Artificial Intelligence

A course about foundations



Probabilistic Reasoning: Supervised Learning

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Artificial Intelligence 2023-2024 Supervised Learning [1]

Machine Learning

Artificial Intelligence 2023-2024 Supervised Learning [2]

Types of machine learning problems

Consider a number of observations (i.e. a dataset) made by an agent $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$

Supervised learning

Learning form <u>complete</u> observations: each of the observations $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ include values for <u>all</u> the random variables in the model

The objective is learning a <u>distribution P</u>

Unsupervised learning

Learning form <u>incomplete</u> observations: observations $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ do <u>not</u> necessarily include values for all the random variables in the model The objective is learning a *distribution P*

■ Reinforcement learning

The observations $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ are states o situations, at each state X_i the agent must perform an **action** a_i that produces a **result** r_i .

The objective is learning a distribution π over possible actions in each state which describes a policy that the agent will follow

Such policy should maximize the expected value of a reward function $v(< r_1, r_2, ..., r_n >)$ of the sequence of results

Observations and Independence

Each observation could be the outcome of an experiment or a test

The outcome of a particular experiment can be represented by a set of *random variables*

For example, if the model makes use of the two random variables $\{X, Y\}$, the N outcomes of the experiments are $D^{(1)} = (X^{(1)}, Y^{(1)}), \dots, D^{(N)} = (X^{(N)}, Y^{(N)})$

That is, a dataset

$$D := \{(X^{(i)}, Y^{(i)})\}_{i=1}^{N}$$

Independent observations, same probability distribution

Independent and Identically Distributed (IID) random variables

Definition

A sequence or a set of random variables $\{X_1, X_2, \dots, X_n\}$ is *Independent and Identically Distributed* (IID) iff:

1)
$$\langle X_i \perp X_j \rangle$$
, $\forall i \neq j$ (independence)

2)
$$P(X_i = x) = P(X_j = x)$$
, $\forall i \neq j, \forall x$ (identical distribution)

CAUTION: Being IID is not an obvious property of observations

e.g. different measurements on different patients <u>may</u> be IID, but different measurements over time on the same patient are <u>not</u> IID

ML = Representation + Evaluation + Optimization

Assume that an I.I.D. dataset D is available

Representation

The objective is learning a specific distribution

$$P({X_r};\theta)$$

where $\{X_r\}$ are all the random variables of interest and θ is a set of parameters

Which kind of distribution (i.e. the *model* or also the *learner*) do we select?

Example: assume we select the anti-spam filter (i.e. Naïve Bayesian Classifier) as the model the parameters in such case are the numerical probabilities in the CPTs

Evaluation

Given a dataset D, how well does a specific set of parameter values $\hat{\theta}$ make the distribution P fit the dataset?

An estimator, i.e. a scoring function of some sort, must be selected

Optimization

How can we find the optimal set of parameter values θ^* with respect to the *estimator* of choice?

In general, this is an optimization problem

Maximum Likelihood Estimator (MLE)

Likelihood

A probabilistic model P(X), with parameters θ

 θ is a set of values that characterizes P(X) completely: once θ is defined, P(X) is also defined.

A set of IID observations (data items) $D = \{D^{(1)}, ..., D^{(N)}\}$

Likelihood function (or conditional probability)

A function, or a conditional probability, derived from the model P(X)

$$L(\theta \mid D) = P(D \mid \theta) = P(D^{(1)}, \dots, D^{(N)} \mid \theta)$$

Note the 'trick':

that the parameter θ . likelihood of the dataset given the parameters

where $P(D \mid \theta)$ is the conditional probability that the parameter θ , considered as a random variables, could <u>generate</u> the observations D

When the observations $\{D^{(1)}, \dots, D^{(N)}\}$ are IID:

$$P(D \mid \theta) = P(D^{(1)} \mid \theta) \dots P(D^{(N)} \mid \theta) = \prod_{m} P(D^{(m)} \mid \theta)$$

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Maximum Likelihood Estimator (MLE)

A probabilistic model P(X), with parameters θ

 θ is a set of values that characterizes P(X) completely: once θ is defined, P(X) is also defined.

