Capturing Dependency of Data using Graphical Models

Song Liu
(song.liu@bristol.ac.uk)

Objectives

- Understand **equivalence** of **conditional independence of R.Vs** and **factorizations** of their probability distribution over a graph.

- Simple **undirected graphical models**:
  - Gaussian Markov Network
  - Logistic Model

Dependency in Dataset:
A Unit Score Example

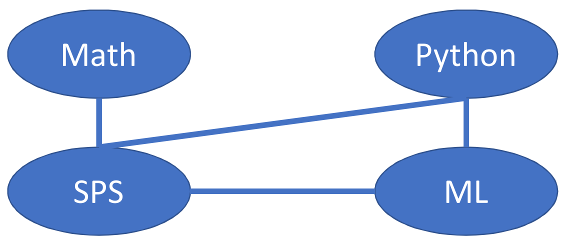
Example: Scores of Units

- Imagine a table of unit scores.

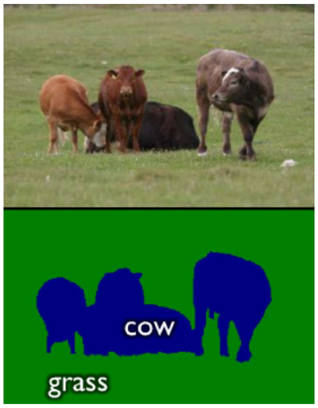
Name	SPS	Math	Python	Mach. Learn.
Song	80	70	50	60
Harry	50	40	70	80
Ron	50	50	…	45
Hermione	90	100	…	100
…	…	…	…	…

Dependency of Datasets and Its Graphical Representation

- Scores of units are **dependent**!
  - Student with **high** Math, Python score is likely to receive **high** SPS score.
  - Vice versa.
- A graphical representation:



Example: Image Segmentation



- The probability of one pixel being labelled as "Cow" is correlated with **adjacent pixels**.
  - A pixel is more likely to be a Cow pixel if surrounding pixels are all Cow pixels

Jamie Shotton et. al. IJCV 2009

Independence and Conditional Independence of R.Vs

Problem Formulation

- Given a dataset $\{\boldsymbol{x}_i\}_{i=1}^{n}$,
  - $\boldsymbol{x}_i = \left[x_i^{(1)}, x_i^{(2)} \ldots x_i^{(d)}\right] \in R^d$
  - $\boldsymbol{x}_i$ is a vector of a student i's scores.
  - e.g., $x^{(1)}$ is SPS, $x^{(2)}$ is Math…

- **What does $p\left(x^{(1)}, x^{(2)} \ldots\ x^{(d)}\right)$ look like?**

Note, here we do not distinguish the lower case x, an assignment of a random variable, and upper case X, a random variable.

Independence of R.V.s

- Let's look at how independence between R.V.s are **expressed in probability:**
- R.V. X is **independent** of Y:
  - $X \perp Y$
  - $\Leftrightarrow p(X, Y) = p(X)p(Y)$
    - Factorization
  - $\Leftrightarrow p(X|Y) = p(X) \Leftrightarrow p(Y|X) = p(Y)$
    - No Information flows between X and Y.

Notice the independence can be expressed via factorization and information flow.

Example: Likelihood with Independent Datapoints:

- Likelihood over the dataset
  - Factorizes into product over each x_i
  - $p(x_1, x_2, \dots x_n; \theta) = \prod_{i=1}^{n} p(x_i; \theta)$
  - We can do so as $x_1 \dots x_n$ are independent.
- Maximum Likelihood Estimation
  - $\max_{\theta} \prod_{i=1}^{n} p(x_i; \theta)$
  - **Lab sheet 4.1**

We can do the factorization of the likelihood function because of the independence of X!!!

