(x)+1 / 96 \sqrt{\sigma_{\text {new }}^{2}}\right]
$$



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## Model choice problem

- What if several model in competition $\left\{M_{k}, k \in\{1, \ldots, K\}\right\}$, with $M_{k}=\left\{\Theta_{k}, \pi_{k}\right\} ?$
- Continuous case : family of models $\left\{M_{\alpha}, \alpha \in \mathcal{A}\right\}$
- $\rightarrow$ How to choose $k$ or $\alpha$ ?
- Examples :
- $M_{1}=\left\{\Theta, \pi_{1}\right\}, M_{2}=\left\{\Theta, \pi_{2}\right\}$ with $\boldsymbol{\pi}_{1}$ a flat prior and $\boldsymbol{\pi}_{2}$ the Jeffreys prior
- $M_{\alpha}$ linear model with normal prior on the noise $\mathcal{N}\left(0, \alpha^{-1}\right)$

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## Hierarchical models

- Bayesian view : put a prior on unknown quantities, then condition upon data.
- Model choice problem : put a 'hyper-prior' on $\alpha \in \mathcal{A}$ (or $k \in\{1, \ldots, K\}) \rightarrow$ hierarchical Bayesian model
- Convenient when dealing with parallel experiments


## Example of hierarchical model

Example : 2 rivers with fishes.

- $X_{i} \in\{0,1\}$ : fished fish ill or sound.
- $X_{i} \sim \mathcal{B e r}(\theta)$, with $\theta=\theta_{1}$ in river 1 and $\theta=\theta_{2}$ in river 2 .
- $\theta_{1}$ and $\theta_{2}$ are 2 realizations of $\boldsymbol{\theta} \sim \mathcal{B e t a}(a, b)$
- $\alpha=(a, b)$ : hyper-parameter for the prior
- hierarchical Bayes : put a prior on $\alpha$ (e.g. product of 2 independent Gammas).


## Posterior mean estimates in a BMA framework

- denote $\boldsymbol{\pi}^{h}$ the hyper-prior on $k$ (or $\alpha$ )
- Let us stick to the discrete case,$k \in\{1, \ldots, M\}$.
- The prior is a mixture distribution $\boldsymbol{\pi}=\sum_{k=1}^{K} \pi^{h}(k) \pi_{k}(\cdot)$, i.e. for all $\boldsymbol{\pi}$-integrable function $g(\boldsymbol{\theta})$,

$$
\mathbb{E}_{\boldsymbol{\pi}}[g(\boldsymbol{\theta})]=\mathbb{E}_{\boldsymbol{\pi}^{h}}[\mathbb{E}(g(\boldsymbol{\theta}) \mid k)]=\sum_{k=1}^{K} \pi^{h}(k) \int_{\Theta_{k}} g(\theta) \mathrm{d} \pi_{k}(\theta)
$$

- by the tower rule for conditional expectations, the posterior mean is a weighted average

$$
\begin{aligned}
\widehat{g}=\mathbb{E}_{\boldsymbol{\pi}}\left[g(\boldsymbol{\theta}) \mid X_{1: n}\right] & =\mathbb{E}_{\boldsymbol{\pi}^{h}}\left[\mathbb{E}\left(g(\boldsymbol{\theta}) \mid k, X_{1: n}\right) \mid X_{1: n}\right] \\
& =\sum_{k=1}^{K} \pi^{h}\left(k \mid X_{1: n}\right) \underbrace{\int_{\Theta_{k}} g(\theta) \mathrm{d} \pi_{k}\left(\theta \mid X_{1: n}\right)}_{\widehat{\mathrm{g}}_{k}: \text { posterior mean in model } k}
\end{aligned}
$$

## Model evidence

Computing the posterior mean in the BMA framework requires

- Computing the posterior means in each individual model $\rightarrow k$ 'moderate' tasks
- Averaging them with weights $\pi^{h}\left(k \mid X_{1: n}\right)$, posterior weight of model k
- Bayes formula

$$
\pi^{h}\left(k \mid X_{1: n}\right)=\frac{\pi^{h}(k) p\left(X_{1: n} \mid k\right)}{\sum_{j=1}^{K} \pi^{h}(j) p\left(X_{1: n} \mid j\right)}
$$

with

$$
\begin{aligned}
p\left(X_{1: n} \mid k\right) & =\text { evidence of model } k \\
& =\int_{\Theta_{k}} p\left(X_{1: n} \mid \theta\right) \mathrm{d} \pi_{k}(\theta) \\
& =m_{k}\left(X_{1: n}\right) \text { marginal likelihood of } X_{1: n} \text { in model } k \\
& \text { hard to compute (integral) }
\end{aligned}
$$

