CS 540 Introduction to Artificial Intelligence

Classification - KNN and Naive Bayes

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Slides created by Sharon Li [modified by Yingyu Liang]

Today's outline

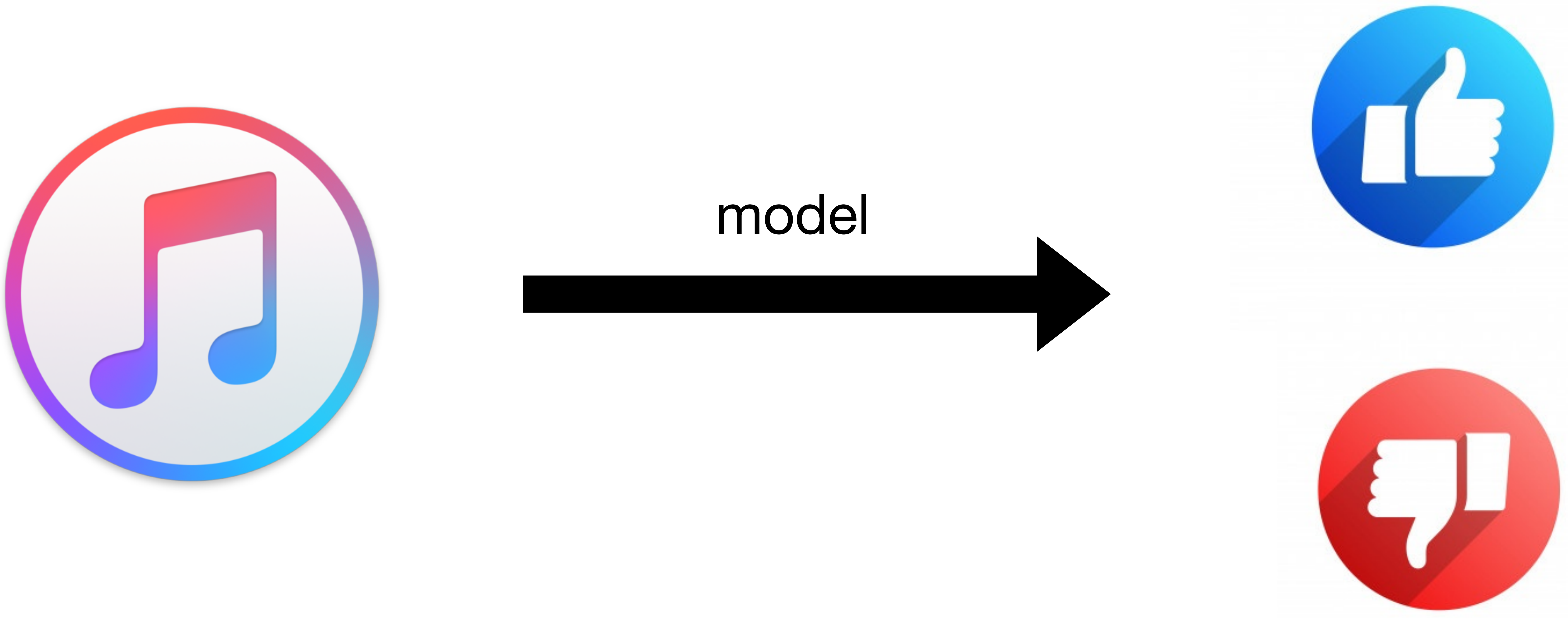
- K-Nearest Neighbors
- Maximum likelihood estimation
- Naive Bayes

Part I: K-nearest neighbors


Wikipedia
The Free Encyclopedia
Main page
Article
Talk
k-nearest neighbors algorithm
From Wikipedia, the free encyclopedia
Not to be confused with k-means clustering.

(source: wiki)

Example 1: Predict whether a user likes a song or not



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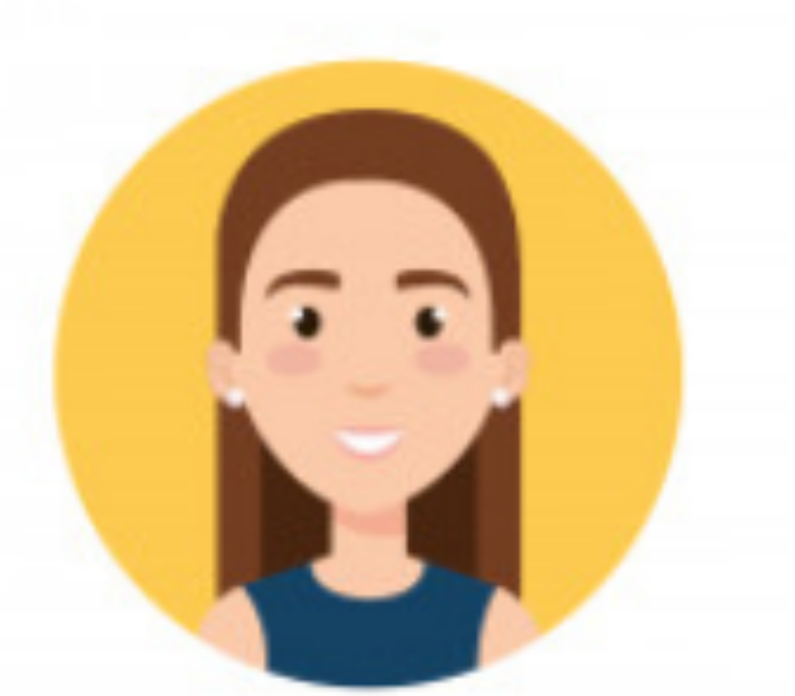
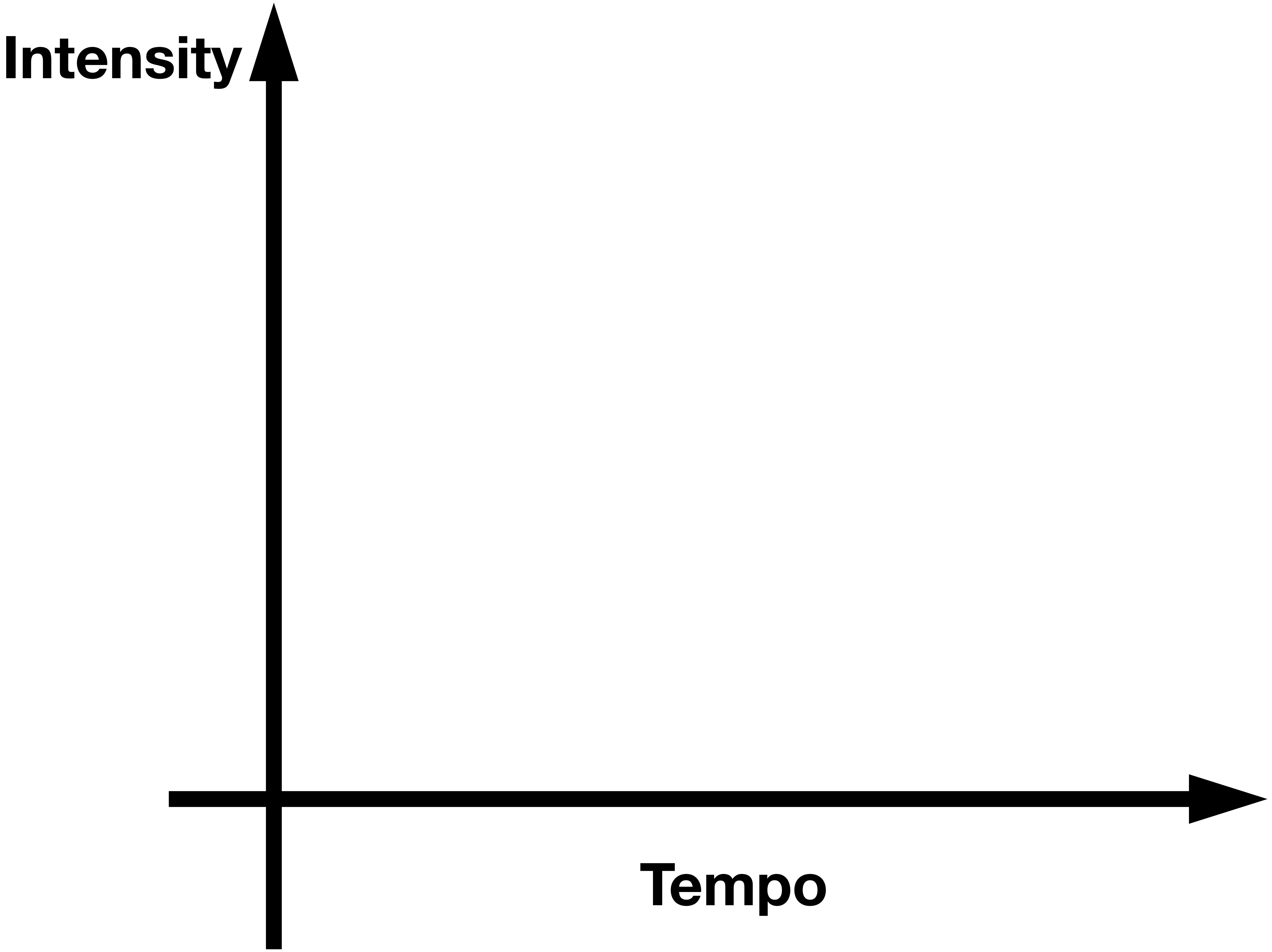
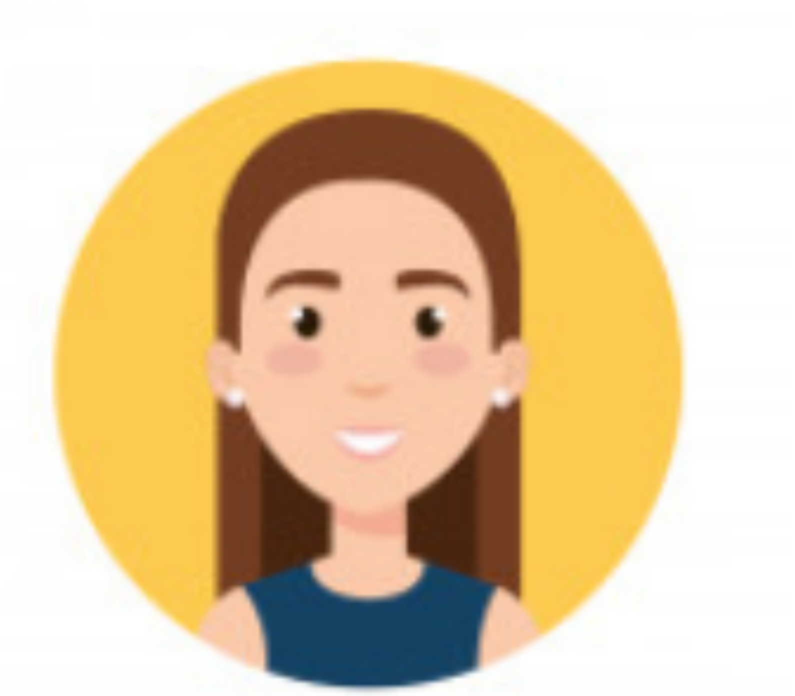


