Data analysis spatio-temporal data and hierarchical models

Bayesian Inference (Part one, Ch3)

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Learning (in materialist world)

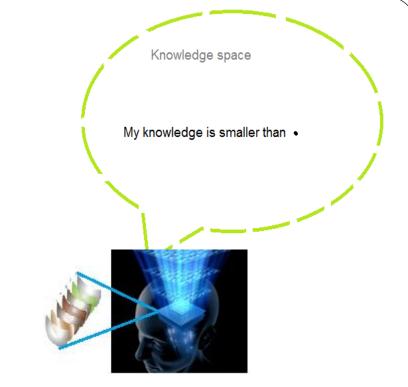
- Goals
 - reproduction of perception, inference, behaviours, conscience, ...
 - extension of the world through the creative imagination
 - enriched world = natural + artificial
- Consequences
 - more rich world, more power
 - confused world, balance of creatures
 - . . .
- Historical evidences
 - the progress can be slowed, but not stopped
 - the progress can be influenced by the creatures including human (knowledge, moral, interest, ...).
 - philosophy, ethics, culture, and social sciences are required.

Plan

- Probability of things
- Generative learning
- Discriminative learning
- Bayesian inference
- Point estimation methods
- Approximations
- Feature selection
- References

- Are we ignorant?
 - reading speed (words/second)
 - understanding (1-20 score)
 - using knowledge (1-20 score)
- To answer, I need a model

$$X = (x_1, x_2, x_3)$$
$$p(X)$$



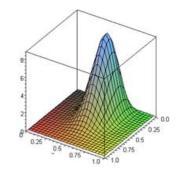


d-dimensional random vector $X = (x_1, \dots, x_d)$

$$X = (x_1, \cdots, x_d)$$

- Joint pdf p(X)
- Simplifications
 - structural (independence)

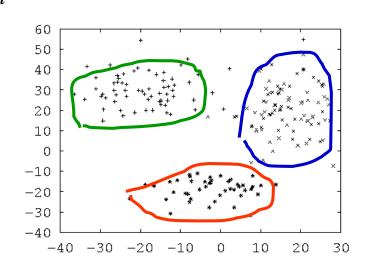
$$p(X) = \prod p(x_i)$$



parametrical

$$p(X) = \sum_{k} \alpha_{k} p_{k}(X)$$

$$\alpha^t \mathbf{1} = 1$$



Conditional pdf

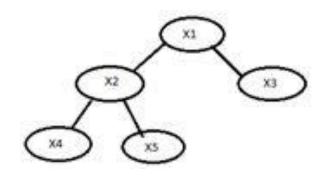
$$p(\cdots,x_i,\cdots|\cdots,x_{i\neq i},\cdots)$$

Joint/conditional

$$p(X) = \prod_{i=1}^{d} p(x_i \mid x_1, \dots, x_{j < i})$$

- Simplifications
 - structural (conditional independence)

$$p(X) = \prod_{i=1}^{d} p(x_i \mid x_{\pi_i})$$



• parametrical (exchangeability): (x_1, \dots, x_d) are exchangeable (De Finetti)

$$p(X) = \int \prod_{i=1}^{a} p(x_i \mid \theta) p(\theta) d\theta$$

The root of the Bayesian school of thought: parameter, prior on that parameter, and data IID given the parameter.

Generative learning

Generative learning

Data: labeled or not

$$D = L \cup U; L = \{Y_i = (X_i, c_i)\}, \quad U = \{Y_i = X_i\}$$

- Generative learning $p(D) = \int p(\Theta) p(D \mid \Theta) d\Theta$
- Approximations $p(D) \approx p(D \mid \hat{\Theta}) \quad \text{where} \quad \hat{\Theta} = \arg\max \begin{cases} p(\Theta) \prod_{y \in D} p(y \mid \Theta) & \textit{MAP} \\ \prod_{y \in D} p(y \mid \Theta) & \textit{ML} \end{cases}$
- Both labeled data L and unlabeled data U can be used.

$$\hat{\Theta} = \arg \max p(\Theta) \prod_{y \in L} p(y \mid \Theta) \prod_{y \in U} p(y \mid \Theta)$$

• $\hat{\Theta}$ which encodes the labels of incomplete data (U) is often required (unsupervised learning).