Conditional Independence of R.V.s

- R.V. X is independent of Y **given** Z
  - $X \perp Y|Z$
  - $\Leftrightarrow p(X,Y|Z) = p(X|Z)p(Y|Z)$
  - $\Leftrightarrow p(X,Y,Z) \propto g_1(X,Z) \cdot g_2(Y,Z)$
    - Factorization
  - $\Leftrightarrow p(X|Y,Z) = p(X|Z)$
    - Information flow**:** Y does not give any additional info which changes the prob. of X given Z.
  - $\Leftrightarrow p(Y|X,Z) = p(Y|Z)$

Z is called conditioning random variable.
What are g_1 and g_2? They are just two functions, does not have to be probability, does not have to be in any specific form. **Their existence guarantees** the conditional independence.

g function is called factor

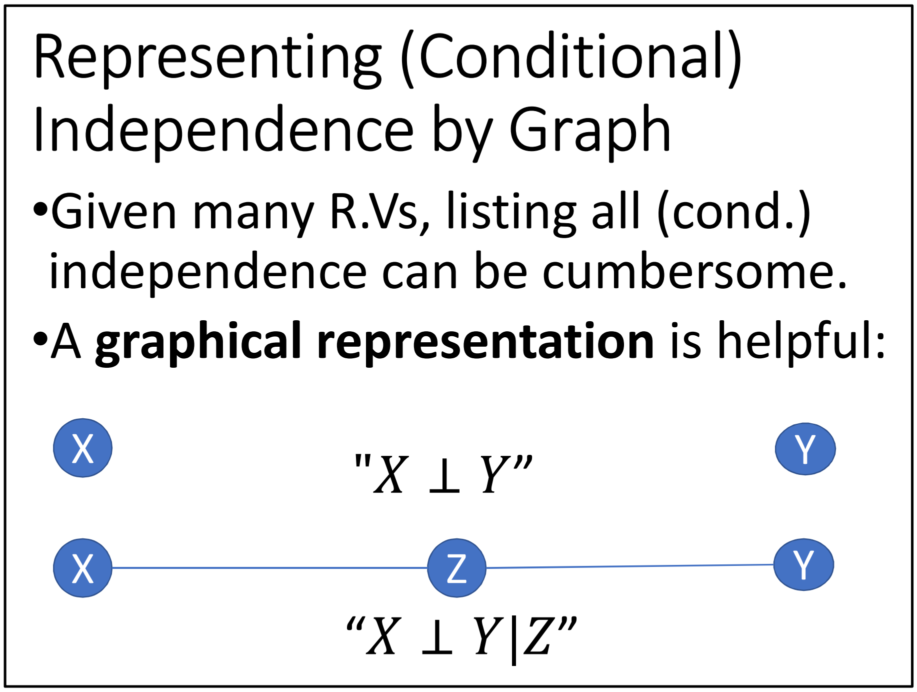
(Conditional) Independence and Information Flow

- (Conditional) Independence tells how information **flows** between R.V.s
  - $X \perp Y \Leftrightarrow$ no information flows in-between X and Y.
  - $X \perp Y|Z \Leftrightarrow$ information **flows between** X and Y **via** Z.

The analogy is like relationship between people.

X and Y are independent: they do not talk to each other.

X and Y are conditional indepdent, they talk to each other via a middle man.



Because in many machine learning tasks, (conditional) independence are **valuable prior knowledge**, you may want to specify (conditional) independence of R.Vs in your dataset.

Imagining listing all the (conditional) independence in a very long document…

Representing Conditional Independence by Graph

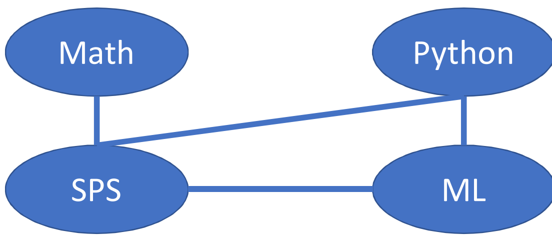
- Given a graph $G =< E, V >$, and three random variables $X, Y, Z \subseteq V$
  - if X and Y are completely "**blocked**" by Z, we say $X \perp Y | Z$ is represented by G.