User Sharon



Example 1: Predict whether a user likes a song or not
1-NN



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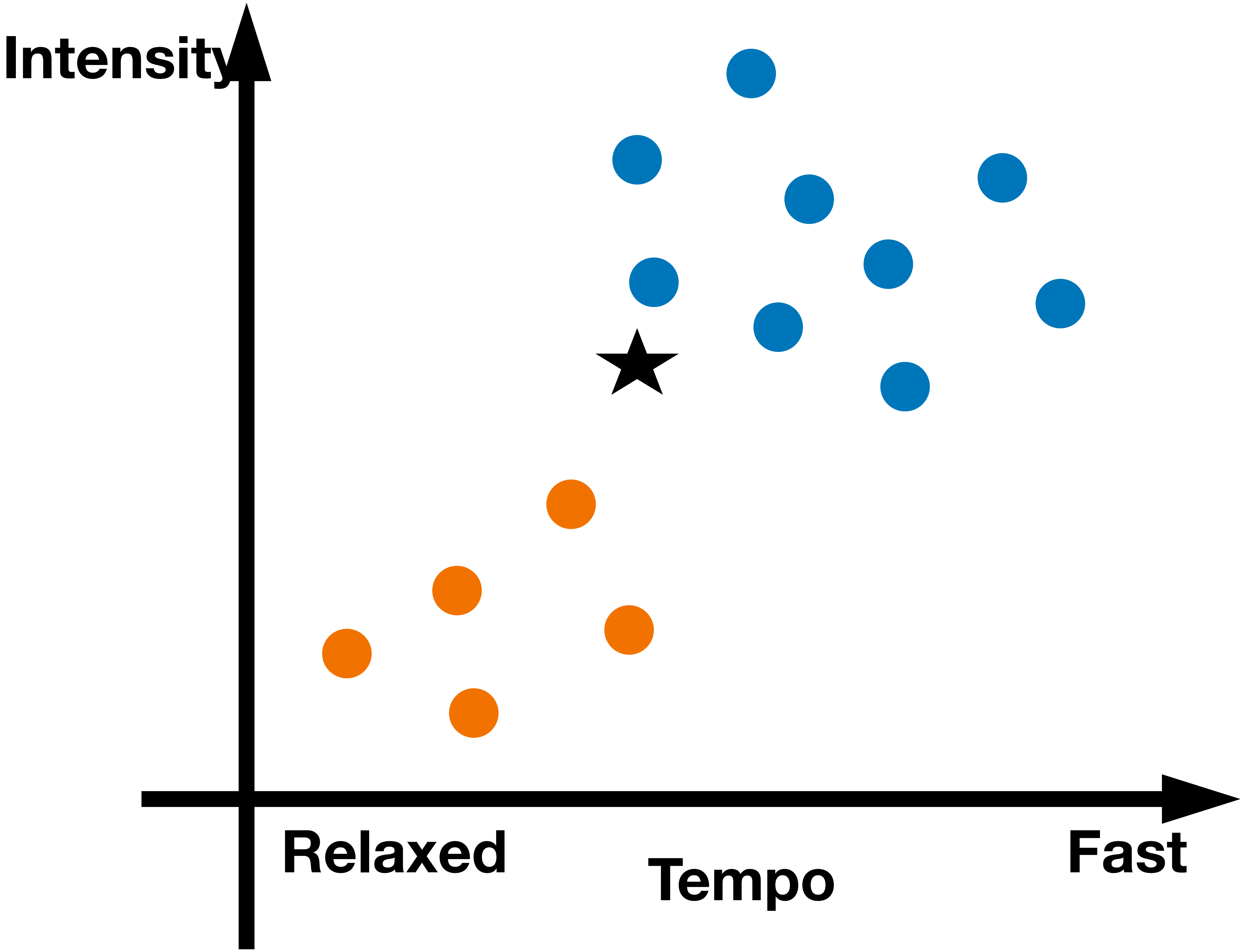
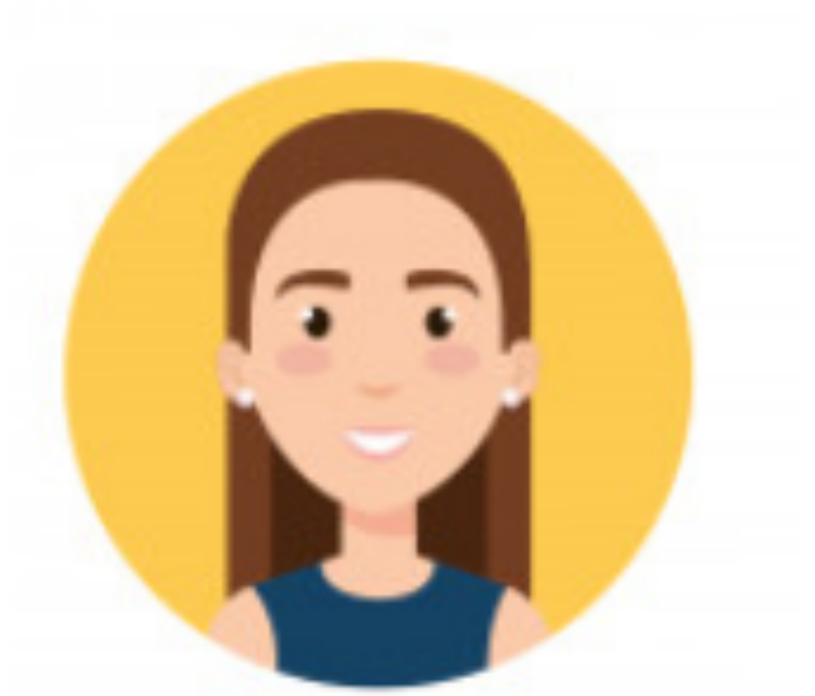


