Supervised vs. Unsupervised Learning

CSE 5334 Data Mining, Spring 2020

Won Hwa Kim

Part of the contents borrowed from Prof. Mark Craven / Prof. David Page Jr. at UW-Madison

Unsupervised Learning

Representation of Objects in Machine Learning

- Given $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$ find patterns in the data

- An instance x (a specific object) represented by k dimensional features

- Each x_i is a coordinate in the feature space (Feature Representation)

Examples…

- Text document: frequency of words (i.e., bag of words)

- Images: color histogram

- Medical information: medical test results

Unsupervised Learning

Training

- Given $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$ find patterns in the data

- Training data is a set of instances for learning (training) phase

- Usually assumed that the data are sampled from an unknown distribution

- Independent and Identically Distributed (i.i.d)

- Learning from the past (experience)

Testing

- Inference, estimation, classification

- Predict future based on the past

Unsupervised Learning

Unsupervised…

- We have data only and no labels.
- What can we learn / infer from the data?
- We can learn what the data looks like, e.g., shape and distribution.

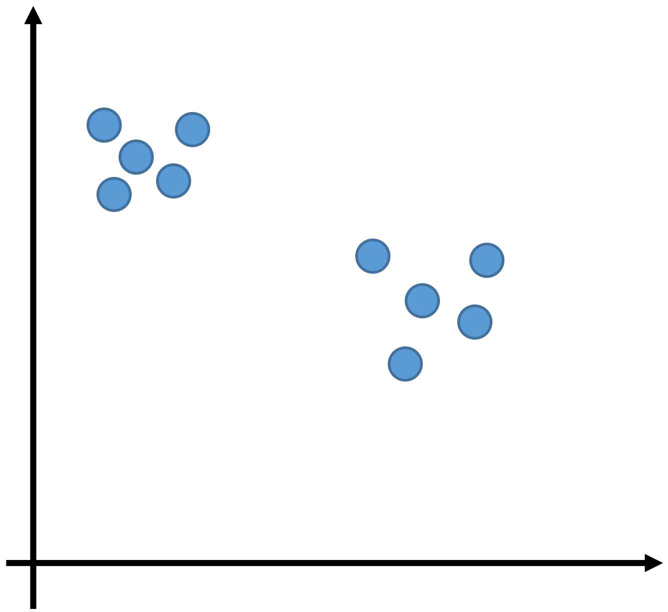
Let’s try to…

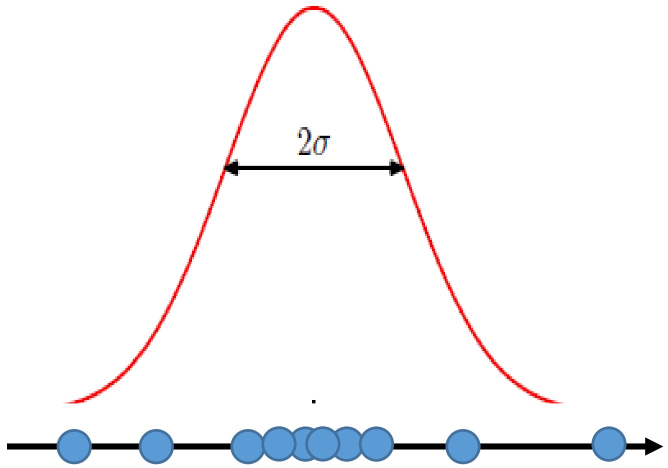
- Model the probability distribution given finite set of observations
- Density estimation, clustering
- Dimension reduction, anomaly detection

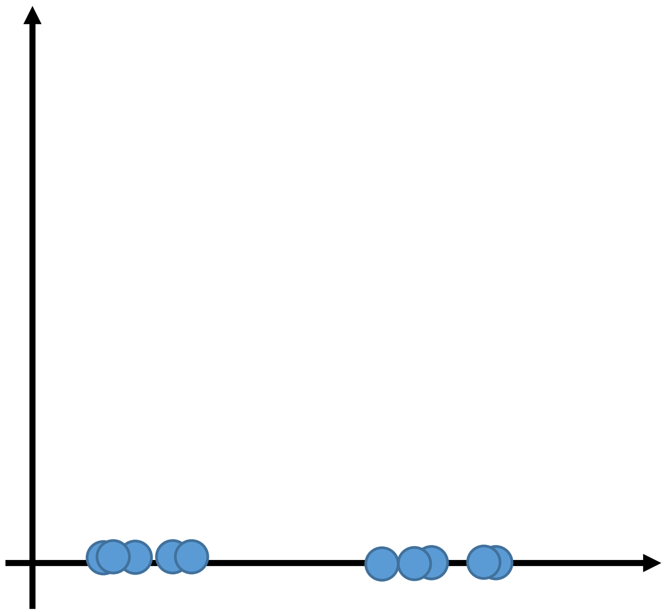
Unsupervised Learning

Unsupervised…

- Given $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$ find patterns in the data





