

Introduction to Bayesian learning

Lecture 2: Bayesian methods for (un)supervised problems

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1. Lecture 1 Cont'd : Conjugate priors and exponential family.

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Prior choice

2. Lecture 1 Cont'd : A glimpse at Bayesian asymptotics

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Laplace approximation and BIC criterion

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Reminder : conjugate priors

last lecture (see lecture notes)

- Definition : hyper parameter, conjugate family
- examples :
 - normal model, known variance - normal prior
 - normal model, known mean - gamma prior on inverse variance
 - normal model , unknown mean and variance : normal-gamma prior on $(\mu, \lambda = 1/\sigma^2)$

conjugate priors for multivariate normal

- $X \sim \mathcal{N}(\mu, \Lambda^{-1})$, $\mu \in \mathbb{R}^d$, $\Lambda \in \mathbb{R}^{d \times d}$ positive, definite (precision matrix : inverse of covariance matrix)
1. unknown mean \rightarrow conjugate prior family on μ : a multivariate Gaussian distributions
 2. unknown precision \rightarrow conjugate prior on Λ : Wishart distributions $\mathcal{W}(\nu, W)$ with ν degrees of freedom ($\nu \in \mathbb{N}^*$) and $W \in \mathbb{R}^{d \times d}$.

Wishart distribution

defined on the cone of positive definite matrices.

- The Wishart distribution $\mathcal{W}(\nu, W)$ has density

$$f_{\mathcal{W}}(\Lambda|\nu, W) = B \det \Lambda^{(\nu-d-1)/2} \exp \left\{ \frac{-1}{2} \text{Tr}(W^{-1}\Lambda) \right\}$$

w.r.t. Lebesgue on $\mathbb{R}^{\frac{d(d+1)}{2}}$: $\prod_{i \leq j} d\Lambda_{(i,j)}$, restricted to the set of positive definite matrices.

- B : a normalizing constant.
- probabilistic representation : let M be a random $\nu \times d$ matrix with *i.i.d.* rows $M_{(i, \cdot)} \sim \mathcal{N}(0, W)$. Then

$$\Lambda \sim \mathcal{W}(\nu, W) \iff \Lambda \stackrel{d}{=} M^{\top} M = \sum_{i=1}^n M_{(i, \cdot)}^{\top} M_{(i, \cdot)}$$

- More details : see *e.g.* *Eaton, Multivariate Statistics : A Vector Space Approach, 2007 (Chapter 8)*

conjugate priors for multivariate normal, Cont'd

3. Unknown mean and precision \rightarrow conjugate prior family on (μ, Λ) : the Gaussian-Wishart distribution with hyper-parameters (W, ν, m, β)

$$\pi(\mu, \Lambda) = \pi_1(\Lambda)\pi_2(\mu|\Lambda)$$

with

$$\begin{aligned}\pi_2 &= \mathcal{W}(W, \nu), \nu \in \mathbb{N}, W \text{ positive definite,} \\ \pi_2(\cdot | \Lambda) &= \mathcal{N}(m, (\beta\Lambda)^{-1}), \quad m \in \mathbb{R}^d, \beta > 0\end{aligned}$$

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Definition : exponential family

A dominated parametric model $\mathcal{P} = \{P_\theta, \theta \in \Theta\}$ is an *exponential family* if the densities write

$$p_\theta(x) = C(\theta)h(x) \exp \left\{ \langle T(x), R(\theta) \rangle \right\}$$

for some functions

$$\begin{aligned} R : \Theta &\rightarrow \mathbb{R}^k, & T : \mathcal{X} &\rightarrow \mathbb{R}^k, \\ C : \Theta &\rightarrow \mathbb{R}_+^*, & h : \mathcal{X} &\rightarrow \mathbb{R}_+^*. \end{aligned}$$

- $C(\theta)$: a normalizing constant
- $R(\theta)$: the *natural parameter* (R : the ‘good’ re-parametrization)
- If $R(\theta) = \theta$, the family is *natural*.
- Most textbook distributions are from the exponential family !

Example I : Bernoulli model

- $\theta \in \Theta =]0, 1[, \mathcal{X} = \{0, 1\}$
- The model is dominated by $\lambda = \delta_0 + \delta_1$

$$\begin{aligned} p_{\theta}(x) &= \theta^x (1 - \theta)^{1-x} \\ &= \exp\{x \log \theta + (1 - x) \log(1 - \theta)\} \\ &= (1 - \theta) \exp\left\{ \underbrace{x}_{T(x)} \underbrace{\log \frac{\theta}{1 - \theta}}_{R(\theta)} \right\} \end{aligned}$$

- The model is an exponential family with
 - $T(x) = x$
 - natural parameter : $\rho = R(\theta) = \log \frac{\theta}{1 - \theta}$.
 - normalizing constant $C(\theta) = (1 - \theta)$

Example II : Gaussian model

- $\theta = (\mu, \sigma^2) \in \Theta = \mathbb{R} \times \mathbb{R}_+^*$
- the model is dominated by Lebesgue on $\mathcal{X} = \mathbb{R}$.

$$\begin{aligned} p_{\theta}(x) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ \frac{-(x^2 - 2\mu x + \mu^2)}{2\sigma^2} \right\} \\ &= \underbrace{\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ \frac{-\mu}{2\sigma^2} \right\}}_{C(\theta)} \exp \left\langle \underbrace{\begin{pmatrix} x \\ x^2 \end{pmatrix}}_{T(x)}, \underbrace{\begin{pmatrix} \mu/\sigma^2 \\ -1/(2\sigma^2) \end{pmatrix}}_{R(\theta)} \right\rangle \end{aligned}$$