Example 1: Predict whether a user likes a song or not

1-NN



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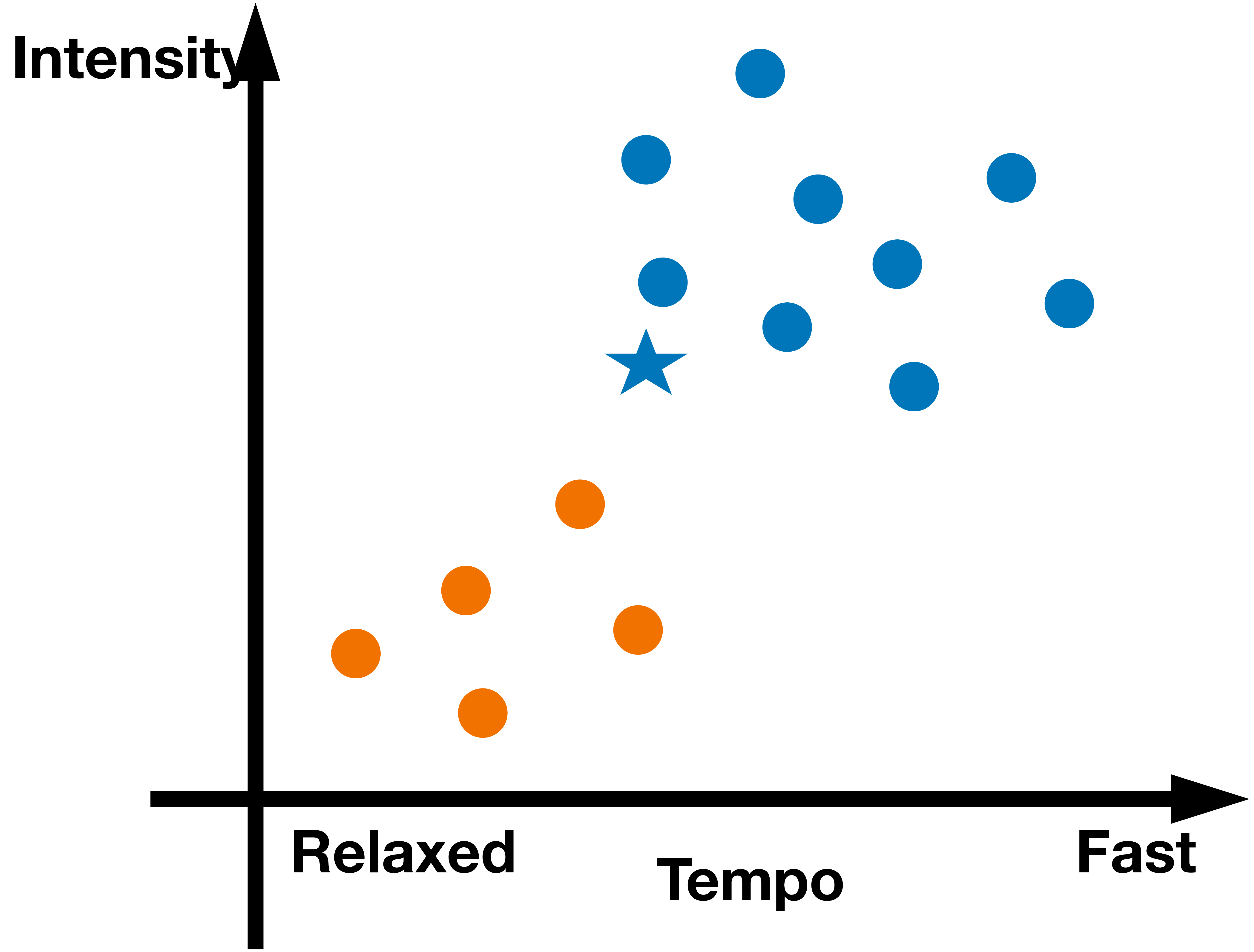


K-nearest neighbors for classification

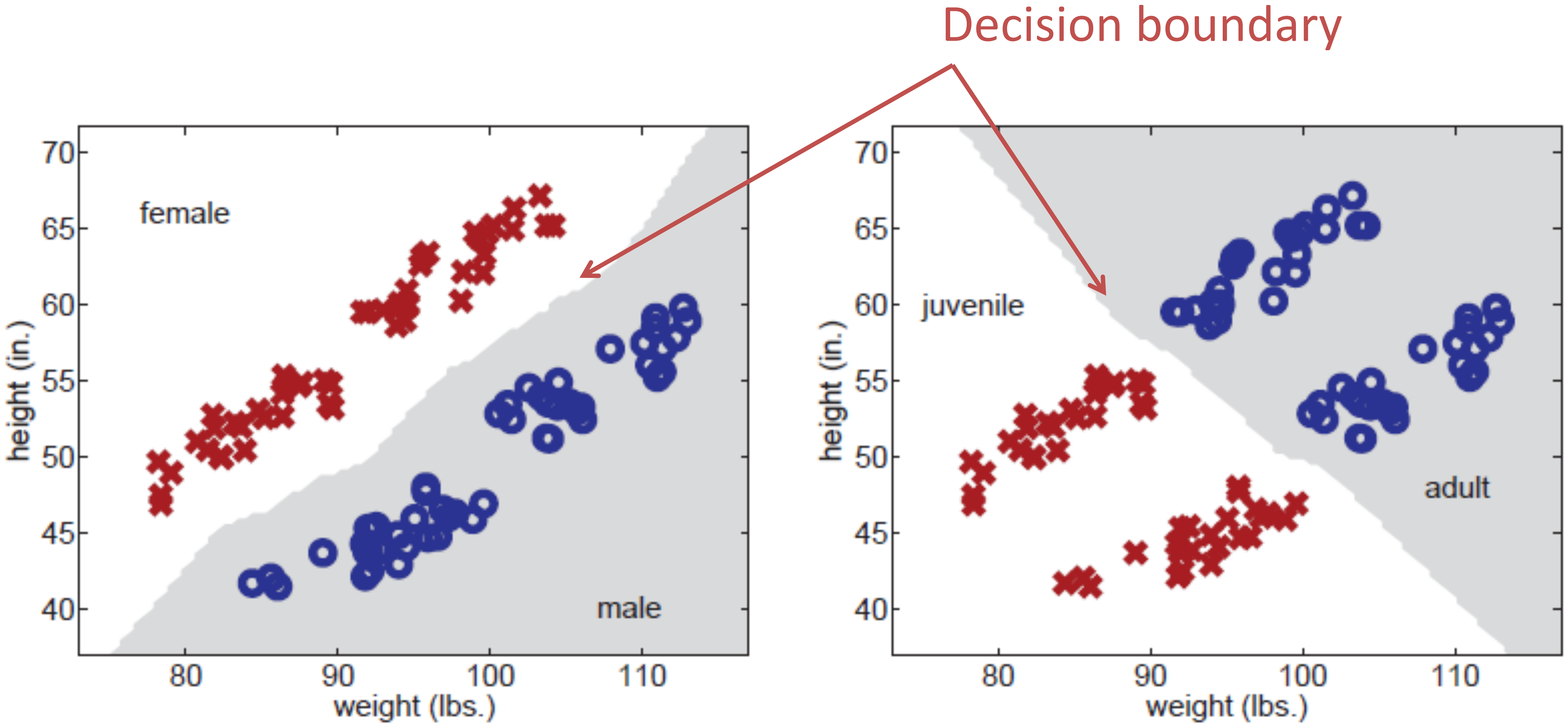
- **Input:** Training data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