A set of IID observations (data items) $D = \{D^{(1)}, ..., D^{(N)}\}$

Maximum Likelihood Estimation

$$\theta_{ML}^* := \operatorname{argmax}_{\theta} L(\theta|D)$$

Since the observations are IID, using *log-Likelihood* could ease computations:

$$\ell(\theta \mid D) = \log L(\theta \mid D) = \log \prod_{m} P(D^{(m)} \mid \theta) = \sum_{m} \log P(D^{(m)} \mid \theta)$$

$$\theta_{ML}^* = \operatorname{argmax}_{\theta} \ell(\theta \mid D)$$
true because log is monotonically increasing

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Example: coin tossing (Bernoulli Trials)

Experiment: tossing a coin X, not necessarily fair (X = 1 head, X = 0 tail)

Parameters: $\theta := \{ \pi \} \Leftrightarrow P(X=1) = \pi, P(X=0) = 1 - \pi \}$

Observations: a sequence of experimental outcomes

$$D = \{D_1 = \{X^{(1)} = x^{(1)}\}, \ D_2 = \{X^{(2)} = x^{(2)}\}, \dots, D_N = \{X^{(N)} = x^{(N)}\}\}$$

Binomial distribution

It is the probability of obtaining $N_{X=1}$ times 'head' in a sequence of N trials In this case, it is assumed to be the likelihood of $\{D^{(1)}, \ldots, D^{(N)}\}$ given the parameters θ

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MLE as optimization

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Example: coin tossing (Bernoulli Trials)

(Log-)Likelihood Function

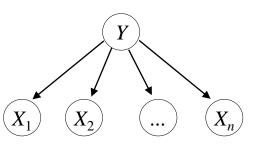
$$\begin{split} &\ell(\theta|D) = \log P(D|\theta) = \log P(\{X^{(i)}\}|\theta) = \log \binom{N}{N_{X=1}} \prod_{i} P(X^{(i)}|\theta) = \log \binom{N}{N_{X=1}} + \sum_{i} \log P(X^{(i)}|\theta) \\ &\text{Rewrite } P(X|\theta) \text{ as:} \\ &P(X\mid\theta) = \pi^{[X=1]} (1-\pi)^{[X=0]} \quad \text{where:} \quad [X^{(i)} = v] := \left\{ \begin{array}{cc} 1 & \text{if} \quad X^{(i)} = v \\ 0 & \text{if} \quad X^{(i)} \neq v \end{array} \right. & \text{Also called} \\ &0 & \text{if} \quad X^{(i)} \neq v \end{array} \\ &\ell(\theta\mid D) = \log \binom{N}{N_{X=1}} + \sum_{i} \log \left(\pi^{[X^{(i)}=1]} \; (1-\pi)^{[X^{(i)}=0]} \; \right) = \\ &= \log \binom{N}{N_{X=1}} + \log \pi \sum_{i} [X^{(i)} = 1] \; + \log (1-\pi) \sum_{i} [X^{(i)} = 0] \\ &= \log \binom{N}{N_{X=1}} + N_{X=1} \log \pi \; + N_{X=0} \log (1-\pi) \end{split}$$

Maximum Likelihood Estimation

$$\frac{\partial \ell}{\partial \theta} = \frac{\partial \ell}{\partial \pi} = \frac{N_{X=1}}{\pi} - \frac{N_{X=0}}{(1-\pi)} \qquad \qquad \frac{\partial \ell}{\partial \theta} = 0 \quad \Rightarrow \quad \theta_{ML}^* = \frac{N_{X=1}}{N_{X=1} + N_{X=0}} = \frac{N_{X=1}}{N}$$

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$$P(Y, X_1, ..., X_n) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y)$$



Parameters: the conditional probability tables in the graphical model

$$\theta := \{ \pi_k, \ \pi_{ijk} \}$$
 , $P(Y = k) =: \pi_k \ P(X_i = j \mid Y = k) =: \pi_{ijk}$

Observations: a set of messages with classification

$$D = \{D^{(1)} = \{Y^{(1)} = 1, X_1^{(1)} = 1, \dots, X_n^{(1)} = 0\},\$$

$$\dots,$$

$$D^{(N)} = \{Y_2^{(N)} = Y_2^{(N)}, X_1^{(N)} = X_1^{(N)}, \dots, X_n^{(N)} = X_n^{(N)}\}\}$$

