Learning

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https://probabll.github.io

Outline and goals

Module 5 introduces *Learning Algorithms* for BNs and MNs (Chapters 17, ...).

ILOs After this module the student

- can estimate parameters for a BN via MLE;
- can estimate parameters for an MN via (approximations to) MLE;

Textbook for this course: Koller and Friedman [1].

Overview of Module 1

HC6a: Parameter estimation for BNs.

LC6: Parameter estimation in code.

HC6b: Parameter estimation for MNs.

WC6: exercises.

Table of contents

Parameter Estimation

Prescribing a Categorical Distribution

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- for any $x \in \mathsf{Val}(X)$, $0 \leq \theta_x \leq 1$
- $\sum_{x \in \mathsf{Val}(X)} \theta_x = 1$

Then, under this choice, $P(X = x) = \theta_x$.

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Suppose we have a dataset $\mathcal{D} = \{x[1], \ldots, x[M]\}$ of M observations of realisations of X.

How can we use **data** to inform our choice of numerical values for the parameters $\boldsymbol{\theta}$?

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Suppose we have a dataset $\mathcal{D} = \{x[1], \ldots, x[M]\}$ of M observations of realisations of X.

How can we use **data** to inform our choice of numerical values for the parameters $\boldsymbol{\theta}$? This is a **statistical inference** problem.

Frequentist Inference

First, characterise the model's likelihood function given the available data $\mathcal{D}$:

$$L(\boldsymbol{\theta}; \mathcal{D}) = \prod_{m=1}^{M} P(X = x[m]) = \prod_{m=1}^{M} \theta_{x[m]}$$

The likelihood function $L(\boldsymbol{\theta}; \mathcal{D})$ assigns 'worth' or 'utility' to a choice of parameter $\boldsymbol{\theta}$. This utility is defined to be the probability mass that our model assigns to $\mathcal{D}$ under the assumption that the data samples were drawn IID from our model using the current choice of $\boldsymbol{\theta}$.

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Second, pick the parameter value that yields maximum likelihood:

$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta} \in \Delta_{K-1}}{\operatorname{argmax}} \; L(\boldsymbol{\theta}; \mathcal{D}) = \underset{\boldsymbol{\theta} \in \Delta_{K-1}}{\operatorname{argmax}} \; \underbrace{\log L(\boldsymbol{\theta}; \mathcal{D})}_{\mathcal{L}(\boldsymbol{\theta}; \mathcal{D})}$$

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$$\boldsymbol{\theta}^\star = \operatorname*{argmax}_{\boldsymbol{\theta} \in \Delta_{K-1}} L(\boldsymbol{\theta}; \mathcal{D}) = \operatorname*{argmax}_{\boldsymbol{\theta} \in \Delta_{K-1}} \underbrace{\log L(\boldsymbol{\theta}; \mathcal{D})}_{\mathcal{L}(\boldsymbol{\theta}; \mathcal{D})} = \sum_{m=1}^{M} \log \theta_{x[m]}$$

This is known as **maximum likelihood estimation (MLE).**

Bayesian Inference

Bayesian inference treats parameters as rvs on their own right.

It also uses the likelihood function, but in a very different way, as a means to update beliefs about parameters:

$$\underbrace{p(\boldsymbol{\theta}|\mathcal{D})}_{\text{posterior}} \propto \underbrace{p(\boldsymbol{\theta})}_{\text{prior}} \underbrace{L(\boldsymbol{\theta};\mathcal{D})}_{\text{likelihood}}$$

Rather than looking for a parameter value judged to be 'right' (or 'optimum')—a point estimate—Bayesian inference attempts to estimate parameters that are *probable* in light of the available data and model assumptions as captured by the likelihood function.

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In this course, we will focus on Frequentist inference (not because it's 'right' or to be preferred in general, simply because Bayesian inference requires a longer course).