  Distance function $d(\mathbf{x}_i, \mathbf{x}_j)$; number of neighbors k; test data $\mathbf{x}^*$

1. Find the k training instances $\mathbf{x}_{i_1}, \ldots, \mathbf{x}_{i_k}$ closest to $\mathbf{x}^*$ under $d(\mathbf{x}_i, \mathbf{x}_j)$
2. Output y^* as the majority class of $y_{i_1}, \ldots, y_{i_k}$. Break ties randomly.

Example 2: 1-NN for little green man

- Predict gender (M,F) from weight, height
- Predict age (adult, juvenile) from weight, height

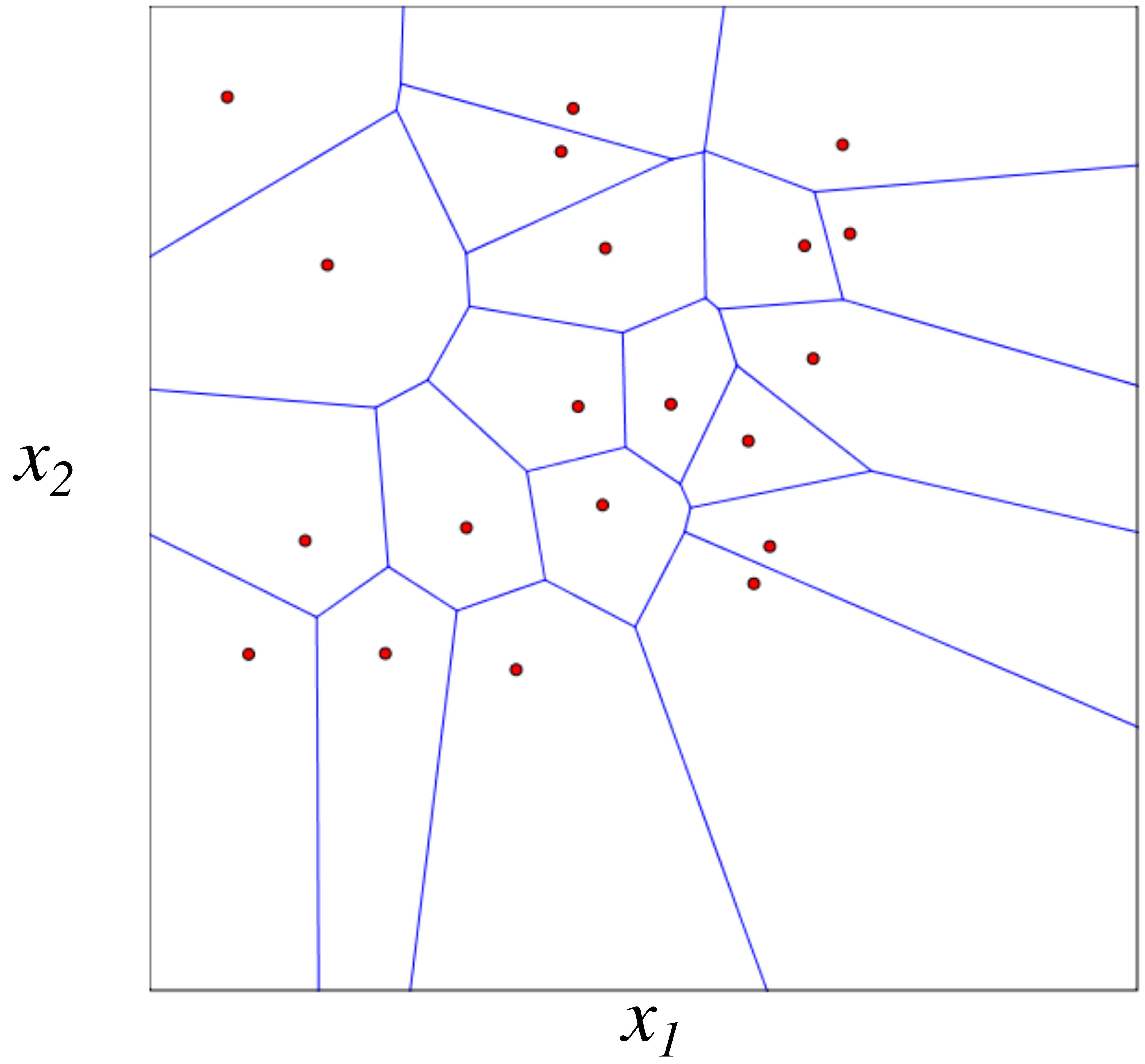


(a) classification by gender

(b) classification by age

The decision regions for 1-NN

Voronoi diagram: each polyhedron indicates the region of feature space that is in the nearest neighborhood of each training instance



K-NN for regression

- What if we want regression?

- Instead of majority vote, take average of neighbors' labels
  - Given test point $\mathbf{x}^*$, find its k nearest neighbors $\mathbf{x}_{i_1}, \ldots, \mathbf{x}_{i_k}$
  - Output the predicted label $\frac{1}{k}(y_{i_1} + \ldots + y_{i_k})$

How can we determine distance?

suppose all features are discrete

- Hamming distance: count the number of features for which two instances differ

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suppose all features are discrete

