CS 2750 Machine Learning
Lecture 12b

Bayesian belief networks

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Density estimation

Data: $D = \{D_1, D_2, .., D_n\}$

$D_i = \mathbf{x}_i$ a vector of attribute values

Attributes:

- modeled by random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ with:
  - **Continuous values**
  - **Discrete values**

E.g. ***blood pressure*** with numerical values

or ***chest pain*** with discrete values

[no-pain, mild, moderate, strong]

Underlying true probability distribution:

$p(\mathbf{X})$

Density estimation

Data: $D = \{D_1, D_2, .., D_n\}$

$D_i = \mathbf{x}_i$ a vector of attribute values

Objective: try to estimate the underlying true probability distribution over variables $\mathbf{X}$, $p(\mathbf{X})$, using examples in D

true distribution $p(\mathbf{X})$ → n samples $D = \{D_1, D_2, .., D_n\}$ → estimate $\hat{p}(\mathbf{X})$

Standard (iid) assumptions: Samples

- **are independent of each other**
- **come from the same (identical) distribution (fixed $p(\mathbf{X})$)**

Learning via parameter estimation

In this lecture we consider **parametric density estimation**

Basic settings:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$
- **A model of the distribution** over variables in ***X*** with parameters Θ :

$$\hat{p}(\mathbf{X} \mid \Theta)$$

- **Data** $D = \{D_1, D_2, .., D_n\}$

Objective: find the parameters Θ that explain best the observed data

Parameter estimation

- **Maximum likelihood (ML)**

  maximize $p(D \mid \Theta, \xi)$

  – yields: one set of parameters Θ_{ML}

  – the target distribution is approximated as:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{ML})$$

- **Bayesian parameter estimation**

  – uses the posterior distribution over possible parameters

$$p(\Theta \mid D, \xi) = \frac{p(D \mid \Theta, \xi)\, p(\Theta \mid \xi)}{p(D \mid \xi)}$$

  – Yields: all possible settings of Θ (and their "weights")

  – The target distribution is approximated as:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid D) = \int_{\mathbf{\Theta}} p(X \mid \mathbf{\Theta})\, p(\mathbf{\Theta} \mid D, \xi)\, d\mathbf{\Theta}$$

Parameter estimation

Other possible criteria:

- **Maximum a posteriori probability (MAP)**

  maximize $p(\mathbf{\Theta} \mid D, \xi)$ (mode of the posterior)

  – Yields: one set of parameters $\mathbf{\Theta}_{MAP}$

  – Approximation:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{MAP})$$

- **Expected value of the parameter**

  $\hat{\mathbf{\Theta}} = E(\mathbf{\Theta})$ (mean of the posterior)

  – Expectation taken with regard to posterior $p(\mathbf{\Theta} \mid D, \xi)$

  – Yields: one set of parameters

  – Approximation:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \hat{\mathbf{\Theta}})$$

Density estimation

- **So far we have covered density estimation for "simple" distribution models:**
  - Bernoulli
  - Binomial
  - Multinomial
  - Gaussian
  - Poisson

But what if:

- The dimension of $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ is large
  - Example: patient data
- Compact parametric distributions do not seem to fit the data
  - E.g.: multivariate Gaussian may not fit
- We have only a "small" number of examples to do accurate parameter estimates

How to learn complex distributions

How to learn complex multivariate distributions $\hat{p}(\mathbf{X})$ with large number of variables?

One solution:

- **Decompose the distribution using conditional independence relations**
- **Decompose the parameter estimation problem to a set of smaller parameter estimation tasks**

Decomposition of distributions under conditional independence assumption is the main idea behind **Bayesian belief networks**

Example

Problem description:

- **Disease:** pneumonia
- **Patient symptoms (findings, lab tests)**:
  - Fever, Cough, Paleness, WBC (white blood cells) count, Chest pain, etc.

Representation of a patient case:

- Symptoms and disease are represented as random variables

Our objectives:

- **Describe a multivariate distribution representing the relations between symptoms and disease**
- **Design of inference and learning procedures for the multivariate model**

Modeling uncertainty with probabilities

- **Full joint distribution:**
  - Assume $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ are all random variables that define the domain
  - Full joint: $P(\mathbf{X})$ or $P(X_1, X_2, \ldots, X_d)$

Full joint it is sufficient to do any type of probabilistic inference:

- Computation of joint probabilities for sets of variables

$$P(X_1, X_2, X_3) \qquad P(X_1, X_{10})$$

- Computation of conditional probabilities

$$P(X_1 \mid X_2 = True, X_3 = False)$$

Marginalization

Joint probability distribution (for a set variables)

- Defines probabilities for all possible assignments to values of variables in the set