Blocked, means there is no path linking X and Y

Example: Encoding (cond.) indep. by graph

Math ⊥ ML | SPS
Math ⊥ Python | SPS
Math ⊥ ML | SPS, Python
Math ⊥ Python, ML | SPS
Math ⊥ Python | SPS, ML

List of conditional independence encoded by Graph!



Graph is a powerful tool to encode/visualize (conditional) indepedence.

Representing Prob. Distribution Factorization by Graph

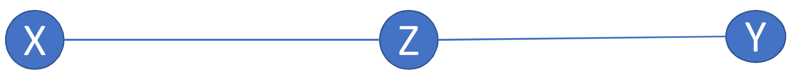
- Factorizing a probability dist. greatly reduces complexity of modelling and computation of a probability dist.
  - Think about that Maximum Likelihood example you did in Lab!

The motivation of factorizing a probability dist.

Representing Prob. Distribution Factorization by Graph

- Writing the factorization of a probability distribution of many factors can be cumbersome.
- Can we also use graph to help??

$$"P(X,Y) = P(X)P(Y)"$$



$$“P(X,Y,Z) \propto g_1(X,Z)g_2(Y,Z)”$$

Representing Prob. Distribution Factorization by Graph

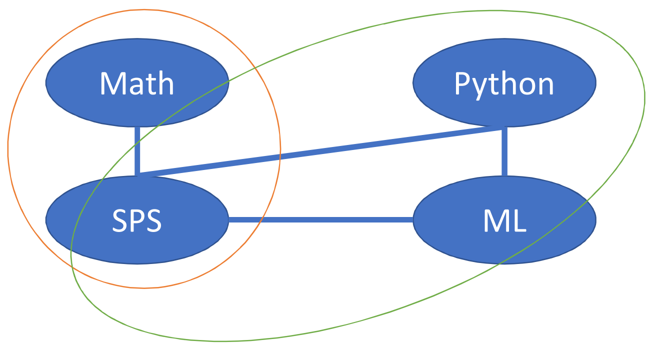
- Given a graph $G = < E, V >$,
- We say $p(X)$ factorizes over G:
- If $p(X) \propto \prod_{c \in C} g_c\left(X^{(c)}\right)$
  - where C is set of all **cliques** in G.
  - Clique: fully connected subgraph.
  - g_c is a function defined on $X^{(c)}$, which is the subset of X **restricted on** c.

Like what we saw before, g_c is a function that can be in any form.

g is called “factor”

Example

$$p(Ma, SPS, Py, ML)$$
$$\propto g_1(Ma, SPS) \cdot g_2(Py, ML, SPS).$$



Equivalency between Factorization and Conditional Independence over G

- Using graph represent a factorization of a probability distribution
- Using graph represent a list of conditional independence
- Remarkably, these two seemingly irrelevant notions are **equivalent!**

Equivalency between Factorization and Conditional Independence over G

- If p factorizes over G, p satisfies all conditional independence represented by G.

- If p satisfies all conditional independence represented by G, then p factorizes over G.

What does that mean

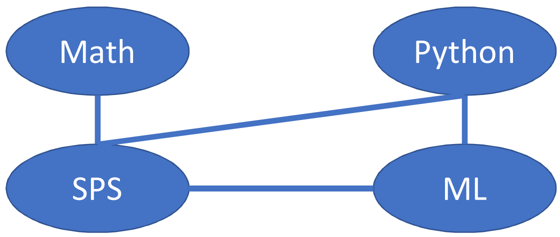
Equivalency between Factorization and Conditional Independence over G

- Verify this on Scores of Units example!

  - Live demonstration.