MLE for the Parameters of a Categorical Distribution

X is a categorical rv with outcomes in $\mathsf{Val}(X) = \{x^1, \ldots, x^K\}$. We model its distribution in tabular form, that is, we introduce a parameter vector $\boldsymbol{\theta}_X = (\theta_{x^1}, \ldots, \theta_{x^K})$ such that $P(X = x) = \theta_x$.

We have a dataset $\mathcal{D} = \{x[1], \ldots, x[M]\}$ of M observations of X.

Define the helper 'counting' function $M[o] = \sum_{m=1}^{M} [x[m] = o]$.

The Iverson bracket $[\alpha]$ is 1 if the logical predicate α is True and 0 otherwise. MLE for Categorical distribution: if you're curious I derived it here.

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We have a dataset $\mathcal{D} = \{x[1], \ldots, x[M]\}$ of M observations of X.

Define the helper 'counting' function $M[o] = \sum_{m=1}^{M} [x[m] = o]$.

The maximum likelihood estimate of θ_x for any $x \in \mathsf{Val}(X)$ is given by

$$\theta_x = \frac{M[x]}{\sum_{x' \in \mathsf{Val}(X)} M[x']} = \frac{M[x]}{M} \tag{1}$$

The Iverson bracket $[\alpha]$ is 1 if the logical predicate α is True and 0 otherwise. MLE for Categorical distribution: if you're curious I derived it here.

MLE for a Categorical Distribution – Example

The coherence C of a course may be high c^1 or low c^0. Let's do MLE for a tabular representation of $P(C)$.

Course	Votes
CS0001	$c^1, c^1, c^1, c^0, c^0, c^0, c^0, c^1, c^1, c^0$
CS0002	$c^1, c^1, c^1, c^0, c^0, c^0, c^1, c^1, c^1, c^1$

Observations from course evaluation surveys.

MLE for $P(C)$ using the data above: $\boldsymbol{\theta} = (\theta_{c^0}, \theta_{c^1}) = (\quad , \quad)$.

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MLE for $P(C)$ using the data above: $\boldsymbol{\theta} = (\theta_{c^0}, \theta_{c^1}) = (^8/_{20}, ^{12}/_{20})$.

MLE for the Parameters of a Tabular CPD

Now, we also have an rv Y taking on values in $\mathrm{Val}(Y) = \{y^1, \ldots, y^V\}$.

We are modelling $P(Y|X)$ in tabular representation. Hence, we introduce a collection of parameter vectors $\boldsymbol{\theta}_{Y|X} = (\boldsymbol{\theta}_{Y|x^1}, \ldots, \boldsymbol{\theta}_{Y|x^K})$.

- Each $\boldsymbol{\theta}_{Y|x}$ is a vector $(\theta_{y^1|x}, \ldots, \theta_{y^V|x})$ for some $x \in \mathrm{Val}(X)$
- such that $P(Y = y|X = x) = \theta_{y|x}$.

Now our observations are M pairs $\mathcal{D} = \{(x[1], y[1]), \ldots, (x[M], y[M])\}$.

Define a new 'counting' function $M[c, o] = \sum_{m=1}^{M} [x[m] = c][y[m] = o]$.

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Define a new 'counting' function $M[c, o] = \sum_{m=1}^{M} [x[m] = c][y[m] = o]$.

The MLE of $\theta_{y|x}$ for any $x \in \mathsf{Val}(X)$ and $y \in \mathsf{Val}(Y)$ is given by

$$\theta_{y|x} = \frac{M[x, y]}{\sum_{y' \in \mathsf{Val}(Y)} M[x, y']} = \frac{M[x, y]}{M[x]} \tag{2}$$

MLE for a Categorical CPD – Example

The course may be difficult d^1 or easy d^0. Let's do MLE for a tabular representation of $P(D|C)$.