$\mathbf{P}(pneumonia, WBCcount)$ 2×3 table

WBCcount

Pneumonia		*high*	*normal*	*low*	$\mathbf{P}(Pneumonia)$
	True	0.0008	0.0001	0.0001	0.001
	False	0.0042	0.9929	0.0019	0.999
$\mathbf{P}(WBCcount)$		0.005	0.993	0.002	

Marginalization (summing of rows, or columns)
- summing out variables

Variable independence

- **The joint distribution over a subset of variables can be always computed from the joint distribution through marginalization**
- **Not the other way around !!!**
  - **Only exception: when variables are independent**

$$P(A, B) = P(A)P(B)$$

$\mathbf{P}(pneumonia, WBCcount)$

WBCcount

Pneumonia		high	normal	low	$\mathbf{P}(Pneumonia)$
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Conditional probability

Conditional probability :

- Probability of A given B

$$P(A \mid B) = \frac{P(A,B)}{P(B)}$$

- Conditional probability is defined in terms of joint probabilities
- Joint probabilities can be expressed in terms of conditional probabilities

$$P(A,B) = P(A \mid B)P(B) \quad \textbf{(product rule)}$$

$$P(X_1, X_2, \ldots X_n) = \prod_{i=1}^{n} P(X_i \mid X_{1,} \ldots X_{i-1}) \quad \textbf{(chain rule)}$$

- Conditional probability – is useful for **various probabilistic inferences**

$$P(Pneumonia = True \mid Fever = True, WBCcount = high, Cough = True)$$

Inference

Any query can be computed from the full joint distribution !!!

- **Joint over a subset of variables** is obtained through marginalization

$$P(A=a, C=c) = \sum_i \sum_j P(A=a, B=b_i, C=c, D=d_j)$$

- **Conditional probability over a set of variables**, given other variables' values is obtained through marginalization and definition of conditionals

$$P(D=d \mid A=a, C=c) = \frac{P(A=a, C=c, D=d)}{P(A=a, C=c)}$$

$$= \frac{\sum_i P(A=a, B=b_i, C=c, D=d)}{\sum_i \sum_j P(A=a, B=b_i, C=c, D=d_j)}$$

Inference

- Any joint probability can be expressed as a product of conditionals via the **chain rule**.

$$P(X_1, X_2, \ldots X_n) = P(X_n \mid X_{1,} \ldots X_{n-1}) P(X_{1,} \ldots X_{n-1})$$

$$= P(X_n \mid X_{1,} \ldots X_{n-1}) P(X_{n-1} \mid X_{1,} \ldots X_{n-2}) P(X_{1,} \ldots X_{n-2})$$

$$= \prod_{i=1}^{n} P(X_i \mid X_{1,} \ldots X_{i-1})$$

- It is often easier to define the distribution in terms of conditional probabilities:
  - E.g.

$$\mathbf{P}(Fever \mid Pneumonia = T)$$

$$\mathbf{P}(Fever \mid Pneumonia = F)$$

Modeling uncertainty with probabilities

- **Full joint distribution:** joint distribution over all random variables defining the domain
  - it is sufficient to represent the complete domain and to do any type of probabilistic inferences

Problems:

- **Space complexity.** To store full joint distribution requires to remember $O(d^n)$ numbers.

  n – number of random variables, d – number of values
- **Inference complexity.** To compute some queries requires $O(d^n)$ steps.
- **Acquisition problem.** Who is going to define all of the probability entries?

Pneumonia example. Complexities.

- **Space complexity**.
  - Pneumonia (2 values: T,F), Fever (2: T,F), Cough (2: T,F), WBCcount (3: high, normal, low), paleness (2: T,F)
  - Number of assignments: 2*2*2*3*2=48
  - We need to define at least 47 probabilities.
- **Time complexity**.
  - Assume we need to compute the probability of Pneumonia=T from the full joint

$$P(Pneumonia = T) =$$

$$= \sum_{i \in T,F} \sum_{j \in T,F} \sum_{k=h,n,l} \sum_{u \in T,F} P(Fever = i, Cough = j, WBCcount = k, Pale = u)$$

  - Sum over 2*2*3*2=24 combinations

Bayesian belief networks (BBNs)

Bayesian belief networks.

- Represent the full joint distribution over the variables more compactly with a **smaller number of parameters**.
- Take advantage of **conditional and marginal independences** among random variables

- **A and B are independent**

$$P(A,B) = P(A)P(B)$$

- **A and B are conditionally independent given C**

$$P(A,B \mid C) = P(A \mid C)P(B \mid C)$$

$$P(A \mid C,B) = P(A \mid C)$$