CS 540 Introduction to Artificial Intelligence

Classification - KNN and Naive Bayes

University of Wisconsin - Madison

Spring 2022

Today's outline

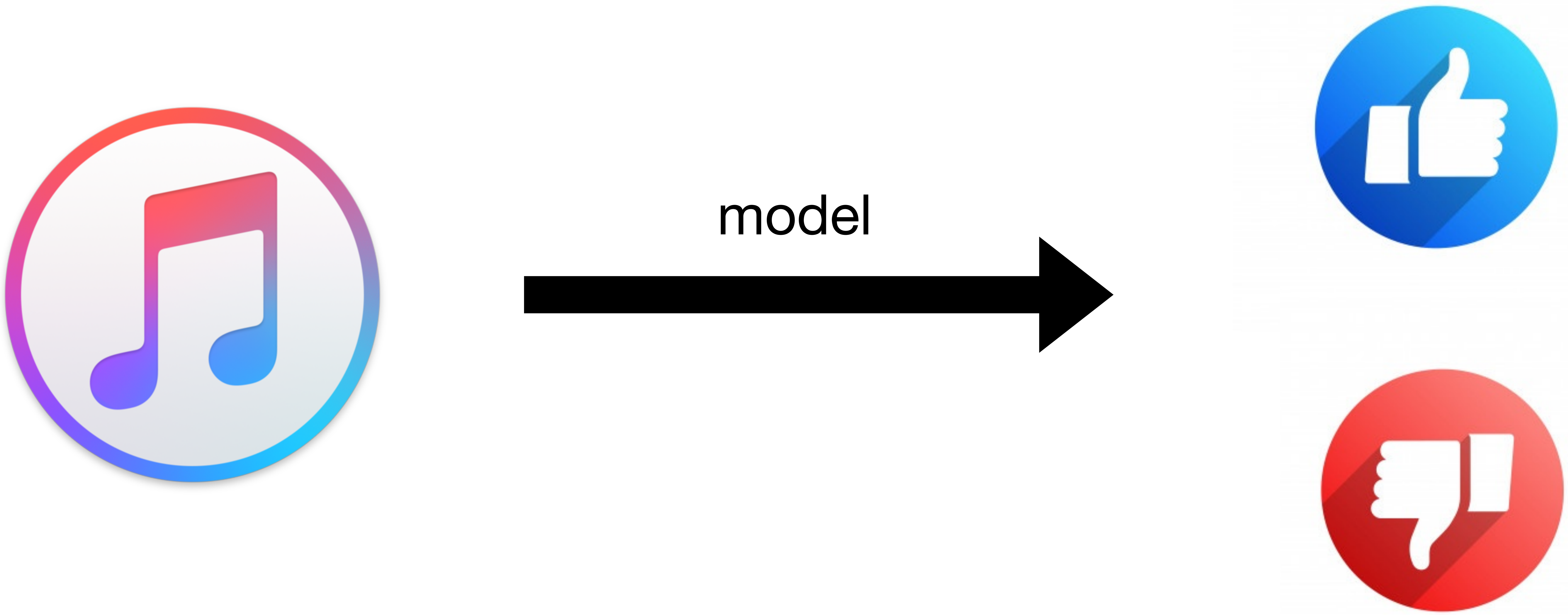
- K-Nearest Neighbors
- Maximum likelihood estimation
- Naive Bayes