Course	Votes
CS0001	$(c^1, d^0), (c^1, d^0), (c^1, d^0), (c^0, d^1), (c^0, d^1)$
	$(c^0, d^0), (c^0, d^1), (c^1, d^0), (c^1, d^0), (c^0, d^1)$
CS0002	$(c^1, d^1), (c^1, d^1), (c^1, d^1), (c^0, d^1), (c^0, d^1)$
	$(c^0, d^1), (c^1, d^1), (c^1, d^1), (c^1, d^1), (c^1, d^0)$

Observations from course evaluation surveys.

MLE for $P(D|C)$ using the data above:

$\boldsymbol{\theta}_{D|c^0} = (\theta_{d^0|c^0}, \theta_{d^1|c^0}) = (\quad , \quad)$

$\boldsymbol{\theta}_{D|c^1} = (\theta_{d^0|c^1}, \theta_{d^1|c^1}) = (\quad , \quad)$

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Observations from course evaluation surveys.

MLE for $P(D|C)$ using the data above:

$$\boldsymbol{\theta}_{D|c^0} = (\theta_{d^0|c^0}, \theta_{d^1|c^0}) = (1/8, 7/8)$$
$$\boldsymbol{\theta}_{D|c^1} = (\theta_{d^0|c^1}, \theta_{d^1|c^1}) = (\quad , \quad)$$

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MLE for $P(D|C)$ using the data above:

$\boldsymbol{\theta}_{D|c^0} = (\theta_{d^0|c^0}, \theta_{d^1|c^0}) = (1/8, 7/8)$

$\boldsymbol{\theta}_{D|c^1} = (\theta_{d^0|c^1}, \theta_{d^1|c^1}) = (6/12, 6/12)$

MLE for Bayesian Networks

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In a BN we have a CPD for each node X_i given the node's parents $\mathrm{Pa}(X_i)$. For CPDs in tabular representation, this means we have a collection of parameters $\boldsymbol{\theta}_{X_i|\mathrm{Pa}(X_i)}$ for each node X_i.

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The likelihood $L(\boldsymbol{\theta}; \mathcal{D})$ of a BN is $L(\boldsymbol{\theta}; \mathcal{D}) = \prod_{m=1}^{M} P(\mathbf{X} = \mathbf{x}[m])$

$$= \prod_{m=1}^{M} \prod_{i} P(X_i = x[m]_i | \mathrm{Pa}(X_i) = \mathrm{pa}(x[m]_i))$$

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$$= \prod_{m=1}^{M} \prod_{i} P(X_i = x[m]_i | \mathrm{Pa}(X_i) = \mathrm{pa}(x[m]_i))$$

$$= \prod_{i} \underbrace{\prod_{m=1}^{M} P(X_i = x[m]_i | \mathrm{Pa}(X_i) = \mathrm{pa}(x[m]_i))}_{L(\boldsymbol{\theta}_{X_i|\mathrm{Pa}(X_i)};\mathcal{D})}$$

decomposes in terms of **local likelihood functions**, one per X_i, where

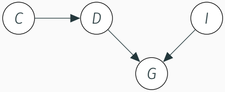
$$L(\boldsymbol{\theta}_{X_i|\mathrm{Pa}(X_i)};\mathcal{D}) = \prod_{m=1}^{M} \theta_{x[m]_i|\mathrm{pa}(x[m]_i)}$$

MLE for Bayesian Networks - Algorithm

Because the BN likelihood decomposes, so long as we have complete observations (that is, we learn by observing joint assignments of *all* rvs), we can solve independent MLE problems, one per rv.