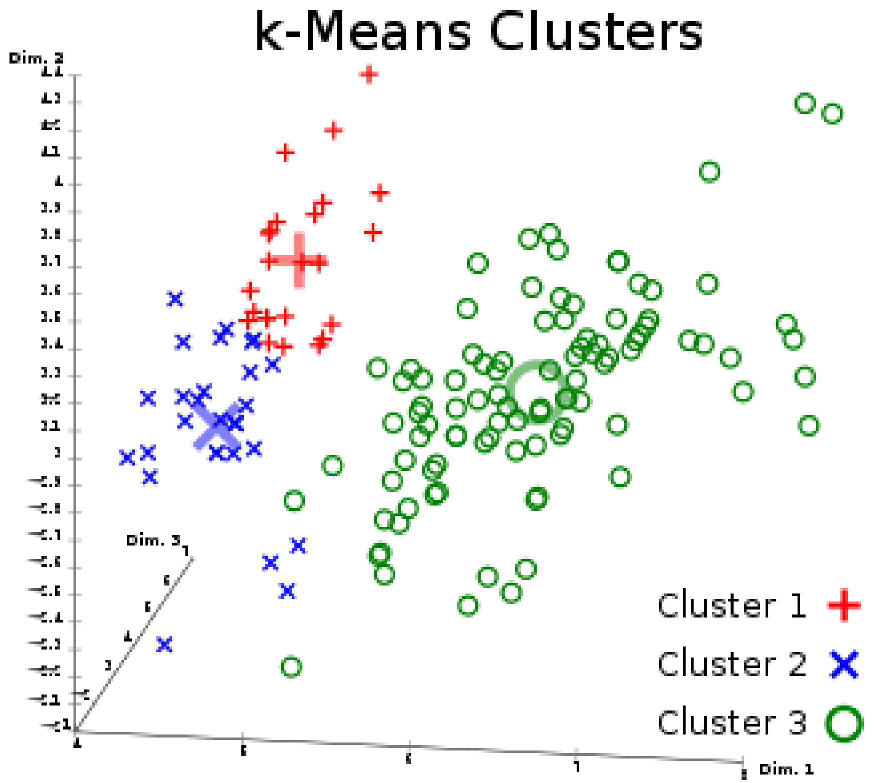


Clustering

K-means

Given: i.i.d. $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^d$ and a parameter k

- Partition N observations into k clusters in which each observation belongs to the cluster with the nearest mean
- NP-hard problem but heuristics exist
- This is not k-nearest neighbor classification



Clustering

K-means

Given: i.i.d. $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^d$ and a parameter k

Step 1: Select k cluster centers, c_1, $c_{2,}$ … c_k

Step 2: Assignment step: for each point in x, determine its cluster based on the distance to the centers

Step 3: Update step: update all cluster centers as the centers of their clusters

$$c_i^{t+1} = \frac{1}{|S_i^t|} \sum_{x_j \in S_i^t} x_j$$

Step 4: Repeat 2 and 3 until converges

Clustering

K-means

- Will it converge?

Yes

- Will it find the global optimal?

Not guaranteed

- How to choose initial centers?

make sure that they are far apart…

- What k shall we use?

domain knowledge / k that minimizes the error

Maximum Likelihood Estimation

Likelihood function

- a function of parameters of a statistical model given data

Given: *independent and identically distributed* (i.i.d.) $\mathbf{x} = (x_1, x_2, \cdots x_N),\ x_i \in \mathbb{R}^k$

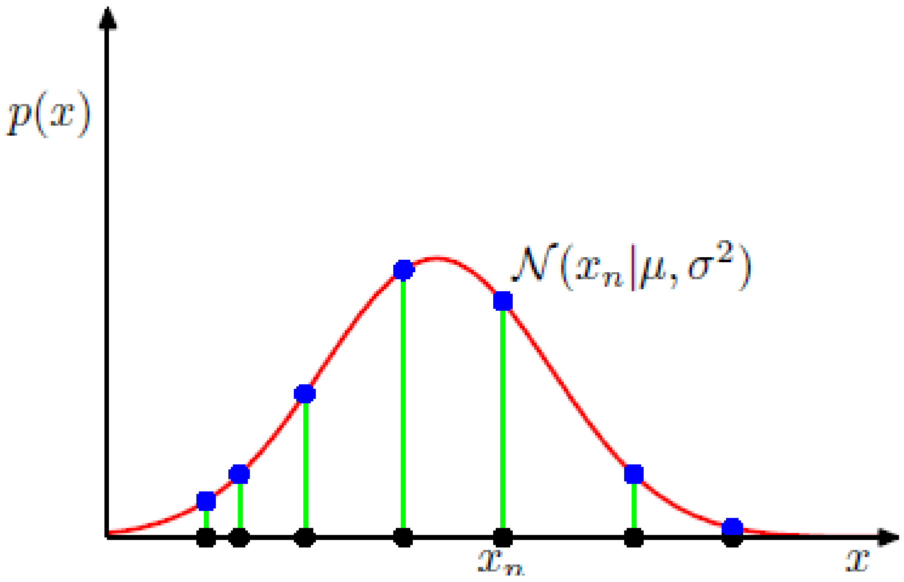
$$L(\theta|\mathbf{x}) = f(x|\theta)$$

$$\hat{\theta}(\mathbf{x}) = \text{argmax}_\theta L(\theta|\mathbf{x})$$

Probability distribution of a dataset

$$N(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} exp(-\frac{1}{2\sigma^2}(x-\mu)^2)$$

$$L(\mu,\sigma) = p(\mathbf{x}|\mu,\sigma^2) = \prod_{i=1}^{N} N(x_i|\mu,\sigma^2)$$