Generative learning – example

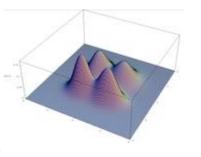
- Finite mixture
 - illiterate
 - non-graduate and cultivated
 - graduate and uncultivated
 - •
 - Applications
 - Astronomy, Biology, Economics, Engineering, Genetics, Marketing, Medicine, Psychiatry, ...

Foundation of finite mixture

Let $X_1, ..., X_N$ denote N random d-dimensional samples with probability density function $f(\mathbf{x}_i)$

$$f(x_i) = \sum_{i=1}^{M} \pi_j f_j(x_i)$$

where $f_j(\mathbf{x}_i)$ are densities, $\pi_i \ge 0$ and $\sum_{i=1}^{M} \pi_i = 1$



A possible interpretation

- Let Z_i be a categorical random variable taking on the values 1, ..., M with probabilities $\pi_1, ..., \pi_M$
- $f_i(x_i)$ (j=1,...,M) is the conditional density of X_i given $Z_i=j$
- $f(x_i)$ is a marginal pdf

$$f(x_i) = \sum_{j=1}^{M} f(x_i, z_i = j) = \sum_{j=1}^{M} p(z_i = j) f(x_i \mid z_i = j) = \sum_{j=1}^{M} \pi_j f_j(x_i)$$

Parametric formulation of mixture model

- The component densities $f_j(\mathbf{x}_i)$ are specified as $f(\mathbf{x}_i|\boldsymbol{\theta}_j)$, where $\boldsymbol{\theta}_i$ is the vector of unknown parameters
- The mixture density $f(\mathbf{x}_i)$ can then be written as

$$f(x_i \mid \Theta) = \sum_{j=1}^{M} \pi_j f(x_i \mid \theta_j)$$

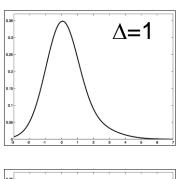
where
$$\Theta = (\pi_1, ..., \pi_{M-1}, \xi^t)^t$$
 and $\xi = (\theta_1, ..., \theta_M)$

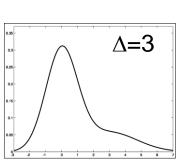
the parameters θ_i are assumed distinct.

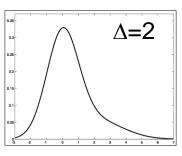
Shapes of an univariate normal mixture

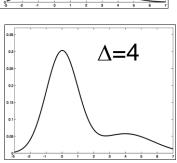
Consider
$$f(x_i | \Theta) = \pi_1 g(x_i / \mu_1, \sigma^2) + \pi_2 g(x_i / \mu_2, \sigma^2)$$

where $g(x_i | \mu, \sigma^2) = (2\pi)^{-\frac{1}{2}} \sigma^{-1} \exp\{-\frac{1}{2}(x_i - \mu)^2 / \sigma^2\}$
 μ and σ^2 are the mean and the variance.









A mixture of two univariate normal components with

$$\pi_1 = 0.75, \, \sigma_1 = \sigma_2 = 1$$

Generative learning

- Some properties
 - data can be incomplete
 - easy and widely used
 - the estimated model encodes information about data and labels
 - the goal is to fit the data, the target problem is not taken into account
 - MAP is more suitable when few labeled data are available

Discriminative learning

Discriminative learning

Discriminative learning

$$p(C \mid X) = \int p(C, \Theta \mid X) d\Theta$$

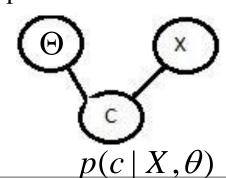
Approximations

$$p(C \mid X) \approx p(C \mid X, \hat{\Theta})$$
 where $\hat{\Theta} = \arg \max \begin{cases} p(\Theta)p(C \mid \Theta, X) & CMAP \\ p(C \mid \Theta, X) & CML \end{cases}$