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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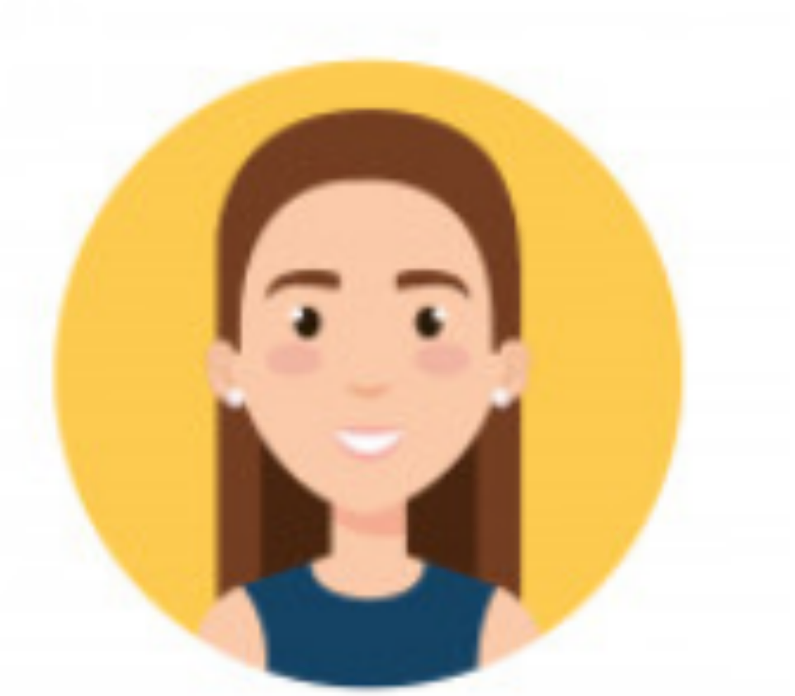
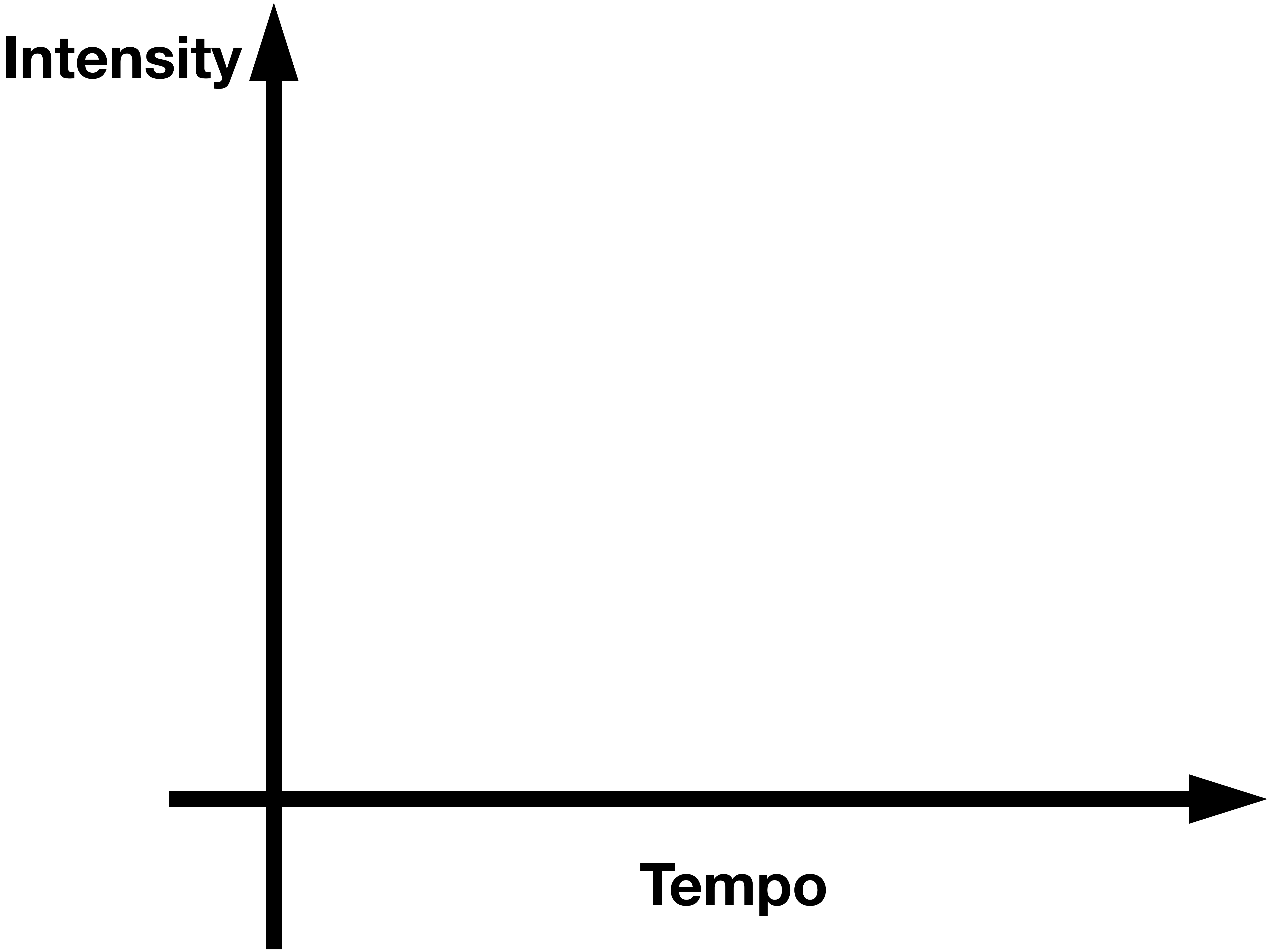