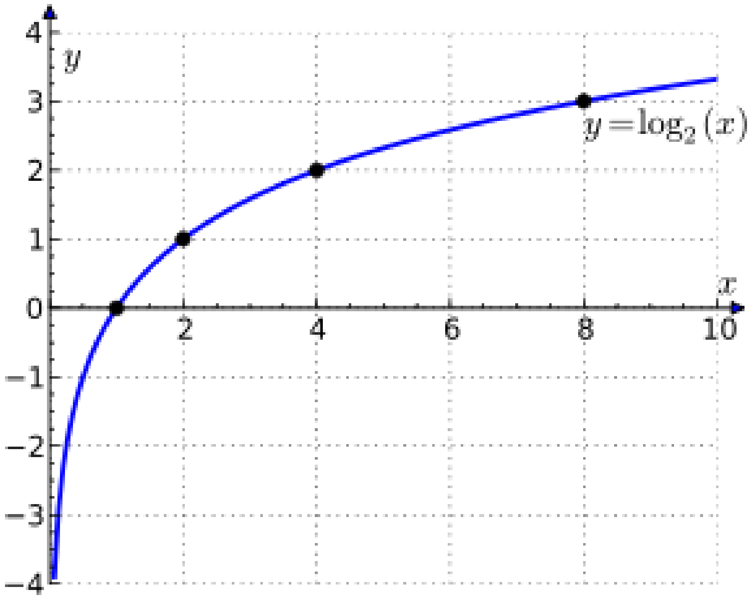
Maximum Likelihood Estimation

Log-likelihood of a Gaussian distribution

Given: *independent and identically distributed* (i.i.d.) $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$

$$L(\mu, \sigma) = p(\mathbf{x}|\mu, \sigma^2) = \prod_{i=1}^{N} N(x_i|\mu, \sigma^2)$$

$$\begin{aligned} \ln p(\mathbf{x}|\mu, \sigma^2) &= \ln \prod_{i=1}^{N} N(x_i|\mu, \sigma^2) \\ &= \sum_{i=1}^{N} \ln N(x_i|\mu, \sigma^2) \\ &= -\frac{1}{2\sigma^2} \sum_{i=1}^{N} (x_i - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi) \end{aligned}$$



Maximum Likelihood Estimation

Maximum (Log) Likelihood Estimation

$$\ell(\mu, \sigma) = \ln p(\mathbf{x}|\mu, \sigma^2) = -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i - \mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

$$\mu_{MLE}, \sigma_{MLE} = \mathrm{argmax}_{\mu,\sigma} \ln p(\mathbf{x}|\mu, \sigma^2)$$

$$\mu_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\sigma^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_{MLE})^2$$

Maximum Likelihood Estimation

Binary Variable (Bernoulli trials)

- Single binary random variable $x \in \{0, 1\}$
- E.g., flipping a coin
- The probability of $x = 1$ denoted by paramter μ

$$p(x = 1|\mu) = \mu, \qquad 0 \leq \mu \leq 1$$
$$p(x = 0|\mu) = 1 - \mu$$

- The probability distribution over x (Bernoulli distribution) written as

$$Bern(x|\mu) = \mu^x (1 - \mu)^{1-x}$$
$$\mathbb{E}[x] = \mu, var[x] = \mu(1 - \mu)$$

Maximum Likelihood Estimation

Binary Variable (Bernoulli trials)

- Single binary random variable $x \in \{0, 1\}$
- E.g., flipping a coin
- The probability of $x = 1$ denoted by paramter p

$$
\begin{aligned}
L(p|x) &= p^{x_1}(1-p)^{1-x_1} \cdots p^{x_N}(1-p)^{1-x_N} \\
&= p^{x_1}p^{x_2} \cdots p^{x_N}(1-p)^{1-x_1}(1-p)^{1-x_2} \cdots (1-p)^{1-x_N} \\
&= p^{(x_1+x_2 \cdots x_N)}(1-p)^{(N-x_1-x_2 \cdots -x_N)}
\end{aligned}
$$

Likelihood function: a function of the **parameters** of a statistical model given **data**.