For each rv X_i, the MLE for the parameters of the tabular CPD $P(X_i|\mathrm{Pa}(X_i))$ is

- $\theta_{o|\boldsymbol{u}} = \frac{M[\boldsymbol{u},o]}{M[\boldsymbol{u}]}$ for any $o \in \mathrm{Val}(X_i)$ and any $\boldsymbol{u} \in \mathrm{Val}(\mathrm{Pa}(X_i))$



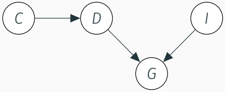
Student	Record
s1000	(c^0, d^1, i^1, g^1)
s1001	(c^0, d^0, i^1, g^1)
s1002	(c^0, d^1, i^0, g^1)
s1003	(c^1, d^0, i^1, g^2)
s1004	(c^1, d^0, i^1, g^2)
s1005	(c^1, d^0, i^0, g^1)
s1006	(c^1, d^0, i^0, g^3)
s1007	(c^0, d^1, i^1, g^3)
s1008	(c^0, d^1, i^1, g^2)
s1009	(c^1, d^0, i^1, g^1)

Observations from CS0001.

θ_{i^0}	θ_{i^1}

pa	$\theta_{g^1\|d,i}$	$\theta_{g^2\|d,i}$	$\theta_{g^3\|d,i}$
d^0, i^0			
d^0, i^1			
d^1, i^0			
d^1, i^1			

MLE for $P(I)$ and $P(G|D, I)$



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s1009	(c^1, d^0, i^1, g^1)

Observations from CS0001.

θ_{i^0}	θ_{i^1}
$3/10$	$7/10$

pa	$\theta_{g^1\|d,i}$	$\theta_{g^2\|d,i}$	$\theta_{g^3\|d,i}$
d^0, i^0			
d^0, i^1			
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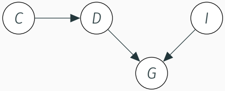
d^1, i^1			

MLE for $P(I)$ and $P(G|D, I)$



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Observations from CS0001.

θ_{i^0}	θ_{i^1}
$^3/_{10}$	$^7/_{10}$

pa	$\theta_{g^1\|d,i}$	$\theta_{g^2\|d,i}$	$\theta_{g^3\|d,i}$
d^0, i^0	$^1/_2$	$^0/_2$	$^1/_2$
d^0, i^1			
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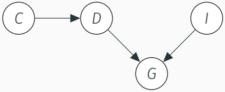
MLE for $P(I)$ and $P(G|D, I)$



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Observations from CS0001.

θ_{i^0}	θ_{i^1}
$3/10$	$7/10$

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d^0, i^0	$1/2$	$0/2$	$1/2$
d^0, i^1	$2/4$	$2/4$	$0/3$
d^1, i^0			
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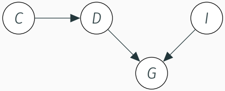
MLE for $P(I)$ and $P(G|D, I)$



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d^1, i^0	$1/1$	$0/1$	$0/1$
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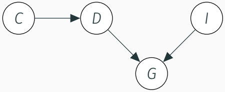
MLE for $P(I)$ and $P(G|D, I)$

MLE for BNs - Example



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pa	$\theta_{g^1\|d,i}$	$\theta_{g^2\|d,i}$	$\theta_{g^3\|d,i}$
d^0, i^0	$1/2$	$0/2$	$1/2$
d^0, i^1	$2/4$	$2/4$	$0/3$
d^1, i^0	$1/1$	$0/1$	$0/1$
d^1, i^1	$1/3$	$1/3$	$1/3$

MLE for $P(I)$ and $P(G|D, I)$

Data Sparsity

Take the example from the previous slide: $\boldsymbol{\theta}_{G|d^1,i^0}$ whose MLE is $(1/1, 0/1, 0/1)$. Clearly, this MLE must not be very robust, after all, it is based on a single observation of $(D = d^1, I = i^0)$.

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Solutions to this take different forms: Bayesian estimation represents uncertainty around parameters, Frequentist estimation use 'regularisers' and/or increase parameter sharing.

