Artificial Intelligence

A course about foundations

Probabilistic Reasoning: Supervised Learning

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Machine Learning

Types of machine learning problems

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

E Supervised learning

 $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ include values for all the random variables in the model

The objective is learning a *distribution P*

▪ **Unsupervised learning**

 $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ do not necessarily include values for all the random variables in the model The objective is learning a *distribution P*

E Reinforcement learning

 $\{D^{(1)}, D^{(2)}, ..., D^{(N)}\}$ X_i the agent must perform an \bm{a} ction $\ a_i$ 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

 $v(< r_1, r_2, ..., r_n>)$ 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 $\{X, Y\}$, *N* outcomes of the experiments are $D^{(1)} = (X^{(1)}, Y^{(1)}), \ldots, D^{(N)} = (X^{(N)}, Y^{(N)})$

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

 $\{X_1, X_2, \ldots, X_n\}$

- 1) $\langle X_i \perp X_j \rangle$, $\forall i \neq j$ (independence)
- 2) $P(X_i = x) = P(X_i = x)$, $\forall i \neq j$, $\forall x$ (identical distribution)

CAUTION: Being IID is not an obvious property of observations

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

ML = Representation + Evaluation + Optimization

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

Example Presentation

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 θ 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.

 $D = \{D^{(1)}, \dots, D^{(N)}\}$

■ Likelihood function (or conditional probability)

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

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

Note the 'trick':

where $P(D | \theta)$ is the conditional probability that the parameter θ , considered as a random variables, could *generate* the observations D $\{D^{(1)}, \, ... \, , D^{(N)}\}$

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

likelihood of the dataset given the parameters

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.

 $D = \{D^{(1)}, \dots, D^{(N)}\}$

• Maximum Likelihood Estimation

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

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

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

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

Example: coin tossing (Bernoulli Trials)

Experiment: tossing a coin X, not necessarily fair $(X = 1 \text{ head}, X = 0 \text{ tail})$ **Parameters:** $\theta := \{ \pi \} \iff P(X = 1) = \pi, P(X = 0) = 1 - \pi$ **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

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

$$
N_{X=1} \text{ is the number of } X=1 \text{ (i.e. heads) in a sequence of } N \text{ trials}
$$

 $N¹$

$$
= {N \choose N_{X=1}} \pi^{N_{X=1}} (1-\pi)^{N_{X=0}}
$$

It is the probability of obtaining $N_{X=1}$ times 'head' in a sequence of N trials $\{D^{(1)}, \ldots, D^{(N)}\}$ given the parameters θ

 \bigwedge

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MLE as optimization

Example: coin tossing (Bernoulli Trials)

■ (Log-)Likelihood Function

$$
\ell(\theta|D) = \log P(D|\theta) = \log P(\{X^{(i)}\}|\theta) = \log \binom{N}{N_{X=1}} \prod_i P(X^{(i)}|\theta) = \log \binom{N}{N_{X=1}} + \sum_i \log P(X^{(i)}|\theta)
$$

Rewrite $P(X|\theta)$ as:

Rewrite $P(X | \theta)$ as:
 $P(X | \theta) = \pi^{[X=1]}(1-\pi)^{[X=0]}$ where: $[X^{(i)} = v] := \begin{cases} 1 & \text{if } X^{(i)} = v \\ 0 & \text{if } X^{(i)} \neq v \end{cases}$ Also called indicator function

$$
\ell(\theta | D) = \log \binom{N}{N_{X=1}} + \sum_{i} \log \left(\pi \binom{[X^{(i)}=1]}{1-\pi} \binom{[X^{(i)}=0]}{1-\pi} \right) =
$$

= $\log \binom{N}{N_{X=1}} + \log \pi \sum_{i} [X^{(i)}=1] + \log(1-\pi) \sum_{i} [X^{(i)}=0]$
= $\log \binom{N}{N_{X=1}} + N_{X=1} \log \pi + N_{X=0} \log(1-\pi)$

• Maximum Likelihood Estimation

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

Naïve Bayesian Classifier

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

Parameters: the conditional probability tables in the graphical model

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

Observations: a set of messages with classification

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

... ,
\n
$$
D^{(N)} = {Y_2}^{(N)} = y^{(N)}, X_1^{(N)} = x_1^{(N)}, ..., X_n^{(N)} = x_n^{(N)}
$$
}

ELikelihood Function

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

\n
$$
= \prod_{m} P(\{Y^{(m)} = y^{(m)}, X_i^{(m)} = x_i^{(m)}\}|\{\pi_k, \pi_{ijk}\})
$$
\n(factorization)

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

\n
$$
= \prod_{m} P(Y^{(m)} = y^{(m)}|\{\pi_k\}) P(\{X_i^{(m)} = x_i^{(m)}\}|Y^{(m)} = y^{(m)}, \{\pi_{ijk}\})
$$
\n($\langle X_i \perp X_j | Y \rangle$) = \prod_{m} P(Y^{(m)} = y^{(m)}|\{\pi_k\}) \prod_{i} P(X_i^{(m)} = x_i^{(m)}|Y^{(m)} = y^{(m)}, \{\pi_{ijk}\})

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Naïve Bayesian Classifier

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

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)