- Hamming distance: count the number of features for which two instances differ

suppose all features are continuous

- Euclidean distance: sum of squared differences

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

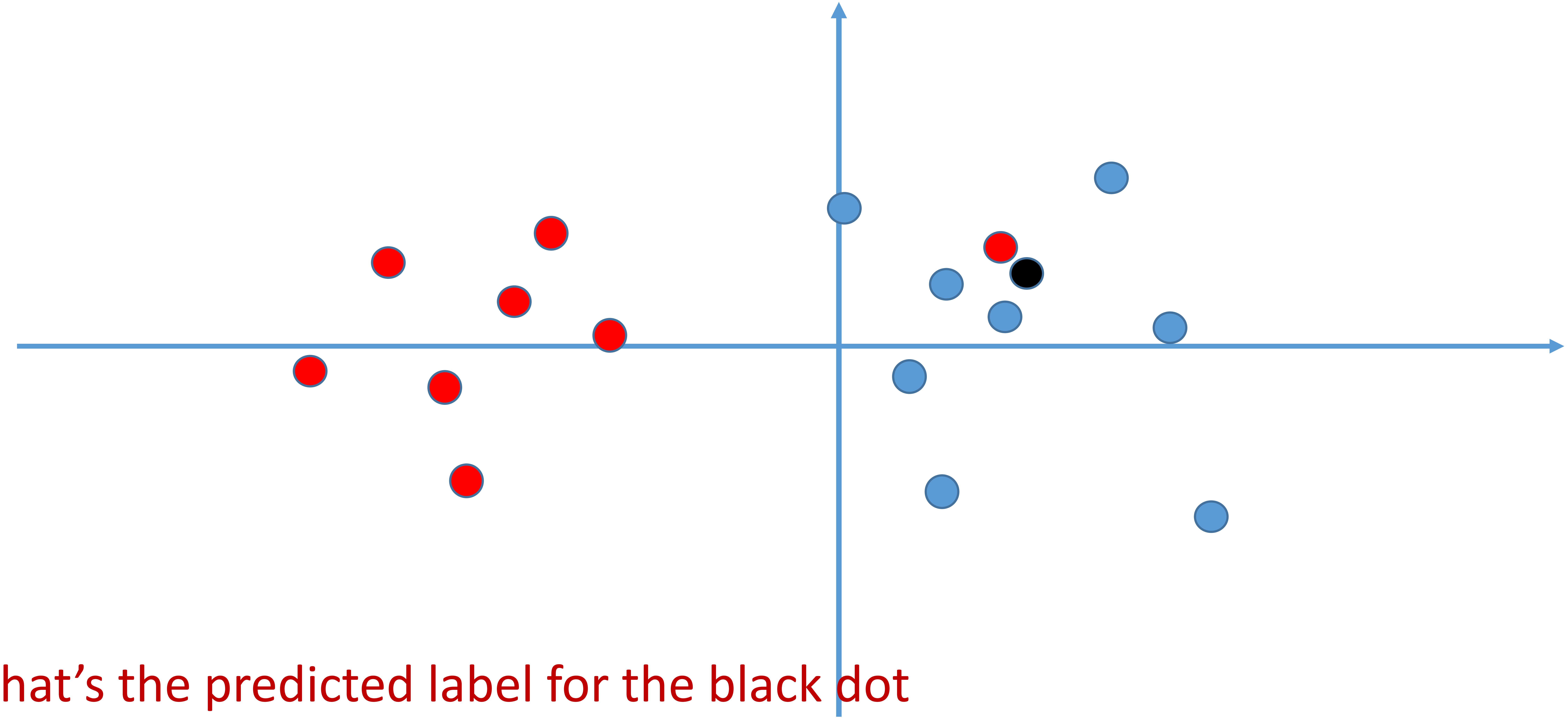
- Manhattan distance:

$$d(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^{n} |p_i - q_i|$$

How to pick the number of neighbors

- Split data into training and **tuning sets**
- Classify tuning set with different k
- Pick k that produces least tuning-set error

Effect of k



What's the predicted label for the black dot using 1 neighbor? 3 neighbors?

Part II: Maximum Likelihood Estimation

Supervised Machine Learning

Non-parametric (e.g., KNN)

vs.

Parametric

Supervised Machine Learning

Statistical modeling approach

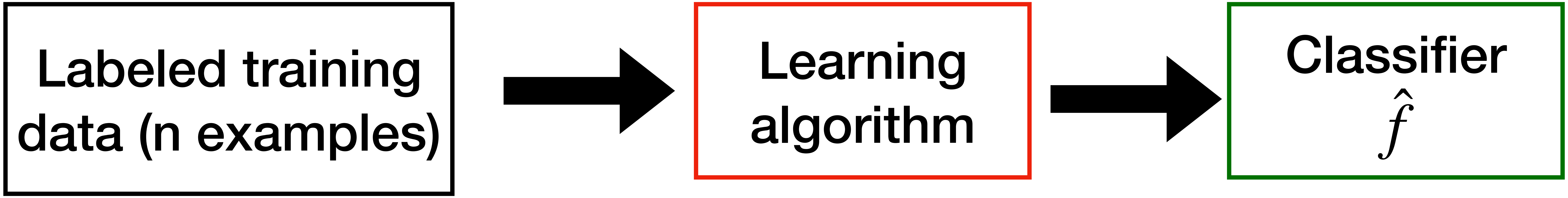
Labeled training data (n examples)

$$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$$

drawn **independently** from
a fixed underlying distribution
(also called the i.i.d. assumption)

Supervised Machine Learning

Statistical modeling approach



$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

drawn **independently** from
a fixed underlying distribution
(also called the i.i.d. assumption)

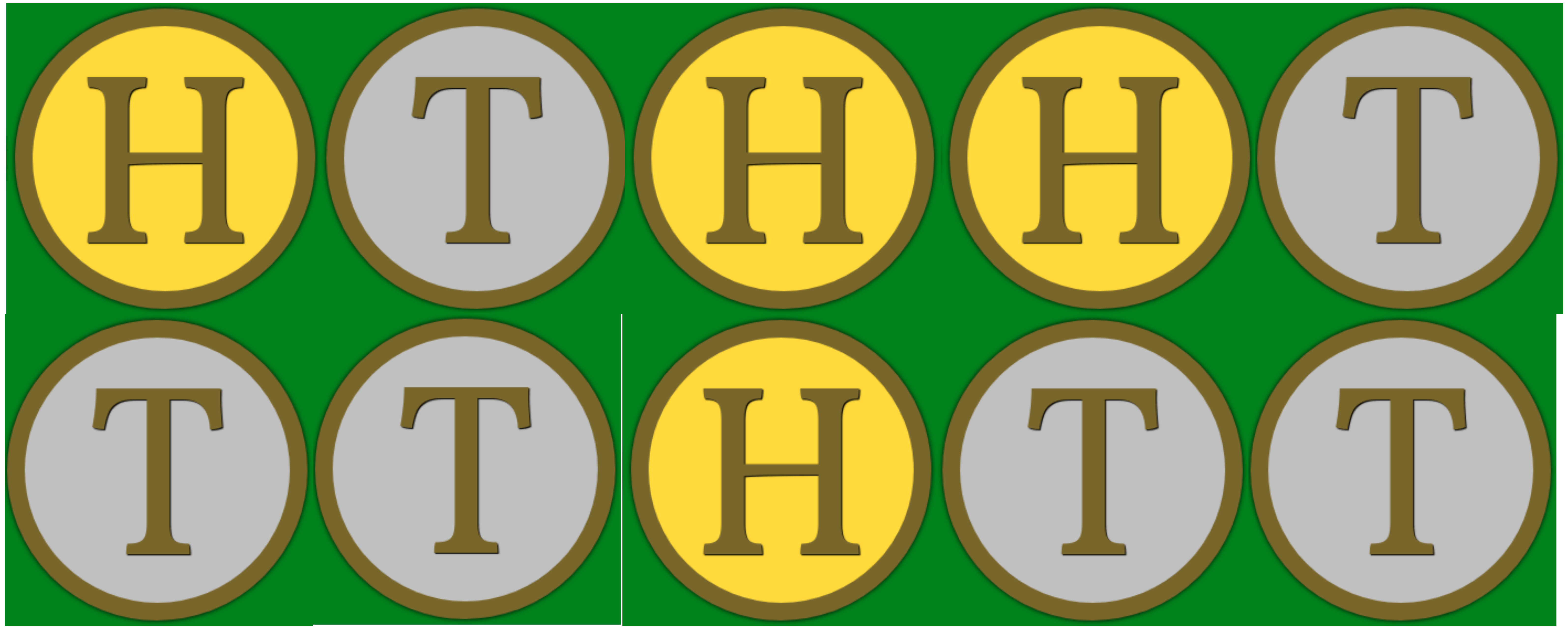
select $\hat{f}(\theta)$ from a pool of models $\mathcal{F}$
that **best describe the data observed**

How to select $\hat{f} \in \mathscr{F}$?

- **Maximum likelihood (best fits the data)**
- Maximum a posteriori (best fits the data but incorporates prior assumptions)
- Optimization of ‘loss’ criterion (best discriminates the labels)

Maximum Likelihood Estimation: An Example

Flip a coin 10 times, how can you estimate $\theta = p(\text{Head})$?



Intuitively, $\theta = 4/10 = 0.4$

How good is θ?

It depends on how likely it is to generate the observed data

$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ (Let's forget about label for a second)

Likelihood function $L(\theta) = \Pi_i p(\mathbf{x}_i \mid \theta)$

↑

Under i.i.d assumption

Interpretation: How **probable** (or how likely) is the data given the probabilistic model p_θ?