- The model is an exponential family with
 - $T(x) = (x, x^2)$
 - natural parameter : $\rho = R(\theta) = (\mu/\sigma^2, -1/2\sigma^2)$.
 - normalizing constant $C(\theta) = (2\pi\sigma^2)^{-1/2}$

likelihood for *i.i.d.* samples in exponential families

$$p_{\theta}(x_1) = C(\theta)h(x) \exp \left\{ \langle R(\theta), T(x_1) \rangle \right\}$$

$$\Rightarrow$$

$$p_{\theta}^{\otimes n}(x_{1:n}) = C(\theta) \underbrace{\prod_{i=1}^n h(x_i)}_{h_n(x_{1:n})} \exp \left\{ \left\langle \underbrace{\sum_{i=1}^n T(x_i)}_{T_n(x_{1:n})}, R(\theta) \right\rangle \right\}.$$

Natural parameter space

- natural parametrization : $\rho = R(\theta)$.
- The density $p_\rho(x) = C(\rho)h(x)\exp\langle T(x), \rho \rangle$ integrates to 1
 $\iff \rho \in \mathcal{E}$, the *natural parameter space*, i.e.

$$\mathcal{E} = \left\{ \rho : \int_{\mathcal{X}} h(x) \exp \langle T(x), \rho \rangle d\lambda(x) < \infty \right\}$$

- If \mathcal{E} is open : the family is *regular*.

Maximum likelihood in regular exponential families

natural parametrization : $\rho = R(\theta)$. λ : reference measure.

lemma : expression for $\mathbb{E}_\rho[T(X)]$

$$\mathbb{E}_\rho[T(X)] = -\nabla_\rho \{\ln C(\rho)\}$$

Proof

$$1 \equiv C(\rho) \int_{\mathcal{X}} h(x) \exp \langle T(x), \rho \rangle d\lambda(x)$$

(with regularity to exchange \int and ∇) \Rightarrow

$$0 = \nabla_\rho C(\rho) \underbrace{\int_{\mathcal{X}} h(x) \exp \langle T(x), \rho \rangle d\lambda(x)}_{C(\rho)^{-1}} + C(\rho) \int_{\mathcal{X}} h(x) T(x) \exp \langle T(x), \rho \rangle d\lambda(x)$$

$$\Rightarrow 0 = \frac{1}{C(\rho)} \nabla_\rho C(\rho) + \mathbb{E}(T(X))$$



Maximum likelihood in regular exponential families, cont'd

proposition

The MLE estimator $\hat{\rho}$ in a regular exponential family satisfies

$$\mathbb{E}_{\hat{\rho}}[T(X)] = \frac{1}{n} \sum_i T(x_i).$$

Proof

$$\begin{aligned} \nabla_{\rho} \log p_{\hat{\rho}}(x) = 0 &\iff \nabla_{\rho} \{n \log C(\rho) + \langle \sum T(x_i), \rho \rangle\} = 0 \\ &\iff \nabla_{\rho} \log C(\hat{\rho}) = \frac{-1}{n} \sum_i T(x_i). \end{aligned}$$

then use the lemma. □

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Conjugate priors in exponential family

Proposition

A natural exponential family with densities

$p_{\theta}(x) = C(\theta)h(x)\exp\langle\theta, T(x)\rangle$, admits a conjugate prior family

$\mathcal{F} = \{\pi_{\lambda,\mu}, \lambda > 0, \mu \in M_{\lambda} \subset \mathbb{R}^k\}$, with

$$\pi_{\lambda,\mu}(\theta) = K(\mu, \lambda)C(\theta)^{\lambda} \exp\{\langle\theta, \mu\rangle\}$$

and $M_{\lambda} = \{\mu : \int_{\Theta} \pi(\mu, \lambda) d\theta < \infty\}$.

The posterior for n observation is

$$\pi_{\lambda,\mu}(\theta|x_{1:n}) \propto C(\theta)^{\lambda+n} \exp\{\langle\theta, \mu + \sum_i T(x_i)\rangle\}$$

so that $\pi_{\lambda,\mu}(\cdot|x_{1:n}) = \pi_{\lambda_n,\mu_n}(\cdot)$, with

$$\lambda_n = \lambda + n; \quad \mu_n = \mu + \sum_i T(x_i)$$

Example : Poisson model

$$\begin{aligned}p_{\theta}(x) &= e^{-\theta} \theta^x / x!, & \mathcal{X} = \mathbb{N}, \theta > 0 \\ &= \frac{1}{x!} e^{-\theta} e^{x \log \theta}\end{aligned}$$

→ an exponential family with

$$T(x) = x, \quad \rho = R(\theta) = \log \theta \in \mathbb{R}, \quad C(\rho) = \exp\{-e^{\rho}\}$$

conjugate prior for ρ :

$$\pi_{a,b}(\rho) \propto \exp\{-be^{\rho}\} \exp\{a\rho\}.$$

Back to θ :

$$\pi(\theta) = " \frac{d\pi}{d\rho} \frac{d\rho}{d\theta} " = \theta^{a-1} \exp\{-b\theta\} \quad (\text{Gamma density})$$

→ The Gamma family is a conjugate prior for θ .

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About the choice of a conjugate prior

- A convenient choice only
- One must still choose hyper-parameters (λ, μ)
- This is an issue of *model choice*
- possible to do so via *empirical Bayes* methods, see lecture 2 and lab session.