Likelihood Function

$$L(\theta|D) \ = \ P(D|\theta) \ = \ P(\{D^{(m)}\}|\{\pi_k,\pi_{ijk}\}) \ = \ \prod_m P(D^{(m)}|\{\pi_k,\pi_{ijk}\}) \quad \text{(data items are IID)}$$

$$= \ \prod_m P(\{Y^{(m)} = y^{(m)},X_i^{(m)} = x_i^{(m)}\}|\{\pi_k,\pi_{ijk}\}) \quad \text{(cond. independence)}$$

$$= \ \prod_m P(Y^{(m)} = y^{(m)}|\{\pi_k,\pi_{ijk}\}) \ P(\{X_i^{(m)} = x_i^{(m)}\}|Y^{(m)} = y^{(m)},\{\pi_k,\pi_{ijk}\}) \quad \text{(cond. independence)}$$

$$= \ \prod_m P(Y^{(m)} = y^{(m)}|\{\pi_k\}) \ P(\{X_i^{(m)} = x_i^{(m)}\}|Y^{(m)} = y^{(m)},\{\pi_{ijk}\}) \quad \text{(adta items are IID)}$$

$$= \ \prod_m P(Y^{(m)} = y^{(m)}|\{\pi_k\}) \ \prod_i P(X_i^{(m)} = x_i^{(m)}|Y^{(m)} = y^{(m)},\{\pi_{ijk}\}) \quad \text{(adta items are IID)}$$

$$P(Y, X_1, \dots, X_n) = P(Y) \prod_{i=1}^n P(X_i \mid Y)$$

$$X_1 \qquad X_2 \qquad \dots \qquad X_n$$

Log-Likelihood Function

$$\ell(\{\pi_k, \pi_{ijk}\}|D) = \sum_{m} \log P(Y^{(m)} = y^{(m)}|\{\pi_k\}) + \sum_{m} \sum_{i} \log P(X_i^{(m)} = x_i^{(m)}|Y^{(m)} = y^{(m)}, \{\pi_{ijk}\})$$

Alternative form for P: (i.e. rewritten using indicator functions)

$$P(Y = k | \{\pi_k\}) = \prod_{k} \pi_k^{[Y=k]}$$

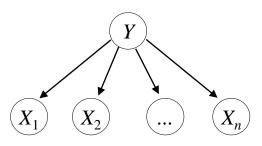
$$P(X_i = j | Y = k, \{\pi_{ijk}\}) = \prod_{j} \prod_{k} \pi_{i,j,k}^{[X_i = j][Y=k]}$$

$$\ell(\{\pi_k, \pi_{ijk}\}|D) = \sum_{m} \sum_{k} [Y^{(m)} = k] \log \pi_k + \sum_{m} \sum_{i} \sum_{j} \sum_{k} [X_i^{(m)} = j][Y^{(m)} = k] \log \pi_{ijk}$$

Being both positive and depending on different variables, the two terms above can be optimized separately

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$$P(Y, X_1, \dots, X_n) = P(Y) \prod_{i=1}^n P(X_i \mid Y)$$



Maximum Likelihood Estimation

$$\ell(\{\pi_k, \pi_{ijk}\}|D) = \sum_{m} \sum_{k} [Y^{(m)} = k] \log \pi_k + \sum_{m} \sum_{i} \sum_{j} \sum_{k} [X_i^{(m)} = j][Y^{(m)} = k] \log \pi_{ijk}$$

Optimizing first term:

Lagrange multiplier

$$\ell^*(\{\pi_k\}|D) = \sum_m \sum_k [Y^{(m)} = k] \log \pi_k + \lambda(1 - \sum_k \pi_k)$$