Regularised MLE and MAP Estimation for Tabular CPDs

A 'regulariser' is a pressure to deviate from the MLE objective in some systematic way. It is common to perform **regularised MLE** instead of (pure) MLE:

$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\mathrm{argmax}}\ \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) - \mathcal{R}(\boldsymbol{\theta}) \tag{3}$$

where $\mathcal{R}(\boldsymbol{\theta})$ is some form of 'penalty' on certain parameters values (for example, those that are too large or too sparse).

Some choices of $\mathcal{R}(\boldsymbol{\theta})$ can be regarded as a form of *prior* about how parameter values would distributed if they were given random treatment. Such objectives are often called maximum-a-posteriori (MAP) estimation, for they coincide with the argmax of the Bayesian posterior $p(\boldsymbol{\theta}|\mathcal{D})$.

Watch Out! MAP Inference $\neq$ MAP Estimation

Don't confuse MAP inference in PGMs (that is, max-product inference), which concerns a max/argmax query about the rvs of a model, to MAP estimation in frequentist statistics (a regularised likelihood objective), which concerns parameter estimation.

MAP Inference in PGMs:

$$x^\star = \underset{x \in \mathrm{Val}(X)}{\operatorname{argmax}} \; P(X = x)$$

$x^\star$ is an assignment of the rvs that are jointly distributed under $P(X)$.

MAP Estimation in Frequentist Statistics:

$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \; \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) - \mathcal{R}(\boldsymbol{\theta})$$

$\boldsymbol{\theta}^\star$ is a collection of parameters that give numerical values for the cells of the tabular CPDs that parameterise $P(X)$.

Laplace Smoothed MLE for Tabular Categorical CPDs

A 'patch' for situations where we don't have enough data to estimate our tabular CPDs is to 'smooth' the MLE by a 'pseudo-count' $\alpha > 0$: a count that we pretend all context-outcome pairs start from before we even gather observations.

The **Laplace smoothed** MLE of $\theta_{X|\boldsymbol{u}}$ for any $x \in \mathrm{Val}(X)$ and $\boldsymbol{u} \in \mathrm{Val}(\mathrm{Pa}(X))$ is given by

$$\theta_{x|\boldsymbol{u}} = \frac{M[\boldsymbol{u}, x] + \alpha}{\sum_{x' \in \mathrm{Val}(X)} (M[\boldsymbol{u}, x'] + \alpha)} = \frac{M[\boldsymbol{u}, x] + \alpha}{\alpha |\mathrm{Val}(X)| + M[\boldsymbol{u}]} \tag{4}$$

In some more advanced versions, α can be specified per context ($\boldsymbol{u}$).

Out of curiosity: Laplace smoothing (or 'add-α smoothing') corresponds to MAP estimation using a Dirichlet prior $\theta_{X|\boldsymbol{u}} \sim \mathrm{Dir}(\alpha)$.

Laplace (add-α) Smoothing - Example

With add-0.1 smoothing, the example of $\boldsymbol{\theta}_{G|d^1,i^0}$ becomes $(^{1.1}/_{1.3}, {}^{0.1}/_{1.3}, {}^{0.1}/_{1.3})$.

Note how 0.1 is added to all 3 outcomes of G and hence affects the denominator in triple dose.

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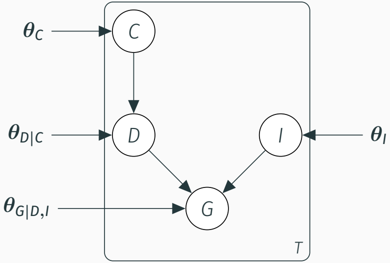
This really is just a 'patch' to avoid 0s. Better strategies cpme from clever forms of parameter sharing. The first of which, we cover next.

Parameter Sharing with Template Models

It is very common to think of a PGM as a *template* to be instantiated given certain meta-data.

For example, we can imagine that our simplified student BN can be used to model T students who take a certain course:

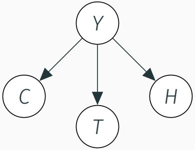


- Students are independent of one another.
- There are 4 tabular CPDs that are reused across all students.