User Sharon



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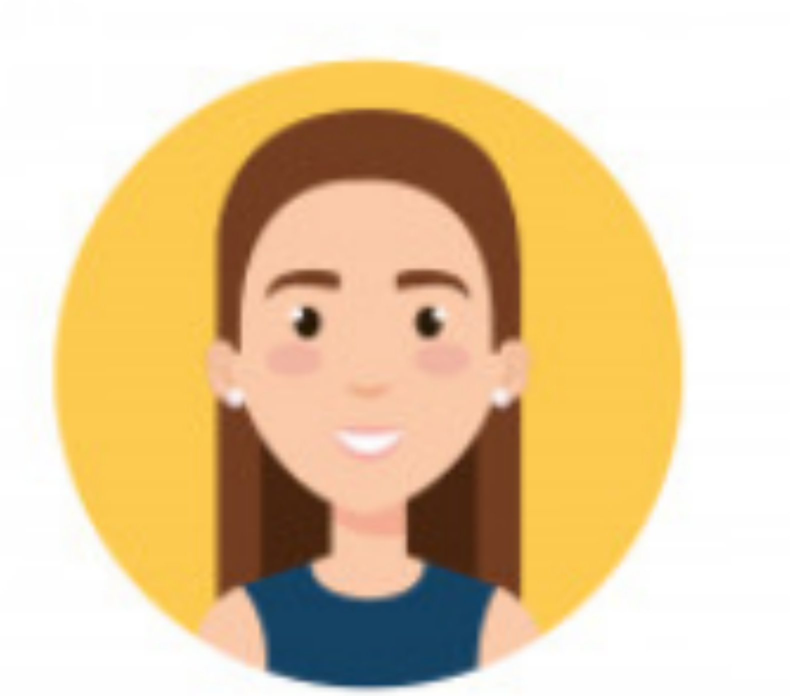
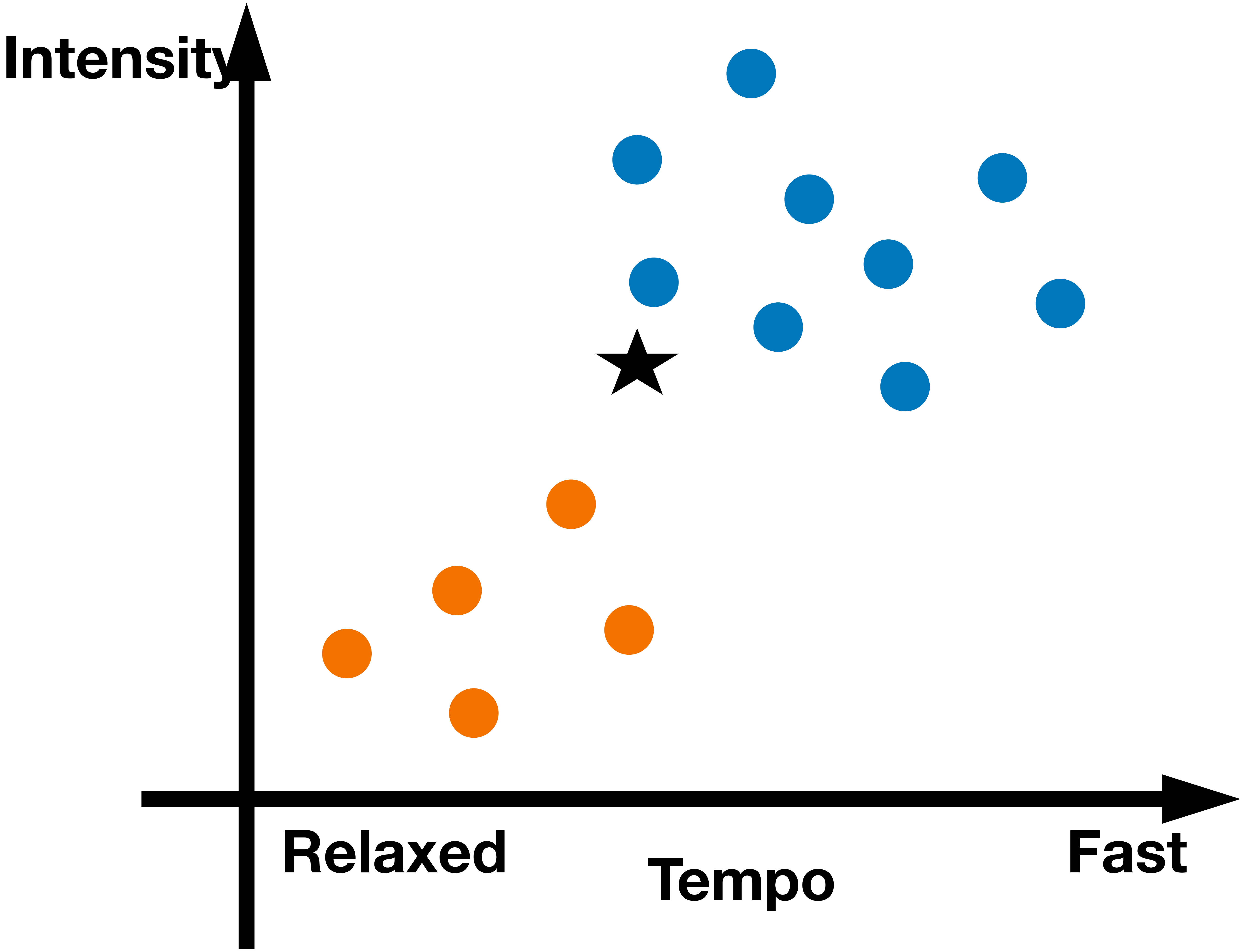
1-NN