Example

$$p(Ma, SPS, Py, ML)$$
$$\propto g_1(Ma, SPS) \cdot g_2(Py, ML, SPS).$$



Hint: $X \perp Y | Z \Leftrightarrow p(X, Y, Z) \propto g_1(X, Z) \cdot g_2(Y, Z)$
$X \perp Y, W | Z \Rightarrow X \perp Y | Z$

Example

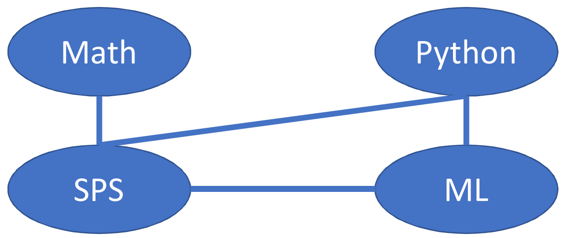
Math ⊥ ML | SPS

Math ⊥ Python | SPS

Math ⊥ ML | SPS, Python

Math ⊥ Python, ML | SPS

Math ⊥ Python | SPS, ML



Hint: $X \perp Y | Z \Leftrightarrow p(X, Y, Z) \propto g_1(X, Z) \cdot g_2(Y, Z)$

Markov Network

- A probability distribution $p(X)$ which uses undirected graph representing its conditional independence, is called an **undirected graphical model**, or a **Markov network**.

The definition of Markov network.

Gaussian Markov Network

- Multivariate Gaussian distribution:
- $\boldsymbol{x} \in R^d, \boldsymbol{x} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$
- $p(\boldsymbol{x}) \propto \exp\left[-\frac{\boldsymbol{x}(\boldsymbol{\Sigma})^{-1}\boldsymbol{x}^\top}{2}\right]$ $\boxed{\text{Let } \boldsymbol{\Theta} = (\boldsymbol{\Sigma})^{-\mathbf{1}}}$.

$$\propto \exp\left[-\frac{\sum_{u,v} \Theta^{(u,v)} x^{(u)}\, x^{(v)}}{2}\right]$$

$$\propto \prod_{u,v;\Theta^{(u,v)} \neq 0} \exp\left(-\Theta^{(u,v)} x^{(u)}\, x^{(v)}\right)$$

aBa^T = \sum_ij B_ij ai aj

You can factorize the joint Gaussian using the pairwise factors

Gaussian Markov Network

- $p(\boldsymbol{x}) \propto \prod_{u,v;\Theta^{(u,v)}\neq 0} g_{u,v}\left(x^{(u)}, x^{(v)}\right)$
- $p(\boldsymbol{x})$ **factorizes over** G**!**
  - G defined by the adjacency matrix

    $$A^{(u,v)} = \begin{cases} 0, \Theta^{(u,v)} == 0 \\ 1, \Theta^{(u,v)} \neq 0 \end{cases}$$
  - G must be an undirected graph (why?)
  - $\Leftrightarrow$ satisfies the conditional independence encoded in G.

This pairwise factorization implies the distribution factorizes over a G whose edges are defined by the structure of Theta

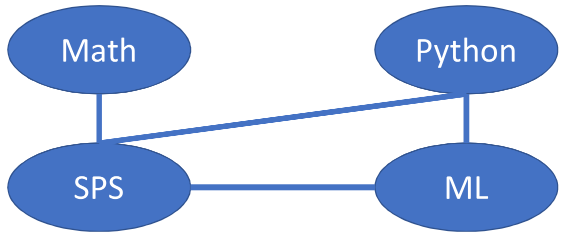
Gaussian Markov Network

- Knowing a graph G that encodes all conditional independence of your dataset, I can use its adjacency matrix G to construct $\mathbf{\Theta}$!
  - Use sparsity of the adjacency matrix
    - NOT its actual values!
  - $\mathbf{\Theta}$ must be positive definite!!

Theta must be positive definite!!

We are using graph to construct our probabilistic model, hence the name, graphical model!!