- Unlike generative learning
 - discriminative learning cannot be used with unlabeled data

$$\hat{\Theta} = \arg \max p(\Theta) \prod_{v \in L} p(c \mid X, \Theta)$$

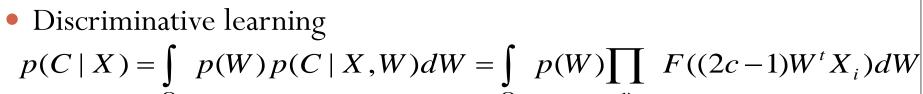
• *X* provides no information about Θ ; i.e., $p(X \mid \Theta) = p(X)$



Discriminative learning - example

- Examples of discriminative learning models
 - logistic regression $p(c \mid X, W) = F((2c-1)W^{t}X)$
 - probabilistic SVM approximation

$$p(c = 1 | y, \alpha, \beta) = F(\alpha y + \beta)$$
$$y = \sum_{i} c_{i} \beta_{i} K(x_{i}, x)$$

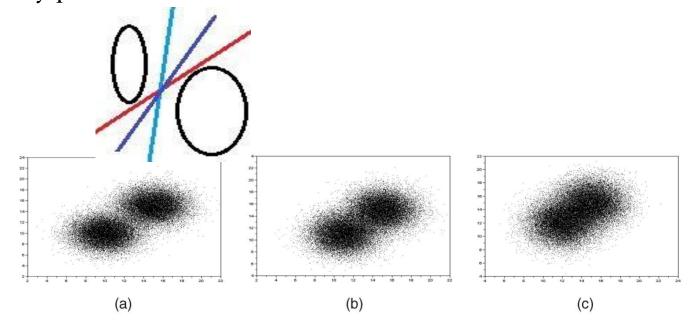


 $F(x) = \frac{1}{1+e^{-x}}$

$$W^* \approx \begin{cases} p(W) \prod_{y} F((2c-1)W^t X_i) & CMAP \\ \prod_{y} F((2c-1)W^t X_i) & CML \end{cases}$$

Discriminative learning

- Some properties
 - data must be complete
 - discriminative learning more accurate than generative learning
 - logistic regression outperform SVM and its variants
 - model encodes information only about labels
 - CMAP is suitable when few labeled data are available
 - separability problem when CML is used



Bayesian inference

Goal

- Data are generated from unknown distribution
- By analyzing the data, we would like to learn about the distribution, predict some future data, and make decision
- The common methodology is to assume that the distribution is known except the value of some of its parameters (parametric methods).
- In this case, one issue is to estimate the parameters (learning).
- Bayesian inference involves prior, posterior, and likelihood distributions.

Bayesian data analysis

- Prediction p(x|D)
- Decision making $r(a \mid x) = \sum_{i} l(a, w_i) p(w_i \mid x)$
- Estimation
 - for fundamentalists, the posterior is the end result and no estimation is allowed
 - in practice, the posterior is summarized by using an estimate $\min_{\hat{\Theta}} \int l(\hat{\Theta},\Theta) p(\Theta\,|\,D) d\Theta$
 - Examples

$$l(\hat{\Theta}, \Theta) = 1 - \delta(\hat{\Theta} - \Theta) \implies \hat{\Theta} = \arg\max_{\theta} p(\Theta \mid D)$$

$$l(\hat{\Theta}, \Theta) = (\hat{\Theta} - \Theta)^2 \implies \hat{\Theta} = \int_{\Theta} \Theta p(\Theta \mid D) d\Theta$$

• Exercise: evaluate the last estimator in the case of a normal pdf with known variance. You consider that the mean is sampled from normal prior.

Bayesian inference - foundation

- Hidden (missed, latent) variables helps in
 - labelling samples, objects, classes, patterns, ...
 - modeling non observed phenomena
 - combining variables in order to reduce dimension
- They are unobserved (non measurable)
- They can be introduced in a model by marginalization
- Example, the marginalized (integrated) likelihood

$$p(D \mid \Theta) = \int_{\Omega} p(z \mid \Theta) p(D \mid z, \Theta) dz$$
$$p(z \mid D, \Theta) = p(D \mid z, \Theta) p(z \mid \Theta) / \int_{\Omega} p(D \mid z, \Theta) p(z \mid \Theta) dz$$