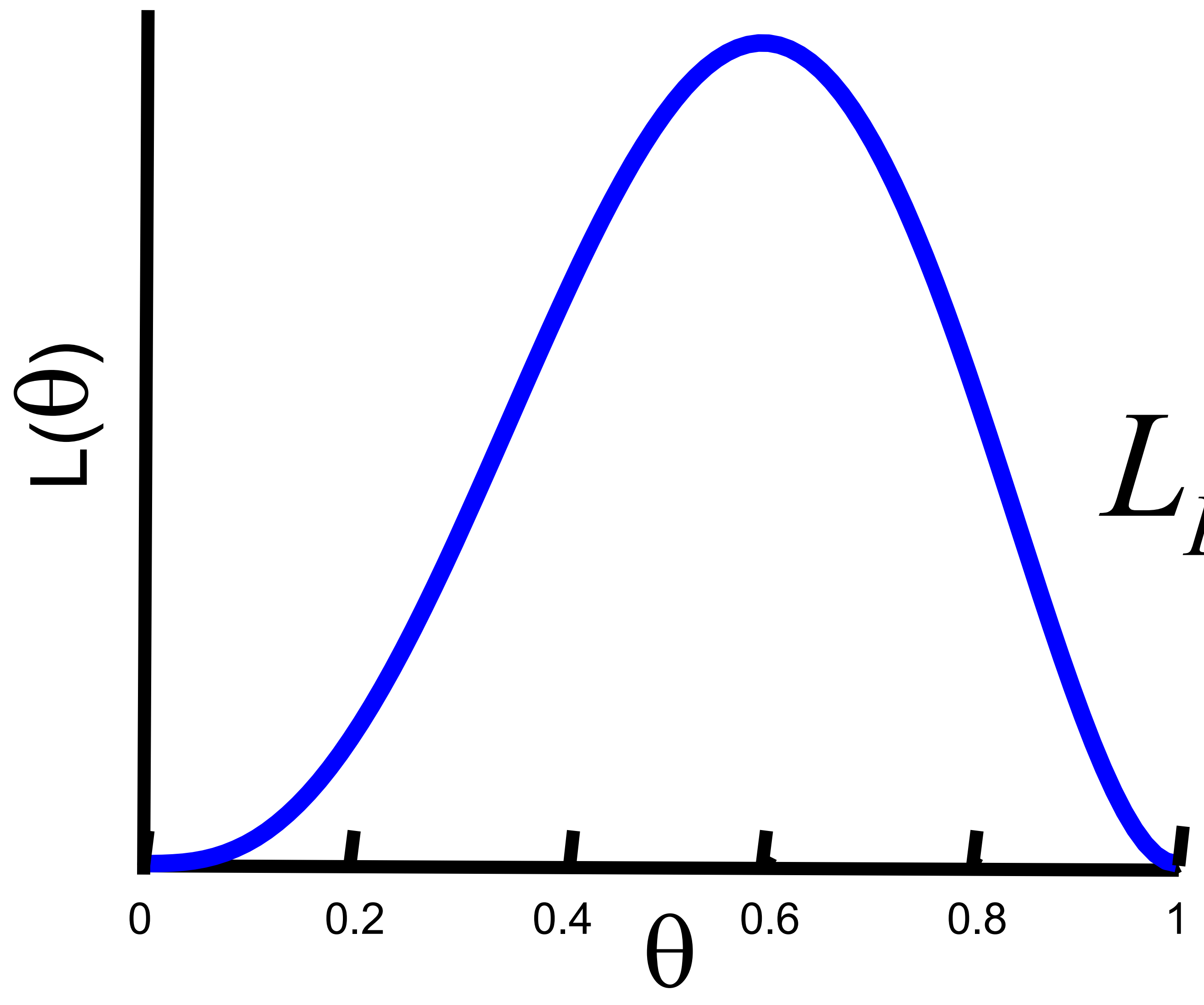
How good is θ?

It depends on how likely it is to generate the observed data

$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ (Let's forget about label for a second)

Likelihood function $L(\theta) = \Pi_i p(\mathbf{x}_i \mid \theta)$

H,T, T, H, H



$$L_D(\theta) = \theta \cdot (1-\theta) \cdot (1-\theta) \cdot \theta \cdot \theta$$

Bernoulli distribution

Log-likelihood function

$$L_D(\theta) = \theta \cdot (1-\theta) \cdot (1-\theta) \cdot \theta \cdot \theta$$

$$= \theta^{N_H} \cdot (1-\theta)^{N_T}$$

Log-likelihood function

$$\ell(\theta) = \log L(\theta)$$

$$= N_H \log \theta + N_T \log(1-\theta)$$

Maximum Likelihood Estimation (MLE)

Find optimal θ^* to maximize the likelihood function (and log-likelihood)

$$\theta^* = \arg\max N_H \log \theta + N_T \log(1-\theta)$$

$$\frac{\partial l(\theta)}{\partial \theta} = \frac{N_H}{\theta} - \frac{N_T}{1-\theta} = 0 \quad \Rightarrow \quad \theta^* = \frac{N_H}{N_T + N_H}$$

which confirms your intuition!

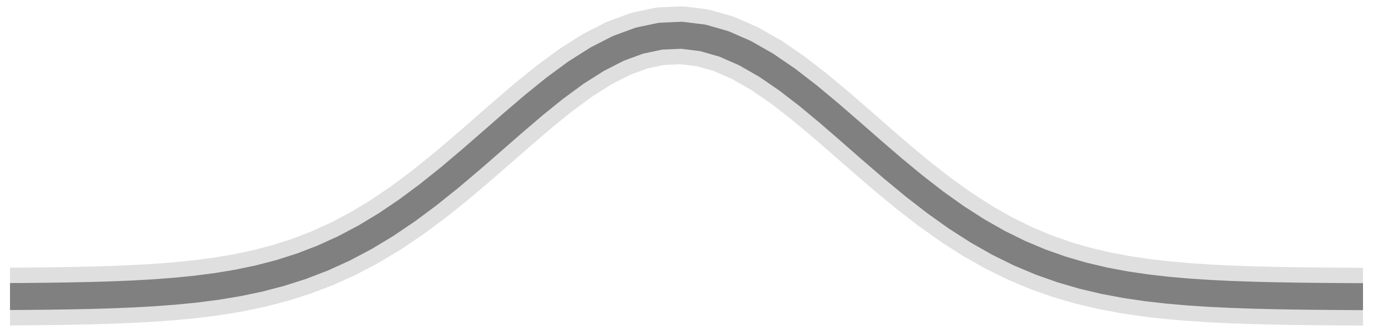
Maximum Likelihood Estimation: Gaussian Model

Fitting a model to heights of females

Observed some data (in inches): 60, 62, 53, 58,… $\in \mathbb{R}$

$$\{x_1, x_2, \ldots, x_n\}$$

Model class: Gaussian model



$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

So, what's the MLE for the given data?

Estimating the parameters in a Gaussian

- **Mean**

$$\mu = \mathbf{E}[x] \text{ hence } \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- **Variance**

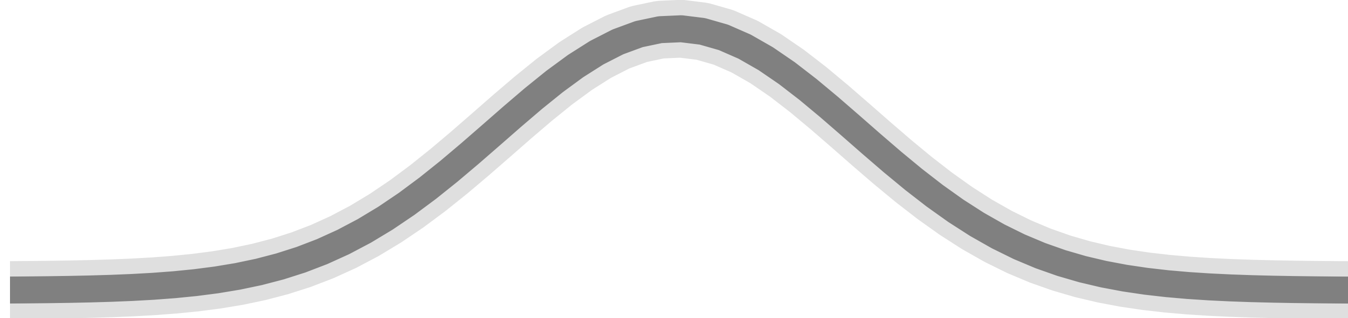
$$\sigma^2 = \mathbf{E}\left[(x-\mu)^2\right] \text{ hence } \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n} (x_i - \hat{\mu})^2$$

Why?