Maximum Likelihood Estimation

Binary Variable (Bernoulli trials)

- Single binary random variable $x \in \{0, 1\}$
- E.g., flipping a coin
- The probability of $x = 1$ denoted by paramter p

$$\ell(p|x) = \ln L(p|x) = \ln p(\sum_{i=1}^{N} x_i) + \ln(1-p)(N - \sum_{i=1}^{N} x_i)$$

$$= N(\bar{x}\ln p + (1-\bar{x})\ln(1-p))$$

$$\frac{\partial}{\partial p}\ell(p|x) = N\frac{\bar{x}-p}{p(1-p)}$$

$$p^* = \bar{x}$$

Density Estimation

Histogram (non-parametric)

- Divide the domain into multiple bins

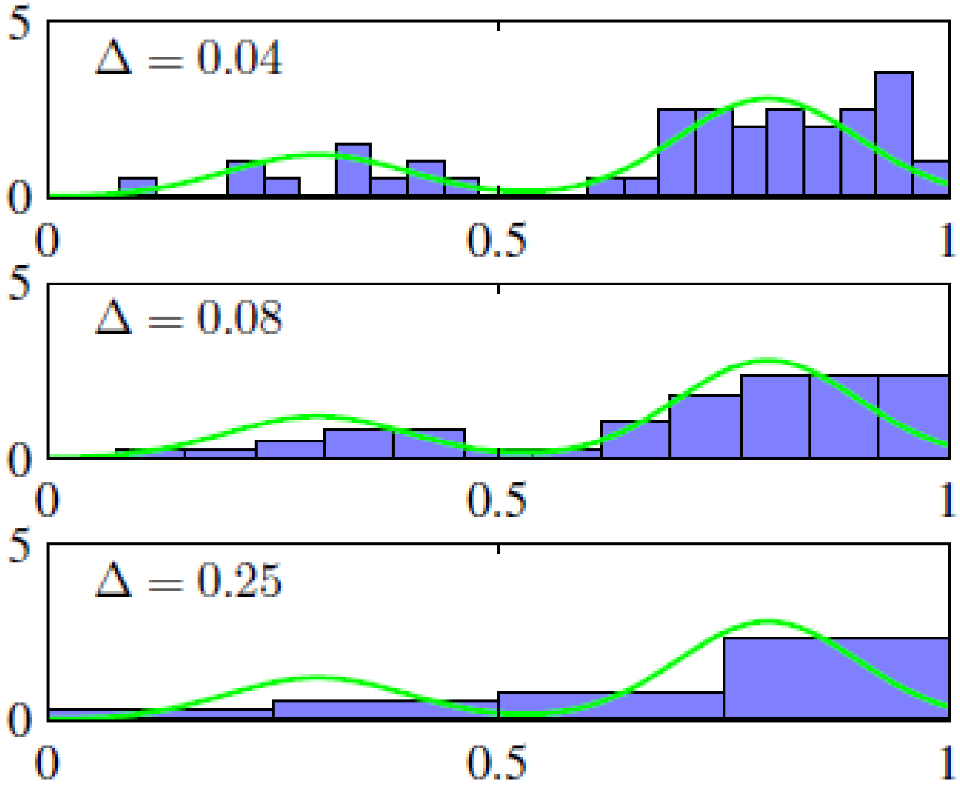
- Probability of a sample falling into each bin

# of observations

$$p_i = \frac{n_i}{N\Delta_i}$$

normalization

Bin width



Density Estimation

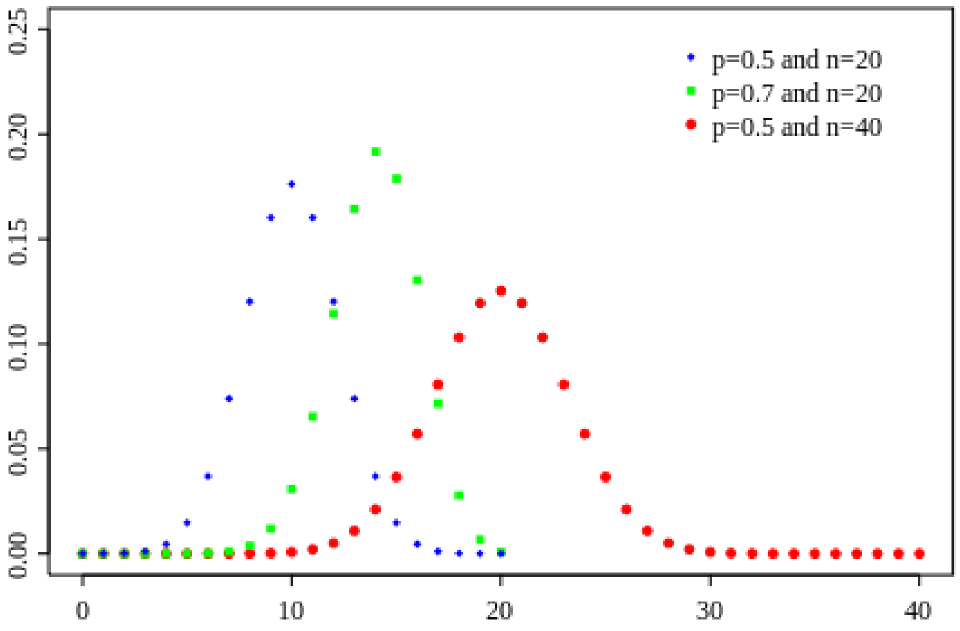
Binomial distribution

- discrete probability distribution of the number of successes in a sequence of n independent experiments

$$\mathrm{Bin}(K|N,P) = \frac{N!}{K!(N-K)!}P^K(1-P)^{N-K}$$

$$\mathbb{E}[K] = NP$$
$$var[K] = NP(1-P)$$

K number of success out of N trials, with p chance of success



Density Estimation

Prob. from histogram

$$p_i = \frac{n_i}{N\Delta_i}$$

Kernel Density Estimation (non-parametric)