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

$$
P(X_i = j | Y = k, \{\pi_{i j k}\}) = \prod_j \prod_k \pi_{i, j, k} [X_i = j] [Y = k]
$$

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

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

Naïve Bayesian Classifier

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

*X*1

Y

 $\left(X_n\right)$

 $\left(X_{2}\right)$

• 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:

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

$$
\frac{\partial \ell^*}{\partial \pi_k} = \frac{\sum_{m} [Y^{(m)} = k]}{\pi_k} - \lambda
$$

number of messages in *D* classified as *k*

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

$$
\sum_{k} \pi_k = 1 \implies \sum_{k} \frac{N_{Y=k}}{\lambda} = 1 \implies \lambda = \sum_{k} N_{Y=k} = N
$$

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

Naïve Bayesian Classifier *Y* $\left[X_n \right]$ (X_1) (X_2) ■ 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:
 $\ell^*(\{\pi_{ijk}\}|D) = \sum_m \sum_i \sum_j \sum_k [X_i^{(m)} = j][Y^{(m)} = k] \log \pi_{ijk} + \sum_i \sum_k \lambda_{ik} (1 - \sum_j \pi_{ijk})$ Optimizing second term: $\frac{\partial \ell^*}{\partial \pi_{ijk}} = \frac{\sum_{m} [X_i^{(m)} = j][Y^{(m)} = k]}{\pi_{ijk}} - \lambda_{ik}$ $\frac{\partial \ell^*}{\partial \pi_{ijk}} = 0 \Rightarrow \pi_{ijk} = \frac{N_{X_i=j, Y=k}}{\lambda_{ik}}$ $\sum_j \pi_{ijk} = 1 \quad \Rightarrow \quad \sum_j \frac{N_{X_i=j,\;Y=k}}{\lambda_{ik}} \;=\; 1 \quad \Rightarrow \quad \lambda \;=\; \sum_j N_{X_i=j,\;Y=k} \;=\; N_{Y=k}$ $\pi_{ijk}^* = \frac{N_{X_i=j, Y=k}}{N_{Y-k}}$ (Maximum Likelihood Estimator of π_{ijk})

Artificial Intelligence 2023-2024 2008 Supervised Learning [15]

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

Learning CPTs for a graphical model via MLE

Model: random variables plus the graph of dependencies Observations: dataset of values, from completely observed outcomes Parameters (to be determined): all conditional probabilities (i.e. all CPTs)

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)

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

\n
$$
\theta = \{\pi_T, \pi_F, \pi_{S|F}, \pi_{A|S,F}, \pi_{L|A}, \pi_{R|L}\}
$$

\n
$$
\pi_T^* := \operatorname{argmax}_{\pi_T} P(D | \pi_T)
$$

\n
$$
\pi_F^* := \operatorname{argmax}_{\pi_F} P(D | \pi_F)
$$

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

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

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

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

 $D_{T,F}$ 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 :

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

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

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? $P(\theta)$

Beta distribution

Artificial Intelligence 2023-2024 2008 Supervised Learning [22]

Conjugate prior distributions

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

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

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)

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

A posteriori probability with Beta prior

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

 $\sqrt{ }$ "is proportional to" $P(D|\theta)P(\theta) \propto \text{Beta}(\theta; \alpha_D + \alpha_P, \beta_D + \beta_P)$

Optimization:

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

which is the same as MLE but with the addition of $\alpha_p + \beta_p$ pseudo-observations \int in the above sense Being a **conjugate prior** $P(\theta)$ of a distribution $P(D|\theta)$ in the above
means that the posterior $P(D|\theta)P(\theta)$ is in the same family of $P(\theta)$

Artificial Intelligence 2023-2024 2003-2004 Supervised Learning [24]

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)

$$
P(D|\theta) = {N \choose N_{X=1}} \prod_i P(D_i|\theta) = {N \choose N_{X=1}} \theta^{N_{X=1}} (1-\theta)^{N_{X=0}}
$$

A posteriori probability with Beta prior

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

Therefore

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

which is the same as MLE but with the addition of $\alpha_p + \beta_p$ pseudo-observations μ in the above sense Being a **conjugate prior** $P(\theta)$ of a distribution $P(D|\theta)$ in the above means that the posterior $P(D|\theta)P(\theta)$ is in the same family of $P(\theta)$

Artificial Intelligence 2023-2024 2003 - Supervised Learning [25]

Anti-spam filter

$$
P(Y, X_1, \dots, X_n) = P(Y) \prod_{i=1}^n P(X_i \mid X_{i-1})
$$
\n
$$
(X_1) (X_2) (X_3) (X_4)
$$

Y

■ Maximum a Posteriori (MAP) Estimation

The adapted computations for:

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

yield:

$$
\pi_k^* = \frac{\alpha_k + N_{Y=k} - 1}{\alpha_k + \beta_k + N - 2}
$$

$$
\pi_{ijk}^* = \frac{\alpha_{ijk} + N_{X_i=j, Y=k} - 1}{\alpha_{ijk} + \beta_{ijk} + N_{Y=k} - 2}
$$

(MAP Estimator of π_k *)*

(MAP Estimator of π_{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

Artificial Intelligence 2023-2024 2008 Supervised Learning [26]

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)

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