User Sharon

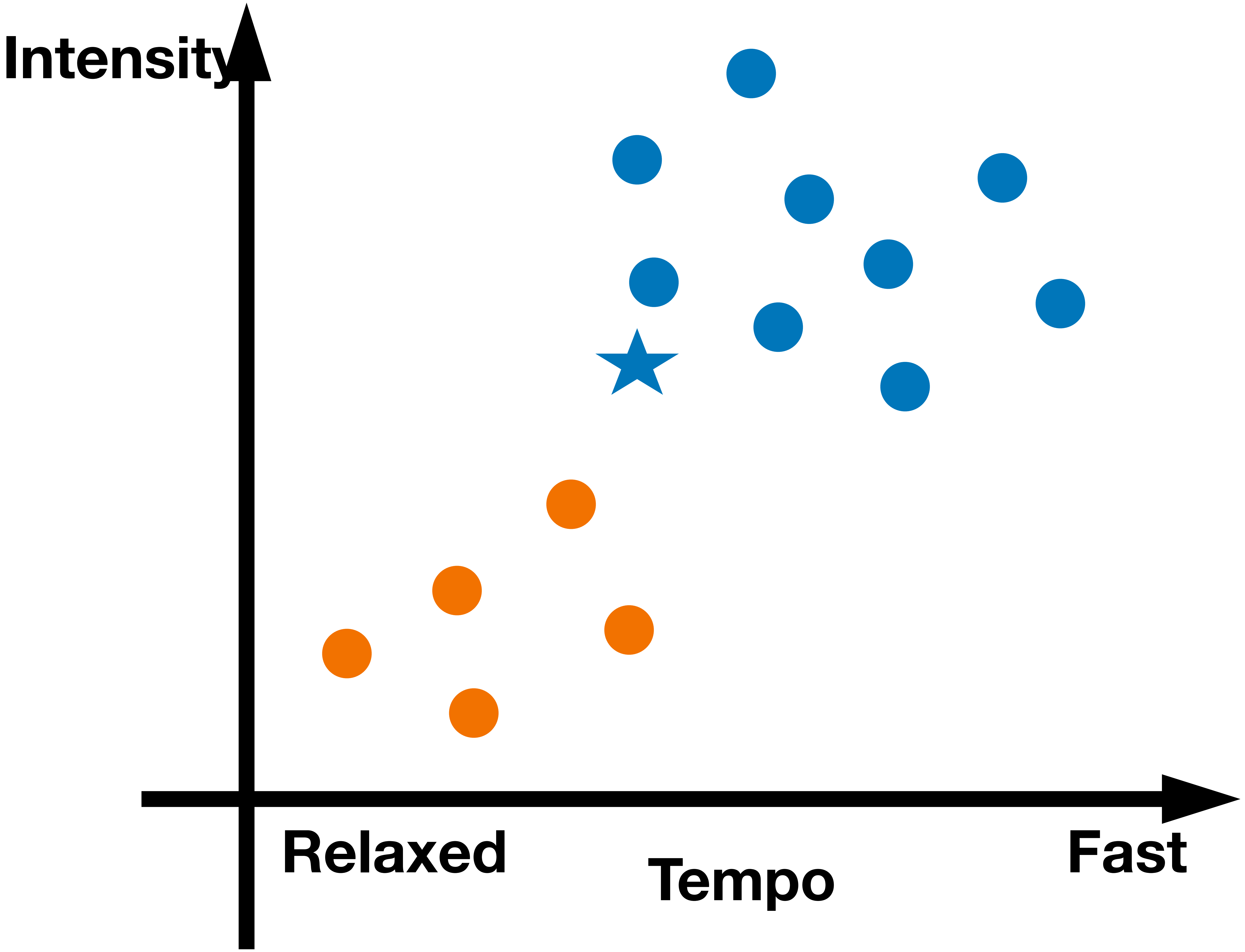
DisLike

Like



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

User Sharon



K-nearest neighbors for classification

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