Other prior choices : non informative priors

- Goal : minimize the bias induced by the prior
- If Θ compact : one can choose $\pi(\theta) = \text{Constant}$
- If Θ non compact, $\int_{\Theta} \pi(\theta) d\theta = \int_{\Theta} C d\theta = +\infty$
OK to do so as long as the posterior is well defined, *i.e.* when

$$\int_{\Theta} p_{\theta}(x) d\pi(\theta) < \infty.$$



uniform only *w.r.t.* the reference measure \rightarrow not invariant under re-parametrization.

e.g. Flat prior on $]0, 1[$ in a $\mathcal{Ber}(\theta)$ model \rightarrow non flat over $\rho = \log[\theta/(1 - \theta)]$

Other prior choices : Jeffreys prior

- For Θ open in \mathbb{R}^d . Reasonable with $d = 1$.
- Remind the Fisher information (in a regular model) :

$$I(\theta) = \mathbb{E}_{\theta} \left[\left(\frac{\partial \log p_{\theta}(X)}{\partial \theta} \right)^2 \right] = -\mathbb{E} \left[\frac{\partial^2 \log p_{\theta}(X)}{\partial \theta^2} \right].$$

- $I(\theta)$ is the expected curvature of the likelihood around θ .
- Interpretation as a an average information carried by X about θ .
- Idea : grant more prior mass to highly informative θ 's

Definition : Jeffreys prior

In a dominated model with densities $p_{\theta}, \theta \in \Theta$, the Jeffreys prior has densities *w.r.t.* Lebesgue on Θ :

$$\pi(\theta) \propto \sqrt{I(\theta)}.$$

- **exercise** compute the Jeffreys prior in the Bernoulli model, in the location model $\mathcal{N}(\theta, \sigma^2)$, σ^2 known and in the scale model $\mathcal{N}(\mu, \theta^2)$, μ known.

Invariance of the Jeffreys prior

- Change of variable : $h(\theta) = \eta$. Then $p_\theta = p_{h(\theta)}$.
- Let $\theta \sim \pi_{J,\theta}$ the Jeffreys prior. Then $\eta \sim \pi_{J,\theta} \circ h^{-1}$ with density

$$\pi(\eta) \stackrel{\text{for } \theta=h^{-1}(\eta)}{=} \pi_{J,\theta}(\theta) \frac{d\theta}{d\eta} = \frac{\sqrt{I(\theta)}}{h'(\theta)}$$

- On the other hand compute the Jeffreys prior on η :

$$\begin{aligned} \pi_{J,\eta}(\eta) &= \sqrt{I_\eta(\eta)} = \mathbb{E}_\eta \left[\left(\frac{\partial \log p_\eta(X)}{\partial \eta} \right)^2 \right]^{1/2} \\ &\stackrel{\theta=h^{-1}(\eta)}{=} \mathbb{E}_\theta \left[\left(\frac{\partial \log p_\theta(X)}{\partial \theta} \frac{d\theta}{d\eta} \right)^2 \right]^{1/2} = \frac{\sqrt{I(\theta)}}{h'(\theta)}. \end{aligned}$$

- Same result : the Jeffreys prior in the η parametrization is the image measure of the Jeffreys prior in the θ parametrization.
- In other words the Jeffreys prior is parametrization-invariant.

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Rough overview

as the sample size $n \rightarrow \infty$

- The influence of the prior choice vanishes
- The posterior distribution concentrates around the true value θ_0 (almost surely)
- The posterior distribution is asymptotically normal with mean $\hat{\theta}$ = the maximum likelihood, and variance $n^{-1}I(\theta)^{-1}$ (same as MLE's)

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Reminder : Beta-Binomial model

- Bayesian model $\begin{cases} \theta \sim \pi = \text{Beta}(a, b) \\ X|\theta \sim \text{Ber}(\theta). \end{cases}$
- P_θ^∞ : distribution over \mathcal{X}^∞ of the random sequence $(X_n)_{n \geq 1} \stackrel{\text{i.i.d}}{\sim} P_\theta$
- posterior distribution (conjugate prior) :

$$\pi(\cdot | x_{1:n}) = \text{Ber}(a + s, b + n - s), \quad s = \sum_1^n x_i.$$

Posterior expectation and variance

$$\begin{aligned}\mathbb{E}_{\pi}(\theta|X_{1:n}) &= \frac{a + \sum_1^n X_i}{a + b + n} \\ &= \frac{a/n + \frac{1}{n} \sum_1^n X_i}{(a + b)/n + 1} \\ &\xrightarrow[n \rightarrow \infty]{a.s.} \theta_0 \quad \text{under } P_{\theta_0}^{\infty}\end{aligned}$$

$$\begin{aligned}\text{Var}_{\pi}(\theta|X_{1:n}) &= \frac{\left(a + \sum_1^n X_i\right)\left(b + n - \sum_1^n X_i\right)}{\left(a + b + n\right)^2\left(a + b + n + 1\right)} \\ &= \frac{1}{n} \frac{\left(a/n + \frac{1}{n} \sum_1^n X_i\right)\left(b/n + 1 - \frac{1}{n} \sum_1^n X_i\right)}{\left((a + b)/n + 1\right)^2\left((a + b + 1)/n + 1\right)} \\ &\underset{P_{\theta_0}^{\infty}\text{-a.s.}}{\sim} \frac{\theta_0(1 - \theta_0)}{n} \quad \underset{\text{exercise}}{=} \quad (n I(\theta_0))^{-1}\end{aligned}$$