Bayesian inference - foundation

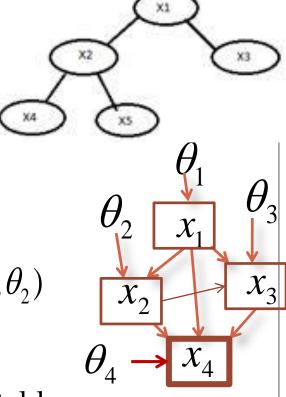
- Graphical model G represents dependencies between variables
- G=(V,E) be a directed acyclic graph

$$p(x_1, ..., x_d) = \prod_{i=1}^d p(x_i \mid x_{\pi_i})$$

Bayesian network

• Example $p(x_1, x_2, x_3, x_4 | \Theta) = p(x_1 | \theta_1) p(x_2 | x_1, \theta_2)$ $p(x_3 | x_1, x_2, \theta_3) p(x_4 | x_1, x_2, x_3, \theta_4)$

• Undirected graph: See Markov random field.



Bayesian inference - foundation

• In order to estimate Θ by using marginalized likelihood, the challenge is to compute the integral

$$p(D \mid \Theta) = \int_{z} p(z \mid \Theta) p(D \mid z, \Theta) dz$$

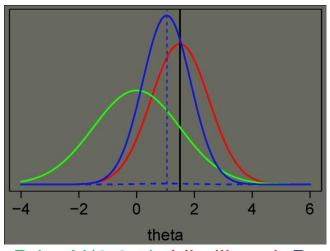
- Example $p(z \mid \alpha) \propto e^{-z^2/\alpha}$ $p(D \mid z, \alpha) \propto \prod_{i=1}^{N} e^{-(zx_i)^4}$
- Several methods exist
 - simulation
 - Laplace approximation
 - •
 - variational approximation

Prior and posterior pdfs

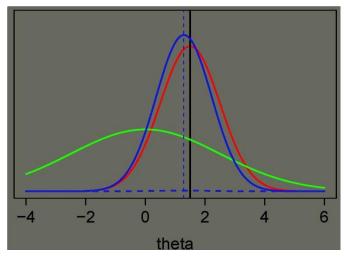
- Let us consider the space of parameters of a pdf. Prior distribution indicates the region in which lies the parameters.
- Prior pdf can be determined from information about frequencies (e.g., previous experimentation) or subjective information.
- They can be a pdf or not.
- Improper prior pdf $f(\theta)$ are such that $\int_{\Omega} f(\theta) d\theta = +\infty$. In this case, the posterior is not necessarily proper. This is used when we would like to give more importance to the data.
 - $\theta^{-1}(1-\theta)^{-1}$ where $\theta \in [0,1]$ and $f(\sigma) = \sigma^{-1}$ are improper priors
- Non informative prior is often determined by assigning equal probability to all values (principle of indifference). Unlike improper prior, it is a pdf and therefore the posterior.
 - $f(\theta)$ =constant is non normative. In this case, the maximum likelihood and the MAP are the same.

Posterior and prior

- Conjugate prior is a pdf in the same family as the posterior. This choice of prior may allows to make the integral in the denominator tractable.
 - example, $g(x \mid \mu)$ a Gaussian, $g(\mu \mid \mu_0, \sigma_0)$ a Gaussian, and σ known



Prior N(0,0.5), Likelihood, Posterior Prior not very informative



Prior N(0,2.5), Likelihood, Posterior Informative prior

Estimation methods

- The posterior is used for the estimation of parameters
 - Full-Bayesian: use of loss function

$$l(\hat{\Theta}, \Theta) = (\hat{\Theta} - \Theta)^2 \implies \hat{\Theta} = \int_{\Theta} \Theta p(\Theta \mid D) d\Theta$$

not easy to determine the suitable loss function

- Bayesian-point: maximum likelihood, maximum *a posteriori*, simulation...
- approximations are sometimes required: Laplace approximation, variational approximation...