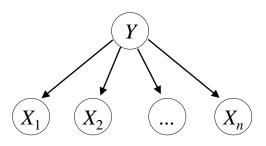
$$\frac{\partial \ell^*}{\partial \pi_k} = \frac{\sum\limits_{m} [Y^{(m)} = k]}{\pi_k} - \lambda$$
 number of messages in D classified as k

$$\frac{\partial \ell^*}{\partial \pi_k} = 0 \quad \Rightarrow \quad \pi_k = \frac{N_{Y=k}}{\lambda}$$

$$\sum_{k} \pi_{k} = 1 \quad \Rightarrow \quad \sum_{k} \frac{N_{Y=k}}{\lambda} = 1 \quad \Rightarrow \quad \lambda = \sum_{k} N_{Y=k} = N$$

$$\pi_k^* = \frac{N_{Y=k}}{N}$$
 (Maximum Likelihood Estimator of π_k)

$$P(Y,X_1,\ldots,X_n)=P(Y)\prod_{i=1}^n P(X_i\mid Y)$$



Maximum Likelihood Estimation

$$\ell(\{\pi_k, \pi_{ijk}\}|D) = \sum_{m} \sum_{k} [Y^{(m)} = k] \log \pi_k + \sum_{m} \sum_{i} \sum_{j} \sum_{k} [X_i^{(m)} = j][Y^{(m)} = k] \log \pi_{ijk}$$

Optimizing second term:

Lagrange multipliers

$$\ell^*(\{\pi_{ijk}\}|D) = \sum_m \sum_i \sum_j \sum_k [X_i^{(m)} = j][Y^{(m)} = k] \log \pi_{ijk} + \sum_i \sum_k \lambda_{ik} (1 - \sum_j \pi_{ijk})$$

$$\frac{\partial \ell^*}{\partial \pi_{ijk}} = \frac{\sum_m [X_i^{(m)} = j][Y^{(m)} = k]}{\pi_{ijk}} - \lambda_{ik}$$

$$\frac{\partial \ell^*}{\partial \pi_{ijk}} = 0 \quad \Rightarrow \quad \pi_{ijk} = \frac{N_{X_i = j, Y = k}}{\lambda_{ik}}$$

$$\sum_j \pi_{ijk} = 1 \quad \Rightarrow \quad \sum_j \frac{N_{X_i = j, Y = k}}{\lambda_{ik}} = 1 \quad \Rightarrow \quad \lambda = \sum_j N_{X_i = j, Y = k} = N_{Y = k}$$

$$\pi^*_{ijk} = rac{N_{X_i=j, \ Y=k}}{N_{Y=k}}$$
 (Maximum Likelihood Estimator of π_{ijk})

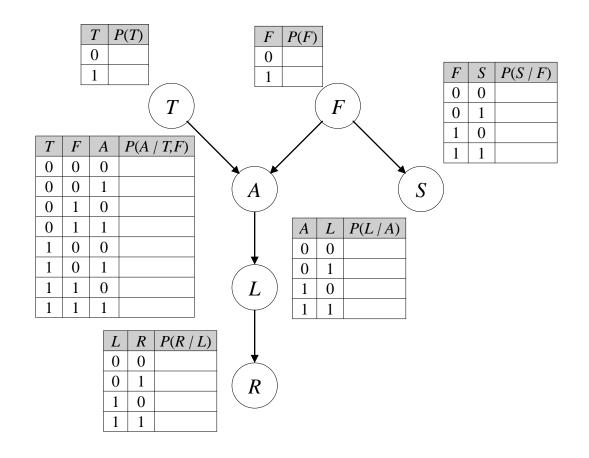
MLE for Graphical Models: A Practical Rule

Learning CPTs for a graphical model via MLE

Model: random variables plus the graph of dependencies

Observations: dataset of values, from <u>completely observed</u> outcomes

Parameters (to be determined): all conditional probabilities (i.e. all CPTs)