Maximum Likelihood Estimation: Gaussian Model

Observe some data (in inches): $x_1, x_2, \ldots, x_n \in \mathbb{R}$

Assume that the data is drawn from a Gaussian



$$L(\mu, \sigma^2 \,|\, X) = \prod_{i=1}^{n} p(x_i; \mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{2\pi\sigma^2} \exp\left(- \frac{(x_i - \mu)^2}{2\sigma^2} \right)$$

Fitting parameters is maximizing likelihood w.r.t μ, σ^2
(maximize likelihood that data was generated by model)

MLE

$$\arg\max_{\mu, \sigma^2} \prod_{i=1}^{n} p(x_i; \mu, \sigma^2)$$

Maximum Likelihood

- Estimate parameters by finding ones that explain the data

$$\underset{\mu,\sigma^2}{\arg\max} \prod_{i=1}^{n} p(x_i; \mu, \sigma^2) = \underset{\mu,\sigma^2}{\arg\min} - \log \prod_{i=1}^{n} p(x_i; \mu, \sigma^2)$$

- **Decompose likelihood**

$$\sum_{i=1}^{n} \frac{1}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2}(x_i - \mu)^2 = \frac{n}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (x_i - \mu)^2$$

Minimized for $\mu = \frac{1}{n} \sum_{i=1}^{n} x_i$

Maximum Likelihood

- Estimating the variance

$$\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$

Maximum Likelihood

- Estimating the variance

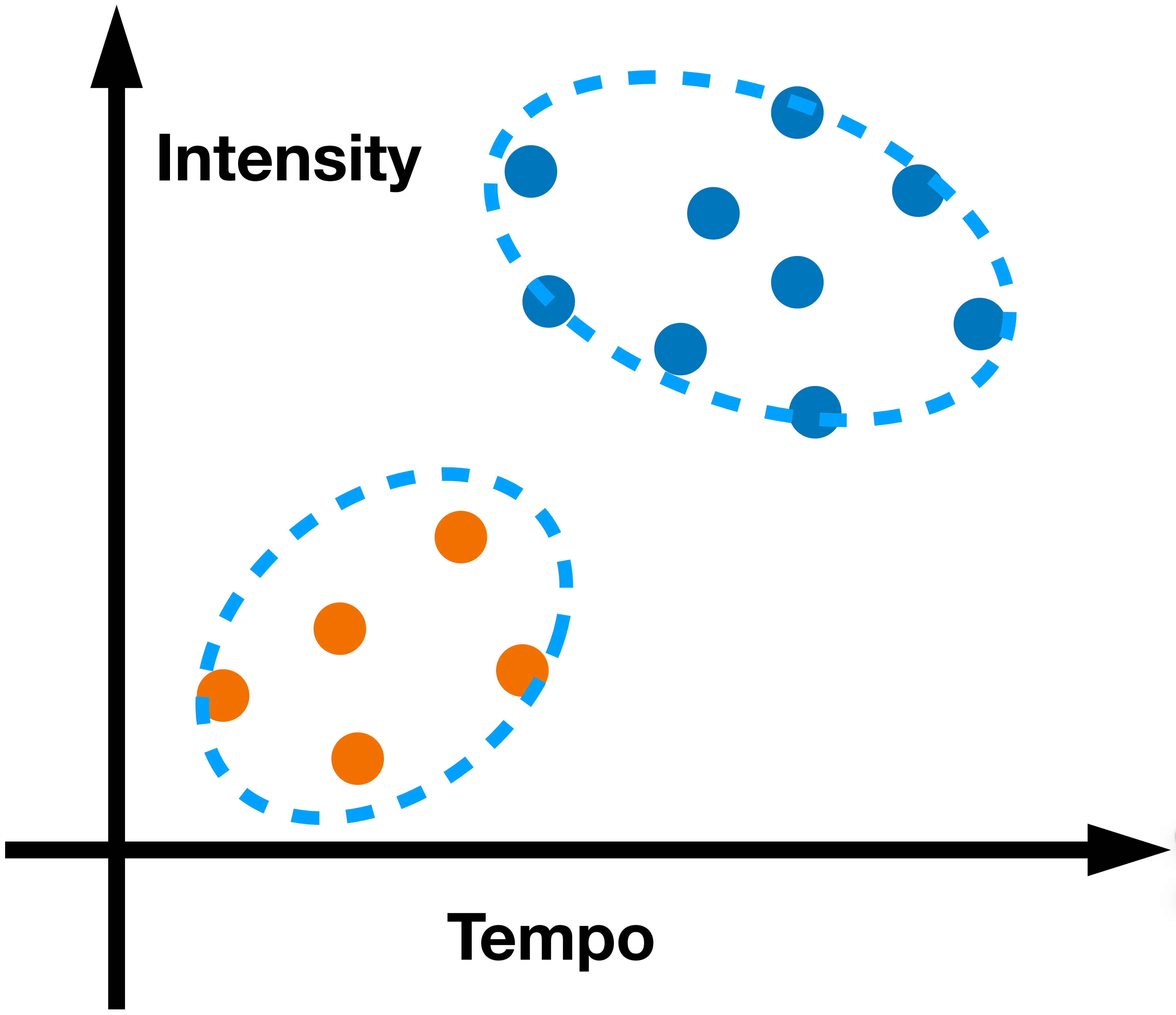
$$\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$