Concentration of the posterior distribution

- Write $\theta_n^* = \theta_n^*(X_{1:n}) = \mathbb{E}_\pi(\theta|X_{1:n})$.
- Tchebychev inequality $\Rightarrow \forall \delta > 0, \forall U = (\theta_n^* - \delta, \theta_n^* + \delta)$,

$$\begin{aligned}\mathbb{P}_\pi(\theta \notin U|X_{1:n}) &= \mathbb{P}_\pi\left((\theta - \theta_n^*)^2 > \delta^2|X_{1:n}\right) \\ &\leq \frac{\text{Var}_\pi(\theta|X_{1:n})}{n\delta^2} \\ &\underset{\text{P}_{\theta_0}^\infty - \text{a.s.}}{\sim} \frac{\theta_0(1 - \theta_0)}{n\delta^2} \underset{n \rightarrow \infty}{\overset{\text{a.s.}}{\rightarrow}} 0.\end{aligned}$$

- summary : $\text{P}_{\theta_0}^\infty$ - a.s., we have that
 - The posterior distribution concentrates around the posterior expectancy θ_n^*
 - $\theta_n^* \xrightarrow[n \rightarrow \infty]{} \theta_0$.

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Posterior consistency

Definition

Let $\{P_\theta, \theta \in \Theta\}$, π be a Bayesian model and let $\theta_0 \in \Theta$. The posterior is *consistent* at θ_0 if For all neighborhood U of θ_0 ,

$$\pi(U|X_{1:n}) \xrightarrow[n \rightarrow \infty]{} 1, \quad P_{\theta_0}^\infty\text{-a.s.}$$

- In general consistency holds when Θ is finite dimensional if π assigns positive mass to θ_0 's neighborhoods.
- See *e.g.* [Ghosh and Ramamoorthi, 2003], Chapter 1.3, 1.4 for details

Doob's theorem

Theorem

If Θ and \mathcal{X} are complete, separable, metric spaces endowed with their Borel σ -field, if $\theta \mapsto P_\theta$ is 1 to 1, then for any prior π on Θ , $\exists \Theta_0 \subset \Theta$ with $\pi(\Theta_0) = 1$ such that for all $\theta_0 \in \Theta_0$, the posterior is consistent at θ_0 .

- **issue** The π -negligible set where consistency does not hold may be large.
- Under additional regularity conditions, consistency holds at a given θ_0 .

Consistency at a given θ_0 .

Theorem([Ghosh and Ramamoorthi, 2003], Th. 1.3.4)

Let Θ be compact, metric and $\theta_0 \in \Theta$. Let $T(x, \theta) = \log \frac{p_\theta(x)}{p_{\theta_0}(x)}$. Assume

1. $\forall x \in \mathcal{X}, \theta \mapsto T(x, \theta)$ is continuous
2. $\forall \theta \in \Theta, x \mapsto T(x, \theta)$ is measurable
3. $\mathbb{E}(\sup_{\theta \in \Theta} |T(\theta, X_1)|) < \infty$.

Then

1. The maximum likelihood estimator is consistent at θ_0 (CV in proba)
2. If $\theta_0 \in \text{Supp}(\pi)$, then the posterior is consistent at θ_0 .

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Bayesian asymptotic normality : Overview

- Tells us about the rate of convergence of $\pi(\cdot | X_{1:n})$ towards δ_{θ_0} .
- With a \sqrt{n} re-scaling, a Gaussian limit centered at the MLE (under appropriate regularity conditions)
- Good references : [Van der Vaart, 1998], [Ghosh and Ramamoorthi, 2003], [Schervish, 2012]

Bernstein - Von Mises Theorem

(stated for $\Theta \subset \mathbb{R}$, similar statements for $\Theta \subset \mathbb{R}^d$).

Theorem

Under appropriate regularity conditions (detailed in [Ghosh and Ramamoorthi, 2003], Th. 1.4.2),

Let $\mathbf{s} = \sqrt{n}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_n(X_{1:n}))$, with $\hat{\boldsymbol{\theta}}(X_{1:n})$ the MLE. Let $\pi^*(s|X_{1:n})$ be the posterior density of \mathbf{s} . Then

$$\int_{\mathbb{R}} \left| \pi^*(s|X_{1:n}) - \sqrt{\frac{I(\theta_0)}{2\pi}} e^{\frac{-s^2 I(\theta_0)}{2}} \right| ds \xrightarrow[n \rightarrow \infty]{a.s.} 0 \text{ under } P_{\theta_0}^\infty$$

- Interpretation : as $n \rightarrow \infty$,

$$\sqrt{n}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_n(X_{1:n})) \overset{d}{\approx} \mathcal{N}(0, I(\theta_0)^{-1}), \text{ i.e.}$$

$$\boldsymbol{\theta} \overset{d}{\approx} \mathcal{N}\left(\hat{\boldsymbol{\theta}}_n, \frac{I(\theta_0)^{-1}}{n}\right)$$

- Multivariate case : similar result with multivariate Gaussian and Fisher information matrix.

Asymptotic normality of the posterior mean

$$\theta_n^* = \mathbb{E}_{\pi}[\theta | X_{1:n}], \quad \hat{\theta}_n : \text{maximum likelihood.}$$

Theorem

In addition to the assumptions of BVM Theorem, assume $\int_{\mathbb{R}} |\theta| \pi(\theta) d\theta < \infty$. Then under $P_{\theta_0}^{\infty}$,

1. $\sqrt{n}(\theta_n^* - \hat{\theta}_n) \xrightarrow[n \rightarrow \infty]{} 0$ in probability
2. $\sqrt{n}(\theta_n^* - \theta_0) \xrightarrow[n \rightarrow \infty]{d} \mathcal{N}(0, I(\theta_0)^{-1})$.