- P: probability of falling with in R

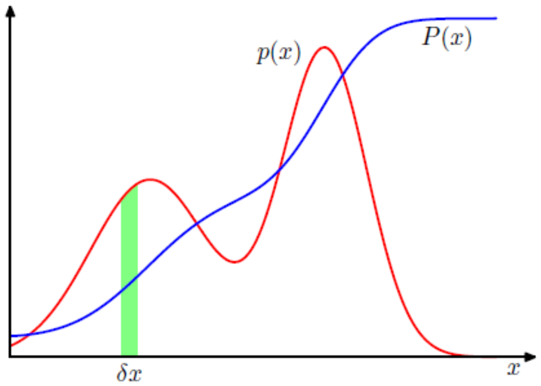
- Need to estimate p(x) given N data points in d-dimensional space

$$P = \int_R p(x)dx$$

K data points falling in R

$$\mathrm{Bin}(K|N,P) = \frac{N!}{K!(N-K)!}P^K(1-P)^{N-K}$$

$$\mathbb{E}[K/N] = P,\ var[K/N] = P(1-P)/N$$



$$K \simeq NP$$

For large N

$$P \simeq p(x)V$$

Sufficiently small R yielding constant prob in a unit volume V

Estimated Probability

$$\boxed{p(x) = \frac{K}{NV}}$$

Density Estimation

Kernel Density Estimation (non-parametric)

- P: probability of falling with in R
- Need to estimate p(x) given N data points

$$\boxed{p(x) = \frac{K}{NV}}$$

$$k(u) = \begin{cases} 1 & |u_i| \leq 1/2, \quad i = 1, \cdots, d \\ 0 & o.w. \end{cases}$$

Parzen window: a kernel function represented as a hypercube

$$K = \sum_{i=1}^{N} k(\frac{x - x_i}{h})$$

Total # of data points in the cube (**side = h**) centered at x

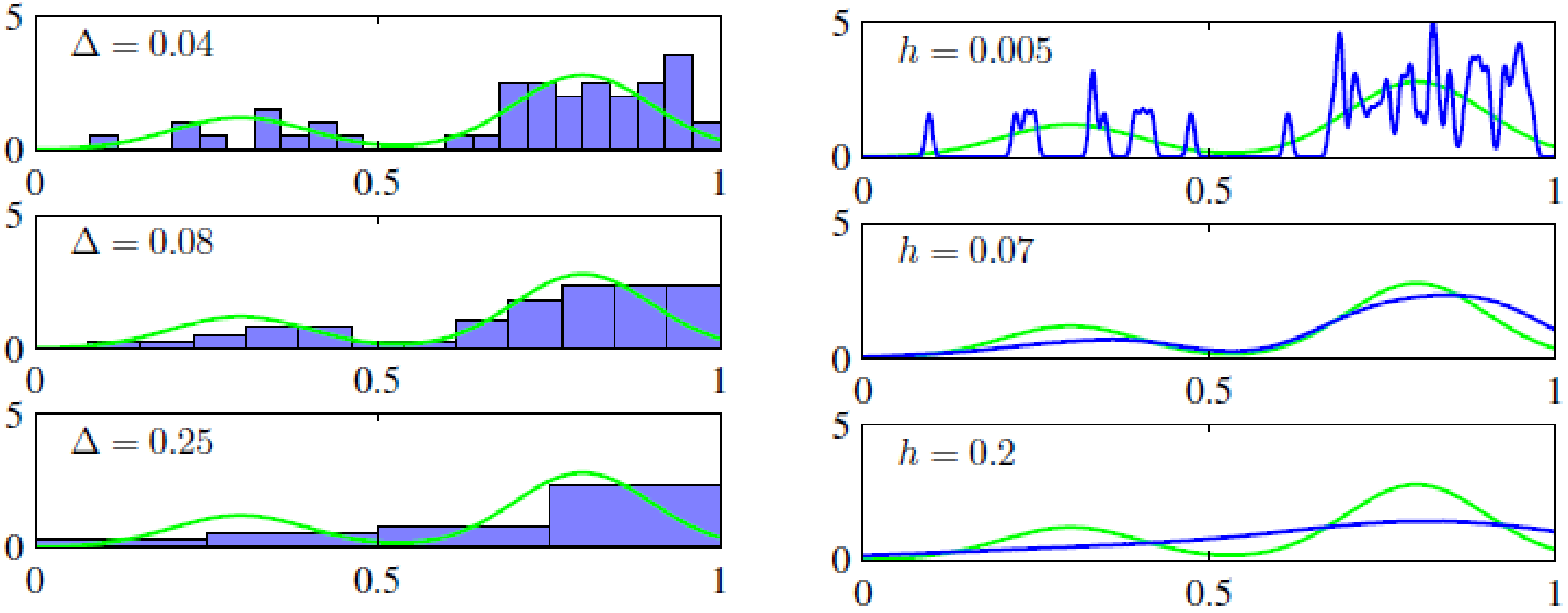
$$p(x) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h^d} k(\frac{x - x_i}{h})$$