Example



- $x^{(1)}$:Math; $x^{(2)}$:Py; $x^{(3)}$:SPS; $x^{(4)}$:ML
- $\boldsymbol{\Theta} = \begin{bmatrix} \Theta_{11} & 0 & \Theta_{13} & 0 \\ 0 & \Theta_{22} & \Theta_{23} & \Theta_{24} \\ \Theta_{13} & \Theta_{23} & \Theta_{33} & \Theta_{34} \\ 0 & \Theta_{24} & \Theta_{34} & \Theta_{44} \end{bmatrix}$

Theta must be positive definite!!

Quiz

- Suppose graph G encodes all cond. indep. in your probability dist. G contains **three edges, five nodes.** How many **non-zero elements** are there in $\mathbf{\Theta}$, the parameter to your Gaussian Markov Net?
- A.3
- B.8
- C.6
- D.10
- E.11

https://bit.ly/2uIFZUu

Constructing Likelihood

- **PC:** If $(x_0, \boldsymbol{x})$ are drawn from a joint Gaussian $p(x_0, \boldsymbol{x})$, show log likelihood $\log p(x_0|\boldsymbol{x})$ has the form:
  - $-(x_0 - \sum_i \beta_i x_i)^2/b$, where $\beta_i \neq 0$ iff (X_0, X_i) is an edge in the Markov network structure of p.
  - How does it help us select good features in least squares fitting?

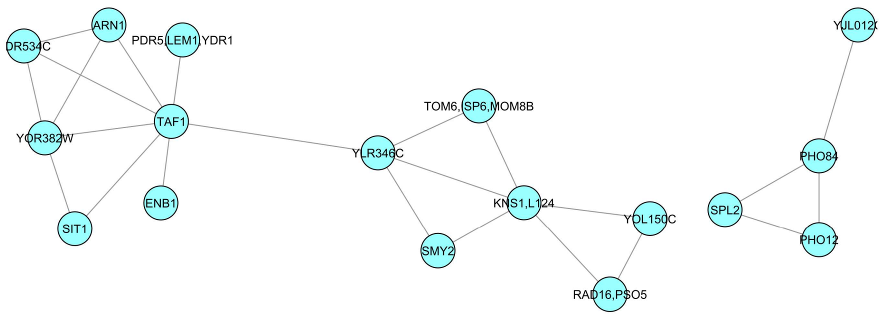
Gaussian Markov Network

- **Not knowing** G encodes all cond. independence of $p(\boldsymbol{x})$. Given dataset D, we can fit a sparse $\widehat{\boldsymbol{\Theta}}$.
  - Using MLE: $\widehat{\boldsymbol{\Theta}} = \underset{\boldsymbol{\Theta}}{\operatorname{argmax}} \log p(D; \boldsymbol{\Theta})$
  - The sparsity of $\widehat{\boldsymbol{\Theta}}$ gives a graphical representation of $p(\boldsymbol{x})$!
  - Such representation reveals how random variables “interacts” with each other!

Example: Gene Expression Data

Time stamp	Gene1	Gene2	Gene3	Gene4
t1	.1	.2	.5	.2
t2	.5	.4	.7	.8
t3	.5	.5	…	.45
t4	.9	.2	…	.01
…	…	…	…	…

Gene Network (Banerjee et al., 2008)



Exponential Family Distribution

- Gaussian Markov network belongs to a wider **family** of distributions, which are defined using a generic form:
- $p(\boldsymbol{x}; \boldsymbol{\theta}) \coloneqq \frac{\exp(\langle \boldsymbol{\theta}, \boldsymbol{f}(\boldsymbol{x}) \rangle)}{Z(\boldsymbol{\theta})}$
  - $\boldsymbol{f}(\boldsymbol{x})$ is a feature transform on $\boldsymbol{x}$.
  - $Z(\boldsymbol{\theta}) \coloneqq \int \exp(\langle \boldsymbol{\theta}, \boldsymbol{f}(\boldsymbol{x}) \rangle) d\boldsymbol{x}$
- PC: show when $\boldsymbol{f}$ is 2nd degree poly. transform with pairwise terms, $p(\boldsymbol{x}; \boldsymbol{\theta})$ is a multivariate Gaussian distribution.