Point estimation methods

Point estimation of parameters

- d-dimensional random vector $x = (x_1, \dots, x_d)^t$
- Observations $D = \{x_1, \dots, x_N\}$
- Model estimation
 - maximum likelihood
 - expectation maximization
 - maximum a posteriori
 - maximum entropy, moment, simulation...
- Model selection

- Indented for the model estimation (not clustering).
- There exist several formulations. We will study the most common.
- Likelihood, under the iid assumption

$$p(D \mid \Theta) = \prod_{n=1}^{N} p(x_n \mid \Theta)$$

• Maximum likelihood estimator $\hat{\Theta}$

$$L(\hat{\Theta}) = \max_{\Theta} p(D \mid \Theta)$$

under constraints (if any).

- Example-Mixture estimation
 - likelihood, under the iid assumption

$$p(D \mid \Theta) = \prod_{n=1}^{N} p(x_n \mid \Theta) = \prod_{n=1}^{N} \sum_{j=1}^{K} \pi_j f(x_n \mid \theta_j)$$

• maximum likelihood

$$\max_{\Theta} L(\Theta) = \prod_{n=1}^{N} \sum_{j=1}^{K} \pi_{j} f(x_{n} \mid \theta_{j})$$
 constraints $\pi_{j} \ge 0$ and
$$\sum_{j=1}^{K} \pi_{j} = 1$$

optimization problem

$$\min_{\Theta} - \sum_{n=1}^{N} \ln(\sum_{j=1}^{K} \pi_{j} f(x_{n} \mid \theta_{j})) + \lambda(1 - \sum_{j=1}^{K} \pi_{j})$$

• first order condition

$$\forall k = 1, ..., K \quad -\sum_{n=1}^{N} \frac{\frac{\partial f(x_n \mid \theta_k)}{\partial \theta_k}}{\sum_{j=1}^{K} \pi_j f(x_n \mid \theta_j)} = 0$$

$$\forall k = 1, ..., K \quad -\sum_{n=1}^{N} \frac{f(x_n \mid \theta_k)}{\sum_{j=1}^{K} \pi_j f(x_n \mid \theta_j)} - \lambda = 0$$

$$\sum_{j=1}^{K} \pi_j f(x_n \mid \theta_j)$$

• solve the (often nonlinear) system of equations

- iterative algorithm
 - input $D, K, \theta_1^0, ..., \theta_K^0, \pi_1^0, ..., \pi_{K-1}^0$
 - ullet output $\hat{ heta}_1,...,\hat{ heta}_K,\hat{\pi}_1,...,\hat{\pi}_K$
 - r=0
 - do

```
for k=1 to K
\Delta^{(r)} = -1
```

r = r+1

$$\pi_k^{(r)} = \dots$$

end for

until convergence

- for convergence, the likelihood function can be used
- for the initial values: see k-means, fuzzy c-means,
- check the second order condition

To illustrate, let us consider a mixture of two univariate Gaussian with common variance

$$f(x \mid \Theta) = \pi_1 g(x \mid \mu_1, \sigma^2) + \pi_2 g(x \mid \mu_2, \sigma^2) \quad \text{where}$$

$$g(x \mid \mu, \sigma^2) = (2\pi)^{-\frac{1}{2}} \sigma^{-1} \exp(-\frac{1}{2}(x - \mu)^2 / \sigma^2) \quad \text{and} \quad \Theta = (\mu_1, \mu_2, \sigma)^t$$

 $\min_{\Theta} - \sum_{n=1}^{N} \ln(\sum_{j=1}^{2} \pi_{j} g(x_{n} \mid \mu_{j}, \sigma)) + \lambda(1 - \sum_{j=1}^{2} \pi_{j})$ the optimization problem the first order condition

$$\forall k = 1, 2 \quad -\sum_{n=1}^{N} \quad \frac{\frac{\partial g(x_n \mid \theta_k)}{\partial \mu_k}}{\sum_{j=1}^{2} \pi_j g(x_n \mid \theta_j)} = 0 \quad \forall k = 1, 2 \quad -\sum_{n=1}^{N} \quad \frac{g(x_n \mid \theta_k)}{\sum_{j=1}^{2} \pi_j g(x_n \mid \theta_j)} - \lambda = 0$$

$$\sum_{j=1}^{2} \pi_{j} - 1 = 0$$

N = 50

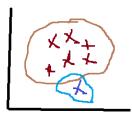
Estimation of mixing proportions

Iteration r	$\pi_{\scriptscriptstyle 1}^{(r)}$	$\log L(\pi_1^{(r)})$
0	0.50000	-91.87811
1	0.68421	-85.55353
2	0.70304	-85.09035
3	0.71792	-84.81398
6	0.74218	-84.60978
7	0.74615	-84.58562
	0.50000	-91.87811
27	0.68421	-85.55353