Regularity conditions for BVM theorem

1. $\{x \in \mathcal{X} : p_\theta(x) > 0\}$ does not depend on θ
2. $L(\theta, x) = \log p_\theta(x)$ is three times differentiable *w.r.t.* θ in a neighborhood of θ_0 .
3. $\mathbb{E}_{\theta_0} |\frac{\partial}{\partial \theta} L(\theta_0, X)| < \infty, \mathbb{E}_{\theta_0} |\frac{\partial^2}{\partial \theta^2} L(\theta_0, X)| < \infty$ and $\mathbb{E}_{\theta_0} \sup_{\theta \in (\theta_0 - \delta, \theta_0 + \delta)} |\frac{\partial^3}{\partial \theta^3} L(\theta, X)| < \infty$
4. $\int_{\mathcal{X}}$ and ∂_θ may be interchanged.
5. $I(\theta_0) > 0$.

Remark : under these conditions the MLE is asymptotically normal, $\sqrt{n}(\hat{\theta}_n - \theta_0) \xrightarrow{d} \mathcal{N}(0, I(\theta_0)^{-1})$ as well.

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Setting



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

- Sample space $\mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_d$ (d features)
- some features may be categorical, some discrete, some continuous
...
- data $X_i = (X_{i,1}, \dots, X_{i,d})$, $i = 1, \dots, n$.
- Classification problem : X_i may come from anyone of K classes $(\mathcal{C}_1, \dots, \mathcal{C}_K)$.
- 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 $c \in \{1, \dots, K\}$ of a new patient.

Naive Bayes assumption

Conditionally to the class $c(i) \in \{1, \dots, K\}$ of observation i , the features $(X_{i,1}, \dots, X_{i,d})$ 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 $\{(x_{i,j}, c(i)), i \in \{1, \dots, n\}, j \in \{1, \dots, d\}\}$, $c(i) \in \{1, \dots, K\}$.
- for $k \in \{1, \dots, K\}$:
 - Retain observations of class $k \rightarrow i \in I_k$.
 - For $j \in \{1, \dots, d\}$ estimate the class distribution, with density

$$p_{j,k}(x_j) = p(x_{i,j} | c(i) = k),$$

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

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

$$p_k(x) = \prod_{j=1}^k p_{j,k,\hat{\theta}_{j,k}}(x_j)$$

2. computing the predictive class probabilities

input :

- new data point $\mathbf{x} = (x_1, \dots, x_d)$
- From step 1 : conditional distributions of X given $C = k$:
 $p_k(\cdot) = \prod p_{j,k,\hat{\theta}_{j,k}}$ (plug-in method, neglect estimation error of $\hat{\theta}_{j,k}$).

- (a) Assign a prior probability to each class : $\pi = (\pi_1, \dots, \pi_K)$,
 $\pi_k = \mathbb{P}_\pi(C = k)$.

step 1 \rightarrow joint density of (X, C) : $q(x, k) = \pi_k p_k(x)$.

- (b) Apply the discrete Bayes formula :

$$\pi(k|x) = \frac{\pi_k p_k(x)}{\sum_{c=1}^K \pi_c p_c(x)} = \frac{\pi_k \prod_{j=1}^d p_{j,k,\hat{\theta}_{j,k}}(x_j)}{\sum_{c=1}^K \pi_c \prod_{j=1}^d p_{j,c,\hat{\theta}_{j,c}}(x_j)}$$

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

3. final step : class prediction

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

$$\hat{c} = \operatorname{argmax}_{k \in \{1, \dots, k\}} \pi(k|x).$$

(a maximum a posteriori)

Example : text documents classification

- 2 classes : $\{1 = \text{spam}, 2 = \text{non spam}\}$
- vocabulary $\mathcal{V} = \{w_1, \dots, w_V\}$.
- dataset : documents (email) $T_i = (T_{i,j}, j = 1, \dots, N_i), i \leq n$ with
 - N_i : number of words in T_i
 - $t_{i,j} \in \mathcal{V} : j^{th}$ 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 the vocabulary \mathcal{V}
- T_i can be summarized by a ‘bag of words’ $X_i = (X_{i,1}, \dots, X_{i,V}) :$

$X_{i,j}$: number of occurrences of word j in T_i .

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

$$\mathcal{L}(X_i | C = k) = \text{Multi}(\theta_k = (\theta_{1,k}, \dots, \theta_{V,k}), N_i), \quad i.e.$$

$$p_{k, \theta_k}(x) = \frac{N_i!}{\prod_{j=1}^V x_{i,j}!} \prod_{j=1}^V \theta_{j,k}^{x_{i,j}}$$

1. training step (text documents)

Fit separately 2 Multinomial models on spam and non-spam

- Here : the Dirichlet prior $\mathcal{Diri}(a_1, \dots, a_V)$, $a_j > 0$ is conjugate for the Multinomial model, with density

$$\text{diri}(\theta|a_1, \dots, a_V) = \frac{\Gamma(\sum_{j=1}^V a_j)}{\prod_{j=1}^V \Gamma(a_j)} \prod_{j=1}^V \theta_j^{a_j-1}$$

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

- Mean of θ under $\pi = \mathcal{Diri}(a_1, \dots, a_V)$:

$$\mathbb{E}_{\pi}(\theta) = \left(\frac{a_1}{\sum_j a_j}, \dots, \frac{a_V}{\sum_j a_j} \right)$$

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

$$\mathcal{Diri}\left((a_1 + \sum_{i=1}^n x_{i,1}), \dots, (a_V + \sum_{i=1}^n x_{i,V})\right).$$