Think of the plate as a 'for loop', the variables inside are 'instantiated' for each 'data record' out of T such data records. The assignments in iteration t_1 are independent of the assignments in iteration t_2.

Suppose we have 3 'predictors' C, T, H for a condition Y.

A condition might be something like COVID19 y^1 (True) or y^0 (False) and predictors might be things like: cough c^1 or c^0, high temperature t^1 or t^0, headache h^1 or h^0).



This is known as a **naive Bayes** model, commonly used for **classification** via $\operatorname{argmax}_y \; P(Y = y | C = c, T = t, H = h)$ for some given assignment $(C = c, T = t, H = h)$ of the symptoms.

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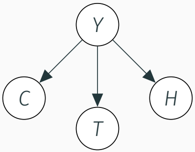

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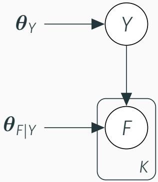
In a naive Bayes model, we assume that the distribution of $C|Y = y$ is the same as the distribution of $T|Y = y$ and of $H|Y = y$.

Instead of 3 CPDs $P(C|Y)$, $P(T|Y)$ **and** $P(H|Y)$, **we have one CPD** $P(F|Y)$ for 'feature value' given 'class' and we take c, t, h to be 3 feature values drawn from that CPD.

MLE for BNs - Example — Naive Bayes Classifier

With K binary 'predictors' $X_1, \ldots, X_K$ (e.g., Cough, Temperature, Headache, loss of sense of Smell) for a condition Y. The NB model is a template BN.



Tabular CPDs

- $P(Y = y) = \theta_y$
- $P(F = f|Y = y) = \theta_{f|y}$

Compute the MLE parameters using the observations in the table.

Y	C	T	H	S
y^0	c^1	t^1	h^1	s^1
y^0	c^0	t^1	h^1	s^0
y^1	c^0	t^1	h^1	s^0
y^1	c^1	t^1	h^1	s^1
y^1	c^1	t^1	h^1	s^1
y^0	c^1	t^0	h^1	s^1
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y^0	c^1	t^0	h^0	s^0
y^0	c^0	t^0	h^0	s^0
y^0	c^1	t^0	h^0	s^0

Solution

$\theta_Y = (^{64}/_{80}, {}^{16}/_{80})$

For $\boldsymbol{\theta}_{F|Y}$, see below:

Y	$\theta_{c^0\|y}$	$\theta_{c^0\|y}$	$\theta_{h^0\|y}$	$\theta_{h^1\|y}$	$\theta_{s^0\|y}$	$\theta_{s^1\|y}$	$\theta_{t^0\|y}$	$\theta_{t^1\|y}$
y^0	$^6/_{64}$	$^{10}/_{64}$	$^6/_{64}$	$^{10}/_{64}$	$^{11}/_{64}$	$^5/_{64}$	$^7/_{64}$	$^9/_{64}$
y^1	$^1/_{16}$	$^3/_{16}$	$^1/_{16}$	$^3/_{16}$	$^1/_{16}$	$^3/_{16}$	$^1/_{16}$	$^3/_{16}$

Because we treat the different symptoms as draws from the same CPD, we have 80 paired data points of the kind (Y, F). It is *as if* we had more data to estimate one CPD $P(F|Y)$ than we would have to estimate 4 CPDs $P(C|Y)$, $P(H|Y)$, $P(S|Y)$, $P(T|Y)$ instead.

Evaluating the MLE Solution

'Intrinsically'

- Assess $L(\boldsymbol{\theta}; \mathcal{H})$ for a dataset 'heldout' from training;

'Extrinsically' (task-driven)

- use the model in a predictive task (e.g., classification) and measure its task performance for some heldout dataset.

MLE for Markov Networks

References

[1] Daphne Koller and Nir Friedman. *Probabilistic graphical models: principles and techniques.* MIT press, 2009.