Conditional Markov Network

- In many tasks, the conditional distribution is the key interest.
  - $p(Y|X)$ measures the randomness on Y given X and help us make a prediction.
  - Both regression and classification requires a **conditional** model.
- How to factorize a conditional distribution over G?

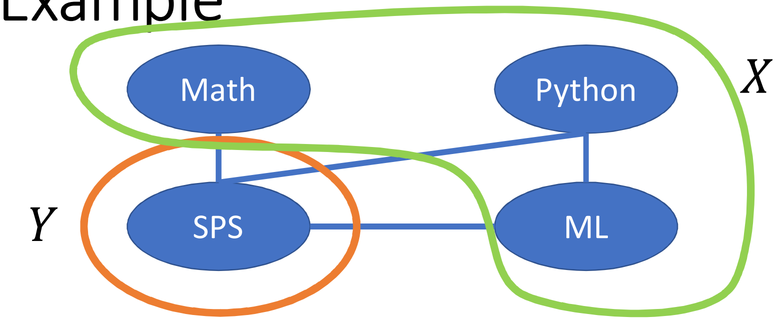
Conditional Markov Network

- We say a conditional probability distribution $P(Y|X)$ factorizes over G whose nodes $V = X \cup Y$, if
- $p(Y|X) = \frac{1}{N(X)} \prod_{c \in C} g_c(Z)\,, Z \subseteq X \cup Y$
- $N(X) \coloneqq \int \prod_{c \in C} g_c(Z)\, dY$
- Normalizing constant:
  - It normalizes the distribution to 1 over the domain of the random variable (Y).

Conditional Markov Network

- PC: show $Z \nsubseteq X$
  - $p(Y|X)$ does not include factors on conditioning variable X!

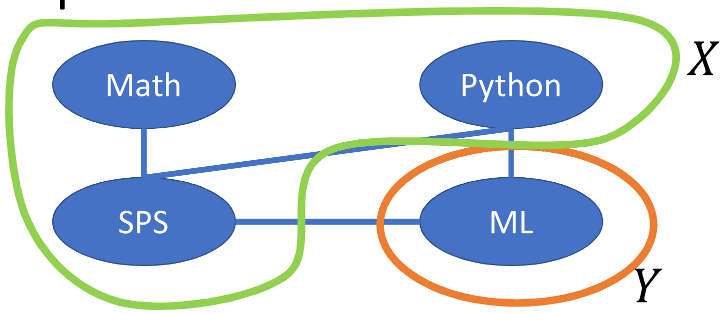
Example



- $p(SPS|Ma, Py, ML)$
  $= \dfrac{1}{Z(Ma, Py, ML)} g_1(SPS, Py, ML) g_2(SPS, Ma)$

- $Z(Ma, Py, ML) = \int g_1(SPS, Py, ML) g_2(SPS, Ma) \color{red}{dSPS}$

Example



- $p(ML|Ma, Py, SPS)$

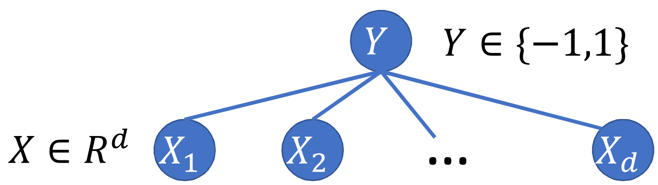
$$= \frac{1}{Z(Ma, Py, SPS)} g_1(SPS, Py, ML)$$

- $Z(Ma, Py, SPS) = \int g_1(SPS, Py, ML) dML$
- g_2 is gone!

Logistic Regression

- The way of constructing a conditional P.D. gives us a simple classification tool: Logistic Regression.