## Shortcomings of BMA

- Inference has to be done in each individual model
- Usually one weight (say $\left.\pi\left(k^{*} \mid X_{1: n}\right)\right) \gg$ all others (reason : concentration of the posterior around the true $\theta_{0} \in \Theta_{k_{0}}$ and $k^{*}=k_{0}$ $\Longrightarrow$ final estimate $\widehat{g} \approx \widehat{g}_{k_{0}}$. Other $\widehat{g}_{k}$ 's are almost useless

> Bottleneck : compute $k^{*}$. model choice problem.

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## Posterior weights, model evidence and Bayes factor

Recall $k^{*}=\underset{k}{\operatorname{argmax}} \pi\left(k \mid X_{1: n}\right)=\underset{k}{\operatorname{argmax}} \underbrace{p\left(X_{1: n} \mid k\right)}_{\text {evidence of model } k} \pi^{h}(k)$

- Uniform prior on $k \Longrightarrow$ only the evidence $p\left(X_{1: n} \mid k\right)$ matters.
- in any case : prior influence vanishes with $n$.
- Relevant quantity to compare model $k$ and $j$ :

$$
B_{k j}=\frac{p\left(X_{1: n} \mid k\right)}{p\left(X_{1: n} \mid j\right)}: \quad \text { Bayes factor (Jeffreys, 61) }
$$

- Suggested scale for decision making :

| $\log _{10} B_{k j}$ | $B_{k j}$ | evidence against $B_{j}$ |
| :---: | :---: | :---: |
| $0 \rightarrow 1 / 2$ | $1 \rightarrow 3.2$ | not significant |
| $1 / 2 \rightarrow 1$ | $3.2 \rightarrow 10$ | substantial |
| $1 \rightarrow 2$ | $10 \rightarrow 100$ | strong |
| $>2$ | $>100$ | decisive |

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## Occam's razor principle

Between 2 models explaining the data equally well, one ought to choose the simplest one.
$\rightarrow$ Avoid over-fitting
$\rightarrow$ Better generalization properties.

## Occam's razor and model evidence

- When selecting $k^{*}$ according to the model evidences $p\left(X_{1: n} \mid k\right)$, the Occam's razor is automatically implemented.
- Reason : the prior plays the role of a regularizer.


## automatic complexity penalty : intuition 1

Complex model $\Longrightarrow$ large $\Theta_{k}$
$\Longrightarrow$ small $\pi_{k}(\theta)$ (if uniform over $\Theta_{k}$ )
$\Longrightarrow \int_{\Theta_{k}} p_{\theta}\left(x_{1: n}\right) \pi_{k}(\theta) \mathrm{d} \theta$ small
(average over large regions where $p_{\theta}\left(x_{1: n}\right)$ small)

## automatic complexity penalty : intuition 2

- if $\Theta_{k} \subset \mathbb{R}:$ assume
- $\pi_{k}$ flat over interval of length $\Delta_{k}^{\text {prior }}$
- $p_{\theta_{k}}\left(X_{1: n}\right)$ peaked around $p_{\hat{\theta}_{\text {MAP }, k}}\left(X_{1: n}\right)$ with 'width' $\Delta_{k}^{\text {posterior }}$.
- then $\pi_{k}(\theta) \approx 1 / \Delta_{k}^{\text {prior }}$ and

$$
p\left(X_{1: n} \mid k\right)=\int_{\Theta_{k}} p_{\theta}(x) \pi_{k}(\theta) \mathrm{d} \theta \approx p_{\widehat{\theta}_{M A P, k}}\left(X_{1: n}\right) \underbrace{\frac{\Delta \theta_{k}^{\text {posterior }}}{\Delta \theta_{k}^{\text {prior }}}}_{\text {complexity penalty }}
$$

- If $\Theta_{k} \subset \mathbb{R}^{d}$ and same approximation in each dimension

$$
\log p\left(X_{1: n} \mid k\right) \approx \log p_{\widehat{\theta}_{M A P, k}}\left(X_{1: n}\right)+\underbrace{d \log \frac{\Delta \theta_{k}^{\text {posterior }}}{\Delta \theta_{k}^{\text {prior }}}}_{\text {dimension }+ \text { complexity penalty }}
$$

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2. Bayesian linear regression
3. Bayesian model choice

Bayesian model averaging
Bayesian model selection
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