Ground truth $\mu_1 = 0$ $\mu_2 = 2$ $\sigma^2 = 1$ $\pi_1 = 0.8$ $\pi_2 = 0.2$

Some properties

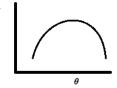
- easy to derive and to use for supervised learning
- good estimator; may be consistent, unbiased, efficient
- invariant; if $t = r(\Theta)$ then $\hat{t} = r(\hat{\Theta})$
- limited to iid
- no prior knowledge
- may not exist



point estimator (poor uncertainty)



• numerical issues; flat maximum, several maxima, degenerate maximum







- EM intended for clustering.
- The main idea is data can be viewed as being complete $(\mathbf{x}_1, \mathbf{z}_1), \ldots, (\mathbf{x}_N, \mathbf{z}_N)$, where $z_i = (\underbrace{0,0,\ldots,1,0,\ldots,0}_{i^{th}})^t$
- We wish to infer the \mathbf{z}_i on the basis of the feature data \mathbf{x}_i .
 - \bullet estimation of the model $\widehat{\Theta}$
 - for each \mathbf{x}_j , \mathbf{f} ($\hat{\theta}_l \mid \mathbf{x}_j$),..., \mathbf{f} ($\hat{\theta}_K \mid \mathbf{x}_j$) are the estimated posterior probabilities that this observation belongs to the 1st, 2nd,..., and K^{th} component. Indeed, the estimated component-label vector \mathbf{z}_i is $\hat{\mathbf{z}}_i$ where $\hat{\mathbf{z}}_{ii} = (\hat{\mathbf{z}}_{ii})$

$$\hat{z}_{ij} = \begin{cases} 1 & if \ j = \arg\max_{h} f(\hat{\theta}_{h} \mid x_{i}) \\ 0 & elsewhere \end{cases}$$

- Algorithm
 - input $D, K, \theta_1^0, ..., \theta_K^0, \pi_1^0, ..., \pi_{K-1}^0$ output $\hat{\theta}_1, ..., \hat{\theta}_K, \hat{\pi}_1, ..., \hat{\pi}_K$

 - do
 - •E-Step, estimate the posterior for each j and i $\tau_{ii} = f(\theta_i^{(r-1)} | x_i) = \pi_i^{(r-1)} f(x_i | \theta_i^{(r-1)}) / f(x_i | \Theta^{(r-1)})$
 - •M-Step, fond (b) by maximizing

$$\sum_{i=1}^{N} \sum_{j=1}^{K} \tau_{nj} \ln(\pi_{j}^{(r-1)} f(x_{i} | \theta_{j}^{(r-1)}))$$

Until convergence

clustering (hard clustering if needed)

$$\hat{z}_{ij} = \begin{cases} 1 & \text{if } j = \arg\max_{h} f(\hat{\theta}_{h} \mid x_{i}) \\ 0 & \text{elsewhere} \end{cases}$$

• Example, let us consider the normal mixture

$$g(x_i \mid \Theta) = \sum_{j=1}^{K} \pi_j g(x_i \mid \theta_j)$$

E-step

$$\tau_{ii}^{(r)} = g(\theta_i^{(r)} | x_i) = \pi_i^{(r)} g(x_i | \theta_i^{(r)}) / g(x_i | \Theta^{(r)})$$

M-Step

$$\pi_j^{(r+1)} = \sum_{i=1}^{N} \tau_{ji}^{(r)} / N$$
 $(j=1,...,K)$

$$\mu_j^{(r+1)} = \sum_{i=1}^N \tau_{ji}^{(r)} x_i / \sum_{i=1}^N \tau_{ji}^{(r)}$$
 (j=1,...,K)

$$\sigma_j^{2(r+1)} = \sum_{i=1}^N \tau_{ji}^{(r)} (x_i - \mu_j^{(r+1)})^2 / \sum_{i=1}^N \tau_{ji}^{(r)} \qquad (j = 1, ..., K)$$

- Some properties
 - converges to the maximum likelihood
 - easy and allows clustering (incomplete data) and supervised learning
 - the *K* dimensional problem is split to 1D problems
 - share properties with the maximum likelihood.