1. training step (text documents) Cont'd

- Concatenate documents of each class separately

$$\rightarrow \mathbf{x}^{(k)} = (x_j^{(k)})_{j=1,\dots,V}, \quad k = 1, 2$$

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

- $\theta_k = (\theta_{k,1}, \dots, \theta_{k,V})$ multinomial parameter for class k .
- Flat priors on θ_k : $\pi_1 = \pi_2 = \text{Diri}(1, \dots, 1)$
- Posterior mean estimates

$$\hat{\theta}_k = \mathbb{E}_{\pi_k}[\theta | \mathbf{x}^{(k)}] = \left(\frac{x_1^{(k)} + 1}{V + \sum_{j=1}^V x_j^{(k)}}, \dots, \frac{x_V^{(k)} + 1}{V + \sum_{j=1}^V x_j^{(k)}} \right)$$

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

2. Prediction step

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

$$\pi(C = k|x^{new}) = \frac{p(x^{new}|C = k)\pi_1}{p(x^{new}|C = k)\pi_1 + p(x^{new}|C = 2)\pi_2}$$

with

$$p(x^{new}|C = k) \propto \prod_{j=1}^V \widehat{\theta}_{k,j}^{x_j^{new}}$$

- The class prediction is

$$k^*(x^{new}) = \operatorname{argmax}_{k=1,2} p(x^{new}|C = k)$$

1. Lecture 1 Cont'd : Conjugate priors and exponential family.

Introduction, examples

Exponential family

conjugate priors in exponential families

Prior choice

2. Lecture 1 Cont'd : A glimpse at Bayesian asymptotics

Example : Beta-Binomial model

Posterior consistency

Asymptotic normality

3. Supervised learning example : Naive Bayes Classification

4. Bayesian linear regression

Regression : reminders

Bayesian linear regression

5. Bayesian model choice

Bayesian model averaging

Bayesian model selection

Automatic complexity penalty

Laplace approximation and BIC criterion

Empirical Bayes

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The regression problem

- Supervised learning : training dataset (x_i, Y_i) , $i \leq n$, 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_{new} , predict Y_{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

$$R_n(x_{1:n}, y_{1:n}, h) = \frac{1}{n} L(x_i, y_i, h) \\ \rightarrow \underset{h \in \mathcal{H}}{\text{minimize}} \quad R_n(x_{1:n}, y_{1:n}, h)$$

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

$$Y_i = h_0(x_i) + \epsilon_i ,$$

$\epsilon_i \sim P_\epsilon$ independent noises, *e.g.* $P_\epsilon = \mathcal{N}(0, \sigma^2)$, σ^2 known or not.

\rightarrow likelihood of h , $p_h(x_{1:n}, y_{1:n}) = \prod_{i=1}^n p_\epsilon(y_i - h(x_i))$.

$$\rightarrow \underset{h \in \mathcal{H}}{\text{minimize}} \quad - \sum_{i=1}^n \log p_\epsilon(y_i - h(x_i))$$

- With Gaussian noises, both strategies coincide.

Linear regression

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

$$h(x) = \sum_{j=1}^p \theta_j \phi_j(x), \quad \theta_j \text{ unknown, } \phi_j \text{ known, } \quad i.e.$$

$$\mathcal{H} = \left\{ \sum_{j=1}^p \theta_j \phi_j : \quad \theta = (\theta_1, \dots, \theta_p) \in \mathbb{R}^p \right\}$$

- 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
- $\mathcal{X} = \mathbb{R}^d, \quad \phi_j(x) = \frac{1}{(2\pi)^{d/2} \det \Sigma_j} \exp -\frac{1}{2}(x - \mu_j)^\top \Sigma_j^{-1}(x - \mu_j),$
Gaussian basis function

Empirical risk minimization for linear regression

- Empirical risk :

$$R_n(\mathbf{x}_{1:n}, \mathbf{y}_{1:n}, \theta) = \frac{1}{2} \sum_{i=1}^n (y_i - \langle \theta, \phi(\mathbf{x}_i) \rangle)^2 = \frac{1}{2} \|\mathbf{y}_{1:n} - \Phi \theta\|^2,$$

with $\Phi \in \mathbb{R}^{n \times p}$: design matrix, $\Phi_{i,j} = \phi_j(\mathbf{x}_i)$.

- Minimizer of R_n : the *least squares* estimator
- explicit solution when $\Phi^\top \Phi$ is of rank p (invertible)

$$\hat{\theta} = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{y}_{1:n}$$

Regularization

- **goals** : prevent
 - over-fitting
 - numerical instabilities (inversion of $(\Phi^\top \Phi)$).
- Add a complexity penalty (function of θ) 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

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \|\mathbf{y}_{1:n} - \Phi\theta\|^2 + \lambda \|\theta\|_2^2 \quad \text{for some } \lambda > 0.$$

$$\rightarrow \text{solution } \hat{\theta} = \left[\Phi^\top \Phi + \lambda I_p \right]^{-1} \Phi^\top \mathbf{y}_{1:n}.$$

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Bayesian linear model

- Again, $Y_i = \langle \theta, \Phi(x_i) \rangle + \epsilon_i$
- Assume $\epsilon_i \sim \mathcal{N}(0, \beta^{-1})$, $\beta > 0$ noise precision viewed as a constant (known or not)
- Prior distribution on $\theta \in \mathbb{R}^p$: $\pi = \mathcal{N}(m_0, S_0)$.
- independence assumption : $\epsilon_1 \perp\!\!\!\perp \epsilon_2 \perp\!\!\!\perp \dots \perp\!\!\!\perp \theta$.
- $Y = Y_{1:n} = \Phi\theta + \epsilon_{1:n}$, with $\Phi \in \mathbb{R}^{n \times p}$, $\Phi_{ij} = \phi_j(x_i)$.