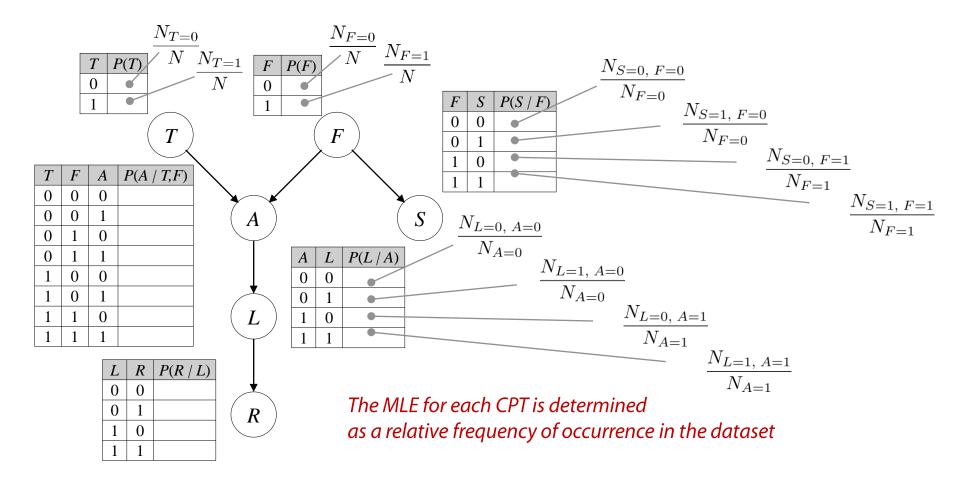
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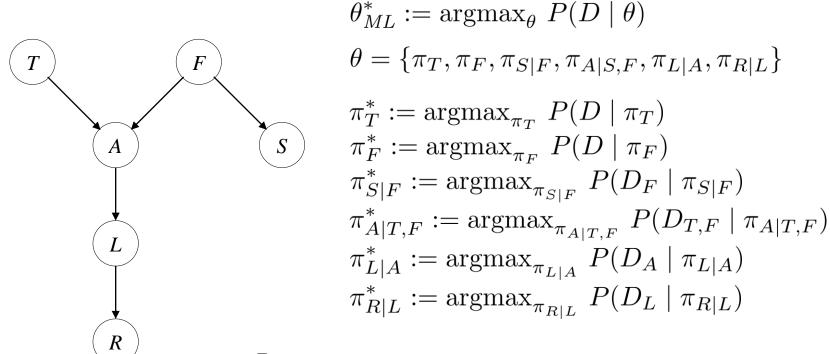


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Learning CPTs for a graphical model via MLE

More in general:

The MLE of a (directed) graphical model is the MLE of each node (in each corresponding observation subset)



 $D_{T,F}\,$ denotes the subset of complete observation in which the random variables T,F have the corresponding values

Bayesian Learning: Maximum a Posteriori (MAP) estimator

Bayesian learning

Maximum a Posteriori Estimation (MAP)

Instead of a likelihood function, the a posteriori probability is maximized

$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)} = \frac{P(D|\theta) P(\theta)}{\sum_{\theta} P(D|\theta) P(\theta)}$$

Which is equivalent to optimize, w.r.t. θ :

$$P(D|\theta) P(\theta)$$

$$\theta_{MAP}^* := \operatorname{argmax}_{\theta} P(D|\theta) P(\theta)$$

Advantages:

- Regularization: not all possible combinations of values might be present in D
- A formula for incremental learning:
 a priori terms could represent what was known before observations D

Problem:

• Which *prior* distribution? $P(\theta)$

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Beta distribution

Gamma function (n integer > 0)

$$\Gamma(n) := (n-1)!$$

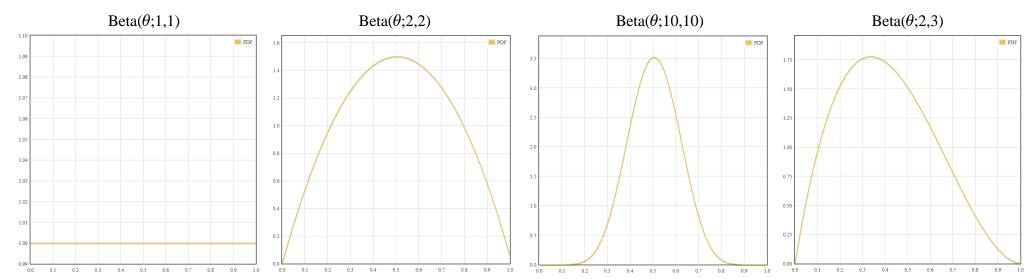
Beta <u>function</u> (α and β integers > 0)

$$B(\alpha,\beta) := \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} = \frac{(\alpha-1)!(\beta-1)!}{(\alpha+\beta-1)!} \quad \text{The definition is more complex when α and β are not integers (see Wikipedia)}$$