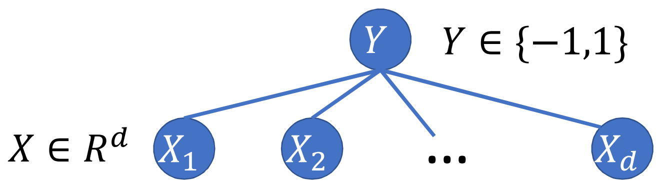
- Consider a simple Markov Net



Y is the variable for class labels, that can be either positive +1 or negative -1 as we saw before.

Logistic Model

- Using the factorization rule above,
  - $p(Y|X) = \frac{1}{N(X)} \prod_i g_i(Y, X^{(i)})$
  - $N(X) = \sum_{c \in \{-1,1\}} \prod_i g_i(Y, X^{(i)})$



Logistic Model

- Let us construct a model of $p(Y|X)$!
- By setting
  $g_i\left(Y = y, X_i = x^{(i)}; \beta_i\right) \coloneqq \exp\left(\beta_i \cdot yx^{(i)}\right)$

- $p(y|\boldsymbol{x}; \beta) = \frac{1}{N(X)} \exp\left(\sum_i \beta^{(i)} \cdot yx^{(i)}\right)$
  $= \frac{1}{N(X)} \exp(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle y).$

- $N(X; \beta) = \sum_{y \in \{1,-1\}} \exp(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle y)$

This is another example, of **graphical modelling**. We have a graph, which encodes the conditional independence. We then create a probabilistic model based on that graph.

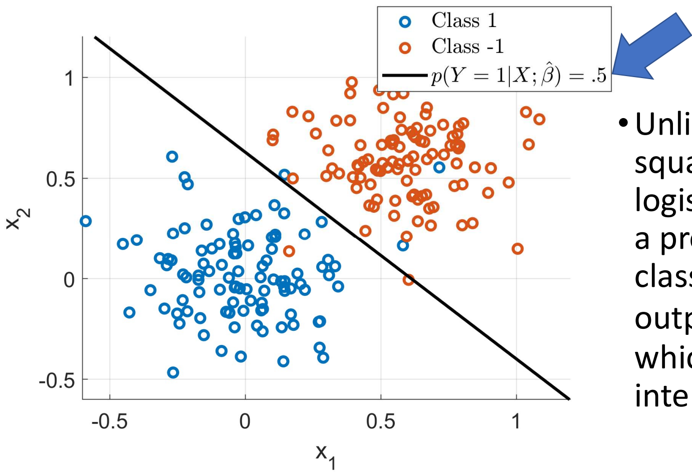
We replaced the integral by sum in the normalizing term, which is required by a discrete variable Y

Logistic Regression

- Logistic model:
- $p(y|\boldsymbol{x};\boldsymbol{\beta}) = \frac{1}{N(X)}\exp(\langle\boldsymbol{\beta},\boldsymbol{x}\rangle y)$
- $N(x) = \exp(\langle\boldsymbol{\beta},\boldsymbol{x}\rangle) + \exp(-\langle\boldsymbol{\beta},\boldsymbol{x}\rangle)$

- $\boldsymbol{\beta}$ can be fitted using MLE.
  - $\widehat{\boldsymbol{\beta}} = \arg\max_{\boldsymbol{\beta}} \sum_{i=1}^{n} \log p(y_i|\boldsymbol{x}_i;\boldsymbol{\beta})$
  - The process of fitting $\boldsymbol{\beta}$ using MLE is called Logistic Regression.
    - sklearn.linear_model.LogisticRegression

Example



- Unlike least squares classifier, logistic classifier is a probabilistic classifier, which outputs $p\left(Y\middle|X;\hat{\beta}\right)$, which is more interpretable!

Conclusion

- Markov network uses a graph to represent its conditional independencies.
  - It visualizes interactions of R.V.s in a P.D.

- Two examples of Markov network
  - Gaussian Markov network factorizes over the graph defined by its **inverse covariance**.
  - Logistic model is a conditional P.D. model factorizes over a classification network.

Quiz

- Which of the following is positive definite?