Maximum a posteriori

- The MAP $\hat{\Theta}_{MAP} = \arg \max_{\Theta} p(\Theta \mid D)$
 - the integral is often intractable

$$p(\Theta \mid D) = p(D \mid \Theta) p(\Theta) / \int_{\Omega} p(D \mid \Theta) p(\Theta) d\Theta$$

• simplification $\hat{\Theta}_{MAP} = \arg \max_{\Theta} p(D \mid \Theta) p(\Theta)$

Maximum a posteriori

Example

prior

likelihood

telihood
$$p(D \mid \Theta) \propto \prod_{j=1}^{N} e^{-\frac{(x_j - \mu)^2}{2\sigma^2}} \qquad \sum_{j=1}^{3.5} \frac{1}{2\sigma^2}$$

$$p(\Theta) = p(\mu) p(\sigma) \propto e^{-\frac{(\mu - \eta)^2}{2\lambda^2}} \frac{\beta^{\alpha}}{\Gamma(\alpha)} \sigma^{\frac{0.5}{\alpha - \alpha - 1}} e^{-\frac{\beta}{\beta} \sigma^{\frac{1.5}{\alpha}}}$$

posterior

posterior
$$\max_{\mu,\sigma} p(\Theta \mid D) \propto \prod_{j=1}^{N} e^{-\frac{(x_j - \mu)^2}{2\sigma^2}} e^{-\frac{(\mu - \eta)^2}{2\lambda^2}} \frac{\beta^{\alpha}}{\Gamma(\alpha)} \sigma^{-\alpha - 1} e^{-\beta/\sigma}$$

 $\eta, \lambda, \beta, \alpha$ hyperparameters

Maximum a posteriori

- Some properties
 - easy to derive and to use for supervised learning
 - another interpretation $\hat{\Theta}_{MAP} = \arg \max_{\Theta} p(D, \Theta)$
 - good estimator; may be consistent, unbiased, efficient
 - looks like the maximum likelihood when N tends to infinity
 - unlike the maximum likelihood, it avoids the overfitting (overfitting: error decrease in learning phase and increase in the test phase)
 - non invariant
 - limited to iid
 - may not exist (see maximum likelihood)
 - point estimator (see maximum likelihood)
 - numerical issues; flat maximum, several maxima, degenerate maximum.

- Find $\Theta \in \{\Theta_1, \Theta_2, ...\}$
- Example of methods
 - Akaike's Information Criterion (AIC) selects the model that minimizes $-2\log L(\hat{\Theta}) + 2d$

where d is equal to the number of parameters in the model.

- the Bayesian information criterion (BIC) of Schwarz (1978) is given by $-2\log L(\Theta) + d\log N$
- many other criteria MDL, MML, ...

- Algorithm
 - input D, $\{\Theta_1, \Theta_2, ...\}$
 - output $\hat{\Theta}$
 - $\min = +\infty$
 - for $\Theta \in \{\Theta_1, \Theta_2, ...\}$

if
$$(v = -2 \log L(\Theta) + complexity term) < \min) then$$

$$\hat{\Theta} = \Theta$$
; min = v; EndIf

Endfor

• The set $\{\Theta_1, \Theta_2, \dots\}_{\text{can}}$ be estimated using the maximum likelihood, EM...

- Example unsupervised learning of a mixture of pdfs
 - input D
 - output $\hat{\Theta}$
 - $min = +\infty$
 - for $j=1..K_{max}$
 - ullet estimate ullet for a mixture of j components

if
$$(v = -2 \log L(\Theta) + complexity term) < \min$$
 then $\hat{\Theta} = \Theta$; $\min = v$; EndIf

Endfor

• The set $\{\Theta_1, \Theta_2, ...\}$ an be estimated using the maximum likelihood, EM...

- Some properties
 - intended for unsupervised learning
 - inherits the ML and MAP properties

References

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- Maximum likelihood
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