Bayesian model

$$\begin{cases} \theta \sim \pi = \mathcal{N}(m_0, S_0) \\ \mathcal{L}[Y|\theta] = \mathcal{N}(\Phi\theta, \frac{1}{\beta}I_n) \end{cases}$$

- Natural Bayesian estimator : $\hat{\theta} = \mathbb{E}_{\pi}(\theta|Y_{1:n})$.
→ posterior distribution ?

Conditioning and augmenting Gaussian vectors

Lemma

Let

$$\begin{cases} W \sim \mathcal{N}(\mu, \Lambda^{-1}) \\ \mathcal{L}[Y|w] = \mathcal{N}(Aw + b, L^{-1}) \end{cases}$$

i.e. $Y = AW + b + \epsilon$ with $\epsilon \sim \mathcal{N}(0, L^{-1}) \perp\!\!\!\perp W$.

Then $\mathcal{L}[W|y] = \mathcal{N}(m_y, S)$ with

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

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

$$\pi(\cdot | Y_{1:n}) = \mathcal{L}[\theta | y_{1:n}] = \mathcal{N}(m_n, S_n)$$

with

$$\begin{cases} S_n = (S_0^{-1} + \beta \Phi^\top \Phi)^{-1} \\ m_n = S_n(\beta \Phi^\top y_{1:n} + S_0^{-1} m_0) \end{cases} \quad (1)$$

Posterior mean estimate

$$\hat{\theta} = \mathbb{E}_\pi[\theta | y_{1:n}] = m_n$$

Special case : diagonal, centered prior

- choose $m_0 = 0$, $S_0 = \alpha^{-1}I_p$, with α : prior precision (it makes sense !)
- Then (1) becomes

$$\left\{ \begin{array}{lcl} S_n = (\alpha I_p + \beta \Phi^\top \Phi)^{-1} & = & \beta^{-1} \left(\frac{\alpha}{\beta} + \Phi^\top \Phi \right)^{-1} \\ m_n = S_n (\beta \Phi^\top y_{1:n}) & = & \underbrace{\left(\frac{\alpha}{\beta} + \Phi^\top \Phi \right)^{-1} \Phi^\top y_{1:n}}_{\text{penalized least squares solution}} \end{array} \right. \quad (2)$$

Adding a prior $\mathcal{N}(0, \alpha^{-1}I_p)$

\iff

Adding a L_2 regularization with parameter $\lambda = \alpha/\beta$.

remark : Narrow prior \iff large α \iff large penalty

Predictive distribution

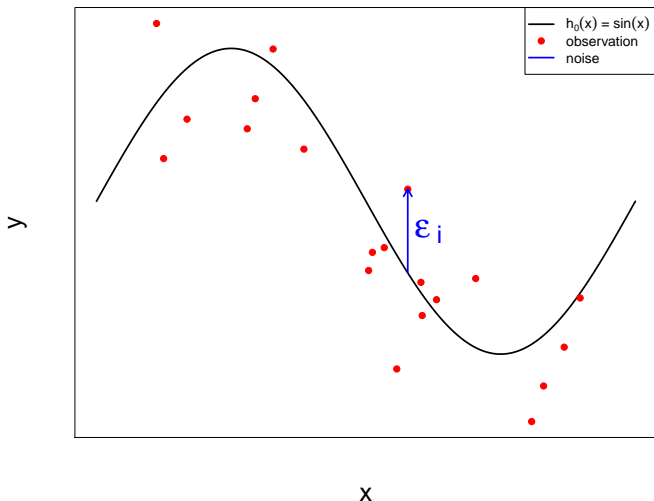
New data point (x_{new}, Y_{new}) , with Y_{new} not observed and x_{new} known :

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

$$\mathcal{L}[Y_{new} | y_{1:n}] = \mathcal{N}\left(\phi(x_{new})^\top m_n, \phi(x_{new})^\top S_n \phi(x_{new}) + \beta^{-1}\right)$$

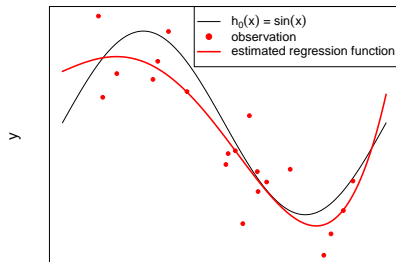
Example : polynomial basis functions

- True regression functions : $h_0(x) = \sin(x)$
- Polynomial basis functions : $\phi(x) = (1, x, x^2, x^3, x^4)$ ($p = 5$).

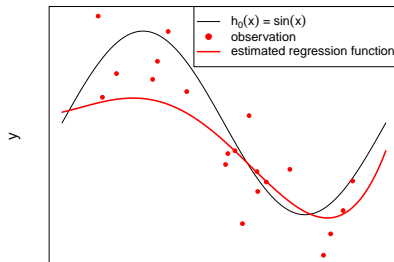


Estimated regression function

- $\hat{h}(x) = \langle \hat{\theta}, \Phi(x) \rangle = \hat{\theta}_1 + \sum_{j=2}^5 \hat{\theta}_j x^{j-1}$
- With the previous dataset