Estimated density at x

Density Estimation

Kernel Density Estimation (non-parametric)

- P: probability of falling within R
- Need to estimate p(x) given N data points



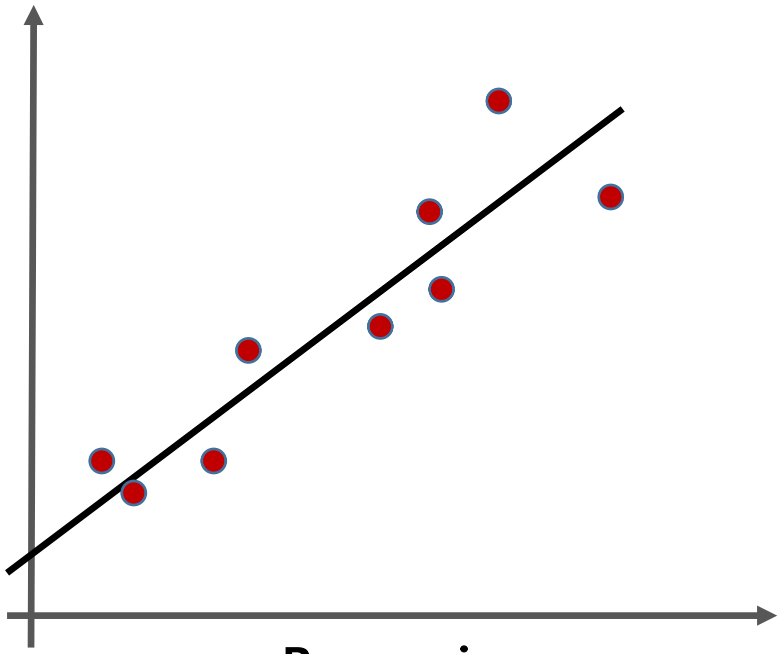
Supervised Learning

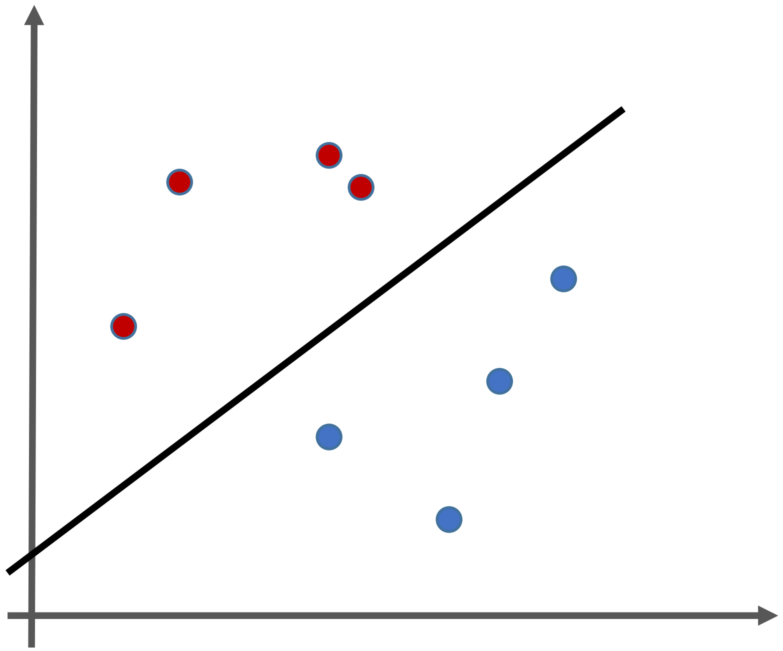
Dataset with Labels

- Given $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$ and labels y_i, find patterns in the data

- Classification: label given as a class

- Regression: label given as a continuous variable


Regression


Classification

Supervised Learning

Training

- Given $\mathbf{x} = (x_1, x_2, \cdots x_N)$, $x_i \in \mathbb{R}^k$ and labels y_i, find patterns in the data

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Testing

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Supervised Learning

Supervised…

- We have data and labels.
- Experience with a teacher!

Let’s try to…

- Make a hypothesis, and find a model that best fits the data

Given a training set of instances X, find a function that best maps X to labels y.