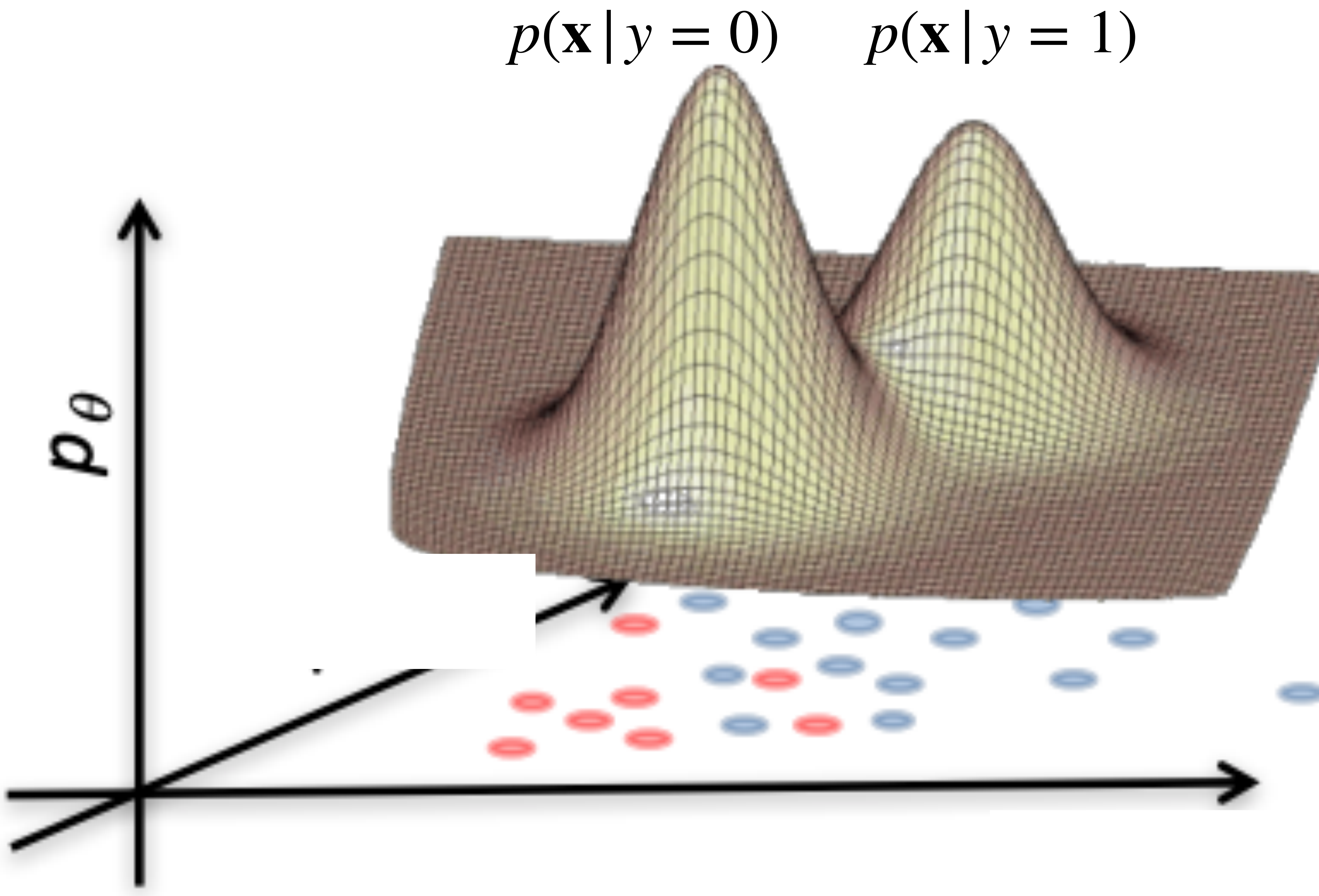
- Take derivatives with respect to it

$$\partial_{\sigma^2}[\,\cdot\,] = \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\sum_{i=1}^{n}(x_i - \mu)^2 = 0$$

$$\implies \sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

Classification via MLE





Classification via MLE

$$\hat{y} = \hat{f}(\mathbf{x}) = \arg\max\, p(y \mid \mathbf{x})$$

(Posterior)

(Prediction)

Classification via MLE

$$\hat{y} = \hat{f}(\mathbf{x}) = \arg\max p(y \mid \mathbf{x})$$ (Posterior)

(Prediction)

$$= \arg\max_y \frac{p(\mathbf{x} \mid y) \cdot p(y)}{p(\mathbf{x})}$$ (by Bayes' rule)

$$= \arg\max_y \; p(\mathbf{x} \mid y) p(y)$$

Using labelled training data, learn **class priors** and **class conditionals**

Part II: Naïve Bayes

Example 1: Play outside or not?

- If weather is sunny, would you likely to play outside?

Posterior probability p(Yes | ) vs. p(No | )

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- If weather is sunny, would you likely to play outside?

Posterior probability p(Yes | ) vs. p(No | )

- Weather = {Sunny, Rainy, Overcast}
- Play = {Yes, No}
- Observed data {Weather, play on day *m*}, m={1,2,…,N}

Example 1: Play outside or not?

- If weather is sunny, would you likely to play outside?

Posterior probability p(Yes | ) vs. p(No | )

- Weather = {Sunny, Rainy, Overcast}
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p(Play | ) = p( | Play) p(Play) / p()

Bayes rule

Example 1: Play outside or not?

- **Step 1**: Convert the data to a frequency table of Weather and Play

Weather	Play
Sunny	No
Overcast	Yes
Rainy	Yes
Sunny	Yes
Sunny	Yes
Overcast	Yes
Rainy	No
Rainy	No
Sunny	Yes
Rainy	Yes
Sunny	No
Overcast	Yes
Overcast	Yes
Rainy	No

Frequency Table		
Weather	No	Yes
Overcast		4
Rainy	3	2
Sunny	2	3
Grand Total	5	9

https://www.analyticsvidhya.com/blog/2017/09/naive-bayes-explained/

Example 1: Play outside or not?

Step 1: Convert the data to a frequency table of Weather and Play

Step 2: Based on the frequency table, calculate **likelihoods** and **priors**

Weather	Play
Sunny	No
Overcast	Yes
Rainy	Yes
Sunny	Yes
Sunny	Yes
Overcast	Yes
Rainy	No
Rainy	No
Sunny	Yes
Rainy	Yes
Sunny	No
Overcast	Yes
Overcast	Yes
Rainy	No

Frequency Table		
Weather	No	Yes
Overcast		4
Rainy	3	2
Sunny	2	3
Grand Total	5	9

Likelihood table				
Weather	No	Yes		
Overcast		4	=4/14	0.29
Rainy	3	2	=5/14	0.36
Sunny	2	3	=5/14	0.36
All	5	9		
	=5/14	=9/14		
	0.36	0.64		

p(Play = Yes) = 0.64

p( | Yes) = 3/9 = 0.33

https://www.analyticsvidhya.com/blog/2017/09/naive-bayes-explained/

Example 1: Play outside or not?

Step 3: Based on the likelihoods and priors, calculate posteriors

P(Yes| )
=P( |Yes)*P(Yes)/P()

?

P(No| )
=P( |No)*P(No)/P()

?

Example 1: Play outside or not?

Step 3: Based on the likelihoods and priors, calculate posteriors

P(Yes| ☀)
=P(☀ |Yes)*P(Yes)/P(☀)
=0.33*0.64/0.36
=0.6

P(No| ☀)
=P(☀ |No)*P(No)/P(☀)
=0.4*0.36/0.36
=0.4

P(Yes| ☀) > P(No| ☀) go outside and play!

Bayesian classification

$$\hat{y} = \arg\max p(y \mid \mathbf{x})$$ (Posterior)

(Prediction)

$$= \arg\max \frac{p(\mathbf{x} \mid y) \cdot p(y)}{p(\mathbf{x})}$$ (by Bayes' rule)

$$= \arg\max \; p(\mathbf{x} \mid y) p(y)$$

Bayesian classification

What if **x** has multiple attributes $\mathbf{x} = \{X_1, \ldots, X_k\}$

$$\hat{y} = \arg\max_{y} p(y \mid X_1, \ldots, X_k)$$

(Posterior)

(Prediction)

Bayesian classification

What if **x** has multiple attributes $\mathbf{x} = \{X_1, \ldots, X_k\}$

$$\hat{y} = \arg\max_y p(y \mid X_1, \ldots, X_k)$$ (Posterior)

(Prediction)

$$= \arg\max_y \frac{p(X_1, \ldots, X_k \mid y) \cdot p(y)}{p(X_1, \ldots, X_k)}$$ (by Bayes' rule)

Independent of y

Bayesian classification

What if **x** has multiple attributes $\mathbf{x} = \{X_1, \ldots, X_k\}$

$$\hat{y} = \arg\max_y p(y \mid X_1, \ldots, X_k)$$ (Posterior)

(Prediction)

$$= \arg\max_y \frac{p(X_1, \ldots, X_k \mid y) \cdot p(y)}{p(X_1, \ldots, X_k)}$$ (by Bayes' rule)

$$= \arg\max_y \; p(X_1, \ldots, X_k \mid y) \; p(y)$$

Class conditional likelihood

Class prior

Naïve Bayes Assumption

Conditional independence of feature attributes

$$p(X_1, \ldots, X_k \mid y)p(y) = \Pi_{i=1}^{k} p(X_i \mid y)p(y)$$

Easier to estimate

(using MLE!)

What we've learned today…

- K-Nearest Neighbors
- Maximum likelihood estimation
  - Bernoulli model
  - Gaussian model
- Naive Bayes
  - Conditional independence assumption

Thanks!