$\alpha = 0.01$

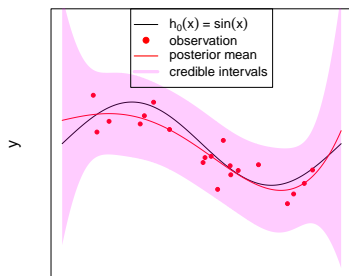


$\alpha = 100$

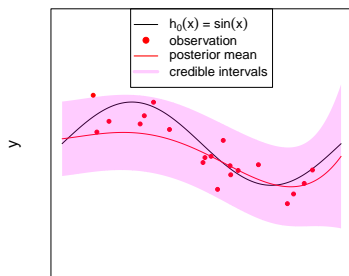
Predictive distribution

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

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



$\alpha = 0.01$



$\alpha = 100$

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 - Prior choice
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Model choice problem

- What if several model in competition $\{M_k, k \in \{1, \dots, K\}\}$, with $M_k = \{\Theta_k, \pi_k\}$?
- Continuous case : family of models $\{M_\alpha, \alpha \in \mathcal{A}\}$
- \rightarrow How to choose k or α ?
- Examples :
 - $M_1 = \{\Theta, \pi_1\}$, $M_2 = \{\Theta, \pi_2\}$ with π_1 a flat prior and π_2 the Jeffreys prior
 - M_α linear model with normal prior on the noise $\mathcal{N}(0, \alpha^{-1})$

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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 $k \in \{1, \dots, K\}$) \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.
- $X_i \sim \text{Ber}(\theta)$, with $\theta = \theta_1$ in river 1 and $\theta = \theta_2$ in river 2.
- θ_1 and θ_2 are 2 realizations of $\boldsymbol{\theta} \sim \text{Beta}(\boldsymbol{a}, \boldsymbol{b})$
- $\boldsymbol{\alpha} = (\boldsymbol{a}, \boldsymbol{b})$: hyper-parameter for the prior
- hierarchical Bayes : put a prior on $\boldsymbol{\alpha}$ (e.g. product of 2 independent Gammas).

Posterior mean estimates in a BMA framework

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

$$\mathbb{E}_{\pi}[g(\theta)] = \mathbb{E}_{\pi^h} \left[\mathbb{E}_{\pi}[g(\theta)|k] \right] = \sum_{k=1}^K \pi^h(k) \int_{\Theta_k} g(\theta) d\pi_k(\theta)$$

- So is the posterior distribution, thus the posterior mean is a weighted average

$$\begin{aligned} \hat{g} &= \mathbb{E}_{\pi}[g(\theta)|X_{1:n}] = \mathbb{E}_{\pi^h} \left[\mathbb{E}_{\pi}[g(\theta)|k, X_{1:n}] | X_{1:n} \right] \\ &= \sum_{k=1}^K \pi^h(k|X_{1:n}) \underbrace{\int_{\Theta_k} g(\theta) d\pi_k(\theta|X_{1:n})}_{\hat{g}_k: \text{posterior mean in model } k} \end{aligned}$$

Model evidence

Computing the posterior mean in the BMA framework requires

- Computing the posterior means in each individual model
→ k ‘moderate’ tasks
- Averaging them with weights $\pi^h(k|X_{1:n})$, *posterior weight of model k*
- Bayes formula

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

with

$$\begin{aligned} p(X_{1:n}|k) &= \text{evidence of model } k \\ &= \int_{\Theta_k} p(X_{1:n}|\theta) d\pi_k(\theta) \\ &= m_k(X_{1:n}) \text{ marginal likelihood of } X_{1:n} \text{ in model } k \end{aligned}$$



hard to compute (integral)

Shortcomings of BMA

- Inference has to be done in each individual model
- Usually one weight (say $\pi(k^*|X_{1:n})$) \gg all others (reason : concentration of the posterior around the true $\theta_0 \in \Theta_{k_0}$ and $k^* = k_0$ \implies final estimate $\hat{g} \approx \hat{g}_{k_0}$. Other \hat{g}_k 's are almost useless

Bottleneck : compute k^* .
model choice problem.

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Posterior weights, model evidence and Bayes factor

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

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

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

- Suggested scale for decision making :

$\log_{10} B_{kj}$	B_{kj}	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.

→ Avoid over-fitting

→ Better generalization properties.

Occam's razor and model evidence

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

automatic complexity penalty : intuition 1

$$\begin{aligned}\text{Complex model} &\implies \text{large } \Theta_k \\ &\implies \text{small } \pi_k(\theta) \text{ (if uniform over } \Theta_k) \\ &\implies \int_{\Theta_k} p_{\theta}(x_{1:n}) \pi_k(\theta) d\theta \text{ small} \\ &\quad \text{(average over large regions where } p_{\theta}(x_{1:n}) \text{ small)}\end{aligned}$$

automatic complexity penalty : intuition 2

- if $\Theta_k \subset \mathbb{R}$: assume
 - π_k flat over interval of length $\Delta\theta_k^{prior}$
 - $p_{\theta_k}(X_{1:n})$ peaked around $p_{\hat{\theta}_{MAP,k}}(X_{1:n})$ with ‘width’ $\Delta_k^{posterior}$.
- then $\pi_k(\theta) \approx 1/\Delta_k^{prior}$ and

$$p(X_{1:n}|k) = \int_{\Theta_k} p_{\theta}(x) \pi_k(\theta) d\theta \approx p_{\hat{\theta}_{MAP,k}}(X_{1:n}) \underbrace{\frac{\Delta\theta_k^{posterior}}{\Delta\theta_k^{prior}}}_{\text{complexity penalty}}$$

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

$$\log p(X_{1:n}|k) \approx \log p_{\hat{\theta}_{MAP,k}}(X_{1:n}) + \underbrace{d \log \frac{\Delta\theta_k^{posterior}}{\Delta\theta_k^{prior}}}_{\text{dimension + complexity penalty}}$$

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