• Beta probability density function (pdf) (α and β integers > 0)

$$\mathrm{Beta}(\theta; \alpha, \beta) \,:=\, \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}$$
 The maximum occurs at:

$$\theta = \frac{\alpha - 1}{\alpha + \beta - 2}$$



Conjugate prior distributions

Coin tossing (i.e. Binomial)

 α_D and β_D are the result counts (i.e. heads and tails)

$$P(D|\theta) = {\binom{\alpha_D + \beta_D}{\alpha_D}} \prod_i P(X_i|\theta) = {\binom{\alpha_D + \beta_D}{\alpha_D}} \theta^{\alpha_D} (1 - \theta)^{\beta_D}$$

A posteriori probability with Beta prior

 α_P and β_P are are the **hyperparameters** of the prior

$$P(D|\theta)P(\theta) = \begin{pmatrix} \alpha_D + \beta_D \\ \alpha_D \end{pmatrix} \theta^{\alpha_D} (1-\theta)^{\beta_D} \cdot \text{Beta}(\theta; \alpha_P, \beta_P) = \begin{pmatrix} \alpha_D + \beta_D \\ \alpha_D \end{pmatrix} \theta^{\alpha_D} (1-\theta)^{\beta_D} \cdot \frac{\theta^{\alpha_P - 1} (1-\theta)^{\beta_P - 1}}{B(\alpha_P, \beta_P)}$$
$$= \begin{pmatrix} \alpha_D + \beta_D \\ \alpha_D \end{pmatrix} \frac{\theta^{\alpha_D + \alpha_P - 1} (1-\theta)^{\beta_D + \beta_P - 1}}{B(\alpha_P, \beta_P)} = \begin{pmatrix} \alpha_D + \beta_D \\ \alpha_D \end{pmatrix} \frac{B(\alpha_D + \alpha_P, \beta_D + \beta_P)}{B(\alpha_P, \beta_P)} \text{Beta}(\theta; \alpha_D + \alpha_P, \beta_D + \beta_P)$$

this factor is a positive constant (for θ)

Conjugate prior distributions

Coin tossing (i.e. Binomial)

 α_D and β_D are the result counts (i.e. heads and tails)

$$P(D|\theta) = {\binom{\alpha_D + \beta_D}{\alpha_D}} \prod_i P(X_i|\theta) = {\binom{\alpha_D + \beta_D}{\alpha_D}} \theta^{\alpha_D} (1-\theta)^{\beta_D}$$

A posteriori probability with Beta prior

$$P(D|\theta)P(\theta) = \binom{\alpha_D + \beta_D}{\alpha_D} \frac{\mathrm{B}(\alpha_D + \alpha_P, \beta_D + \beta_P)}{\mathrm{B}(\alpha_P, \beta_P)} \mathrm{Beta}(\theta; \alpha_D + \alpha_P, \beta_D + \beta_P)$$

$$/ \text{"is proportional to"}$$

$$P(D|\theta)P(\theta) \propto \mathrm{Beta}(\theta; \alpha_D + \alpha_P, \beta_D + \beta_P)$$

Optimization:

$$\theta_{MAP}^* = \operatorname{argmax}_{\theta} \operatorname{Beta}(\theta; \alpha_D + \alpha_P, \beta_D + \beta_P) = \frac{\alpha_D + \alpha_P - 1}{\alpha_D + \alpha_P + \beta_D + \beta_P - 2}$$

which is the same as MLE but with the addition of $\alpha_P + \beta_P$ pseudo-observations

Being a **conjugate prior** $P(\theta)$ of a distribution $P(D|\theta)$ is in the same family of $P(\theta)$

Conjugate prior distributions

Coin tossing (i.e. a specific observation i)

$$P(D_i|\theta) = \theta^{[X_i=1]} (1 - \theta)^{[X_i=0]}$$

Likelihood (of a dataset)

$$P(D|\theta) = \binom{N}{N_{X=1}} \prod_{i} P(D_i|\theta) = \binom{N}{N_{X=1}} \theta^{N_{X=1}} (1-\theta)^{N_{X=0}}$$