Supervised Learning

Methods for supervised learning

- Naïve Bayes classifier
- k-NN classifier
- Decision tree
- Artificial Neural Network
- Ensembles of classifiers

Naïve Bayes

Naïve Bayes Classifier

- Conditional Probabilistic Model
- Assume that each feature is independent from each other
- Maximum Likelihood
- Requires relatively small training set

Naïve Bayes

Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

$$p(h_k | a_1, \cdots, a_N)$$

Probability of class k given x

$$p(h_k|\mathbf{x}) = \frac{p(h_k)p(\mathbf{x}|h_k)}{p(\mathbf{x})}$$

Conditional probability decomposed using Bayes Theorem

$$posterior = \frac{prior \times likelihood}{evidence}$$

Evidence independent from y

$$\begin{aligned} y_{MAP} &= \text{argmax}_{h_k} p(h_k|\mathbf{x}) \\ &= \text{argmax}_{h_k} p(h_k)p(\mathbf{x}|h_k) \end{aligned}$$

Naïve Bayes

Bayes Theorem

$$p(A|B) = \frac{p(B|A)}{p(B)}$$

Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

$$p(h_k|a_1, \cdots, a_N)$$

Probability of class k given x

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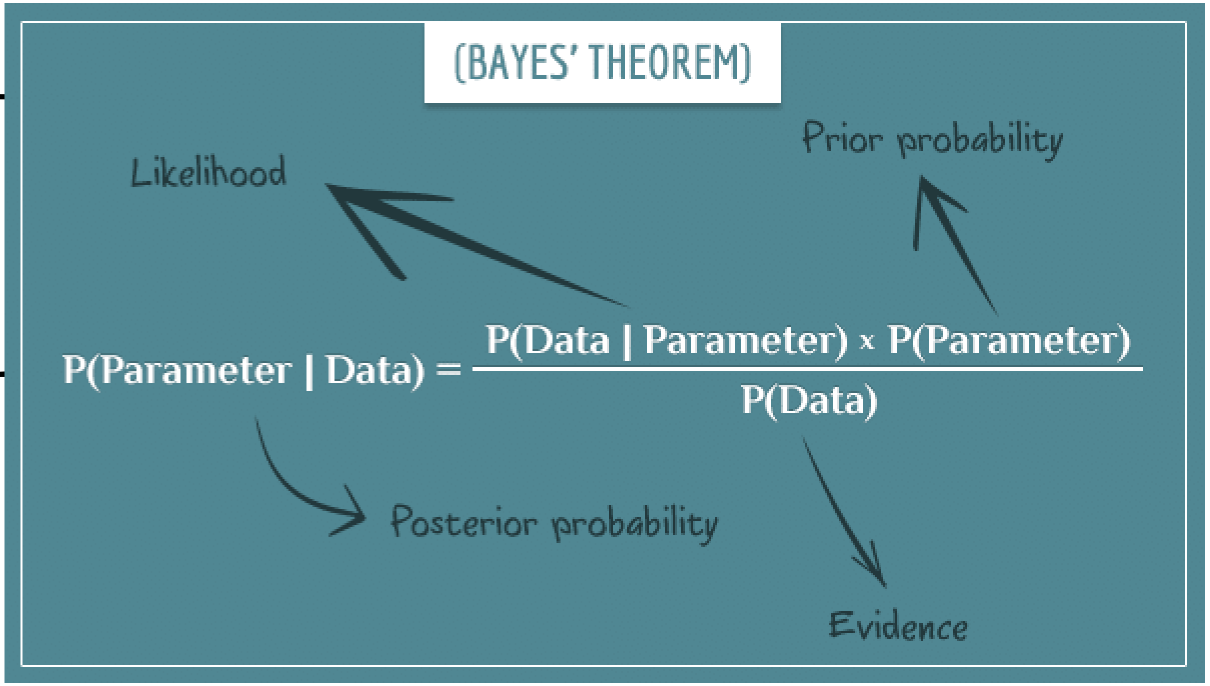

Naïve Bayes

Bayes Theorem

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Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

$$\begin{aligned} y_{MAP} &= \text{argmax}_{h_k} p(h_k|\mathbf{x}) \\ &= \text{argmax}_{h_k} p(h_k)p(\mathbf{x}|h_k) \end{aligned}$$

Maximum a posteriori (MAP)

$$y_{ML} = \text{argmax}_{h_k} p(\mathbf{x}|h_k)$$

With equally probable a priori, it becomes maximum likelihood (ML)

$$\begin{aligned} p(h_k, a_1, \cdots a_N) &= p(a_1, a_2, \cdots, a_p, h_k) \\ &= p(a_1|a_2, \cdots, a_p, h_k)p(a_2, \cdots, a_p, h_k) \\ &= p(a_1|a_2, \cdots, a_p, h_k)p(a_2|a_3, \cdots, a_p, h_k) \cdots \\ &\quad\ p(a_{p-1}|a_p, h_k)p(a_p|h_k)p(h_k) \end{aligned}$$

Using chain rule

$$P(X = x \mid Y = y) = \frac{P(X = x, Y = y)}{P(Y = y)}$$

Naïve Bayes

Bayes Theorem

$$p(A|B) = \frac{p(B|A)}{p(B)}$$

Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

Recall conditional distribution

$$P(X = x \mid Y = y) = \frac{P(X = x, Y = y)}{P(Y = y)}$$

$$y_{MAP} = \text{argmax}_{h_k} p(h_k) p(\mathbf{x}|h_k)$$

$$p(h_k, a_1, \cdots a_p) = p(a_1|a_2, \cdots, a_p, h_k) p(a_2|a_3, \cdots, a_p, h_k) \cdots$$
$$p(a_{p-1}|a_p, h_k) p(a_p|h_k) p(h_k)$$

$$p(a_i|a_{i+1}, \cdots, a_p, h_k) = p(a_i|h_k)$$

Because of independence

$$\begin{aligned} p(h_k|\mathbf{x}) &\propto p(h_k, a_1, a_2, \cdots a_N) \\ &\propto p(h_k) p(a_1|h_k) p(a_2|h_k) \cdots p(a_N|h_k) \\ &\propto p(h_k) \Pi_{i=1}^N p(a_i|h_k) \end{aligned}$$

Naïve Bayes

Bayes Theorem

$p(A|B) = \frac{p(B|A)}{p(B)}$

Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

$$y_{MAP} = \text{argmax}_{h_k} p(h_k)p(\mathbf{x}|h_k)$$

$$\begin{aligned} p(h_k|\mathbf{x}) &\propto p(h_k, a_1, a_2, \cdots a_p) \\ &\propto p(h_k)p(a_1|h_k)p(a_2|h_k) \cdots p(a_p|h_k) \\ &\propto p(h_k)\Pi_{i=1}^{N} p(a_i|h_k) \end{aligned}$$

$$p(h_k|\mathbf{x}) = \frac{1}{Z} p(h_k)\Pi_{i=1}^{p} p(a_i|h_k)$$

Normalize it to be a probability

$$Z = \sum_k p(h_k)p(\mathbf{x}|h_k)$$

Naïve Bayes

Bayes Theorem
$p(A|B) = \frac{p(B|A)}{p(B)}$

Naïve Bayes Classifier

- Given data $\mathbf{x}$ with attributes $a_i \in \mathbb{R}^p$ and labels $h_k \in H$, find patterns in the data

$$y_{MAP} = \text{argmax}_{h_k} p(h_k) p(\mathbf{x}|h_k)$$

$$p(h_k|\mathbf{x}) = \frac{1}{Z} p(h_k) \Pi_{i=1}^{p} p(a_i|h_k) \qquad Z = \sum_k p(h_k) p(\mathbf{x}|h_k)$$

Inference / Prediction using Naïve Bayes

Maximum a posteriori (MAP)

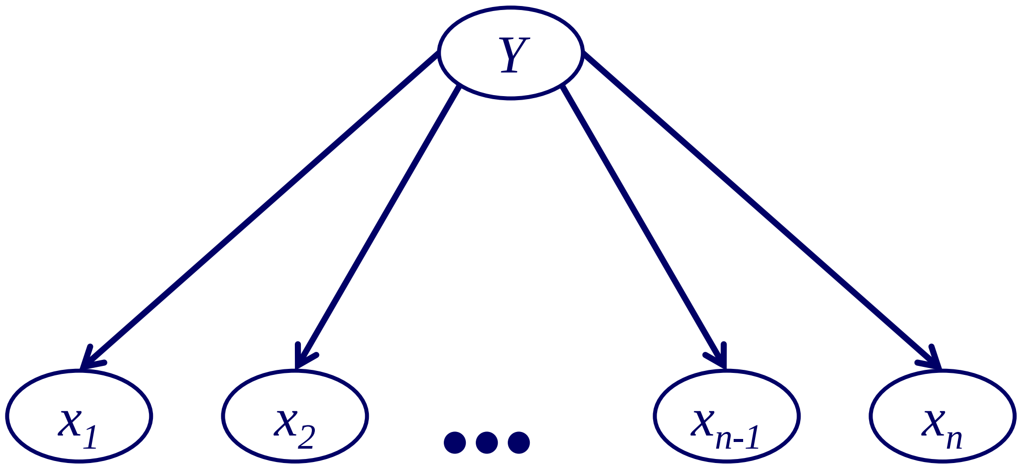
$$\hat{y} = \text{argmax}_k p(h_k) \Pi_{i=1}^{k} p(a_i|h_k)$$

$$\begin{aligned} y_{MAP} &= \text{argmax}_{h_k} p(h_k|\mathbf{x}) \\ &= \text{argmax}_{h_k} p(h_k) p(\mathbf{x}|h_k) \end{aligned}$$

Naïve Bayes

Naïve Bayes Classifier

- One very simple BN approach for supervised tasks is *naïve Bayes*
- In naïve Bayes, we assume that all features X_i are conditionally independent given the class Y



$$\hat{y} = \text{argmax}_k p(h_k) \Pi_{i=1}^{k} p(a_i | h_k)$$