A posteriori probability with Beta prior

"is proportional to"
$$P(D|\theta)P(\theta) \propto \mathrm{Beta}(\theta,\ N_{X=1}+\alpha_P,\ N_{X=0}+\beta_P)$$

Therefore

$$\theta_{MAP}^* = \operatorname{argmax}_{\theta} \operatorname{Beta}(\theta, N_{X=1} + \alpha_P, N_{X=0} + \beta_P) = \frac{N_{X=1} + \alpha_P - 1}{N + \alpha_P + \beta_P - 2}$$

which is the same as MLE but with the addition of $\alpha_P + \beta_P$ pseudo-observations

Being a **conjugate prior** $P(\theta)$ of a distribution $P(D|\theta)$ in the above sense means that the posterior $P(D|\theta)P(\theta)$ is in the same family of $P(\theta)$

Anti-spam filter

$$P(Y, X_1, \dots, X_n) = P(Y) \prod_{i=1}^n P(X_i \mid X_{i-1}) \underbrace{X_1} \underbrace{X_2} \underbrace{X_n}$$

Maximum a Posteriori (MAP) Estimation

The adapted computations for:

$$\theta_{MAP}^* := \operatorname{argmax}_{\theta} P(D|\theta) P(\theta)$$

yield:

$$\pi_k^* = \frac{\alpha_k + N_{Y=k} - 1}{\alpha_k + \beta_k + N - 2} \qquad (\textit{MAP Estimator of } \pi_k)$$

$$\pi_{ijk}^* = \frac{\alpha_{ijk} + N_{X_i=j, Y=k} - 1}{\alpha_{ijk} + \beta_{ijk} + N_{Y=k} - 2} \qquad (\textit{MAP Estimator of } \pi_{ijk})$$

where the

$$\alpha_k, \beta_k, \alpha_{ijk}, \beta_{ijk}$$

are the *hyperparameters* of the prior distribution representing the *pseudo-observations* made *before* the arrival of new, actual observations *D*

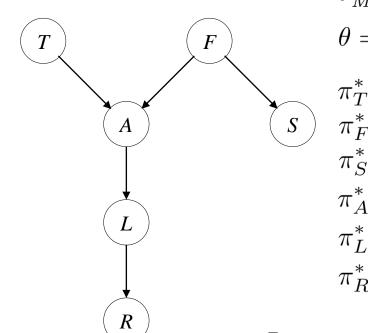
Bayesian Learning: MAP for Graphical Models

Learning CPTs for a graphical model

As Maximum a Posteriori Estimation

More in general:

The MAP of a (directed) graphical model is the MAP of each node (in each corresponding observation subset)



$$\theta_{MAP}^{*} := \operatorname{argmax}_{\theta} P(D \mid \theta) P(\theta)$$

$$\theta = \{\pi_{T}, \pi_{F}, \pi_{S|F}, \pi_{A|S,F}, \pi_{L|A}, \pi_{R|L}\}$$

$$\pi_{T}^{*} := \operatorname{argmax}_{\pi_{T}} P(D \mid \pi_{T}) P(\pi_{T})$$

$$\pi_{F}^{*} := \operatorname{argmax}_{\pi_{F}} P(D \mid \pi_{F}) P(\pi_{F})$$

$$\pi_{S|F}^{*} := \operatorname{argmax}_{\pi_{S|F}} P(D_{F} \mid \pi_{S|F}) P(\pi_{S|F})$$

$$\pi_{A|T,F}^{*} := \operatorname{argmax}_{\pi_{A|T,F}} P(D_{T,F} \mid \pi_{A|T,F}) P(\pi_{A|T,F})$$

$$\pi_{L|A}^{*} := \operatorname{argmax}_{\pi_{L|A}} P(D_{A} \mid \pi_{L|A}) P(\pi_{L|A})$$

$$\pi_{R|L}^{*} := \operatorname{argmax}_{\pi_{R|L}} P(D_{L} \mid \pi_{R|L}) P(\pi_{R|L})$$

 $D_{T,F}$ denotes the subset of complete observation in which the random variables T,F have the corresponding value