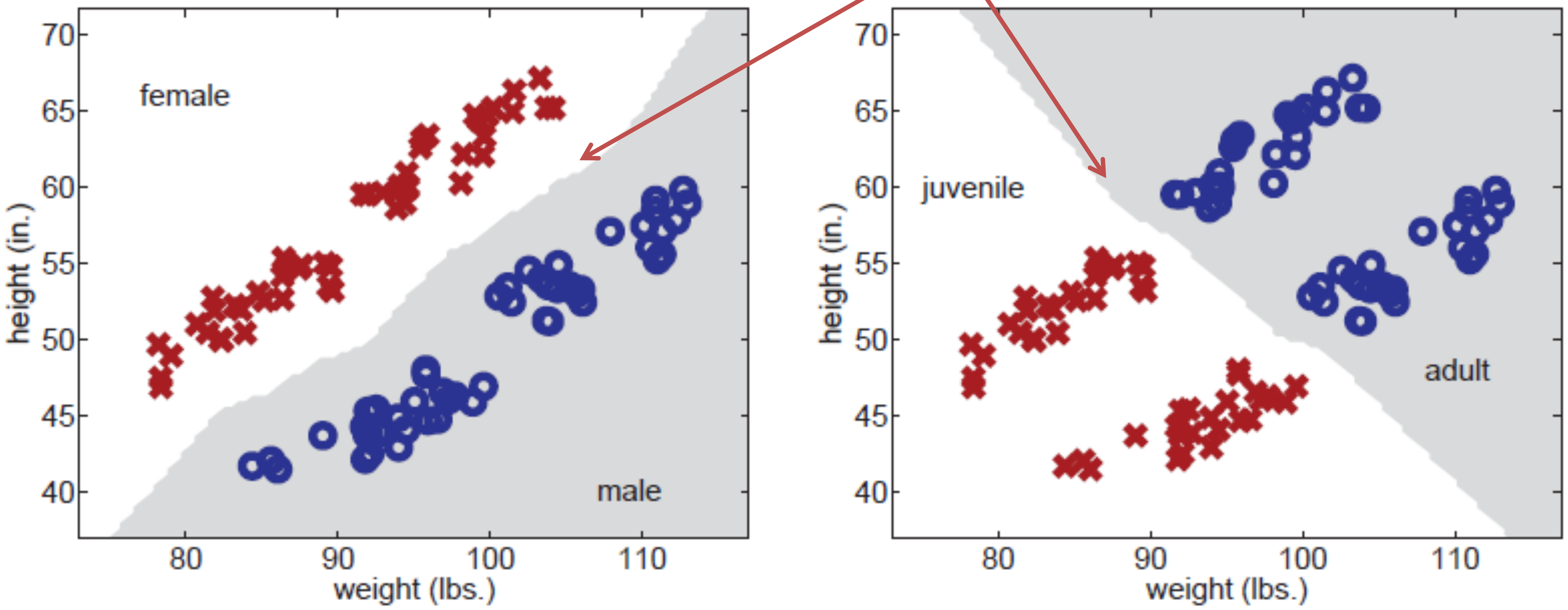
  Distance function $d(\mathbf{x}_i, \mathbf{x}_j)$; number of neighbors k; test data $\mathbf{x}^*$

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

Decision boundary

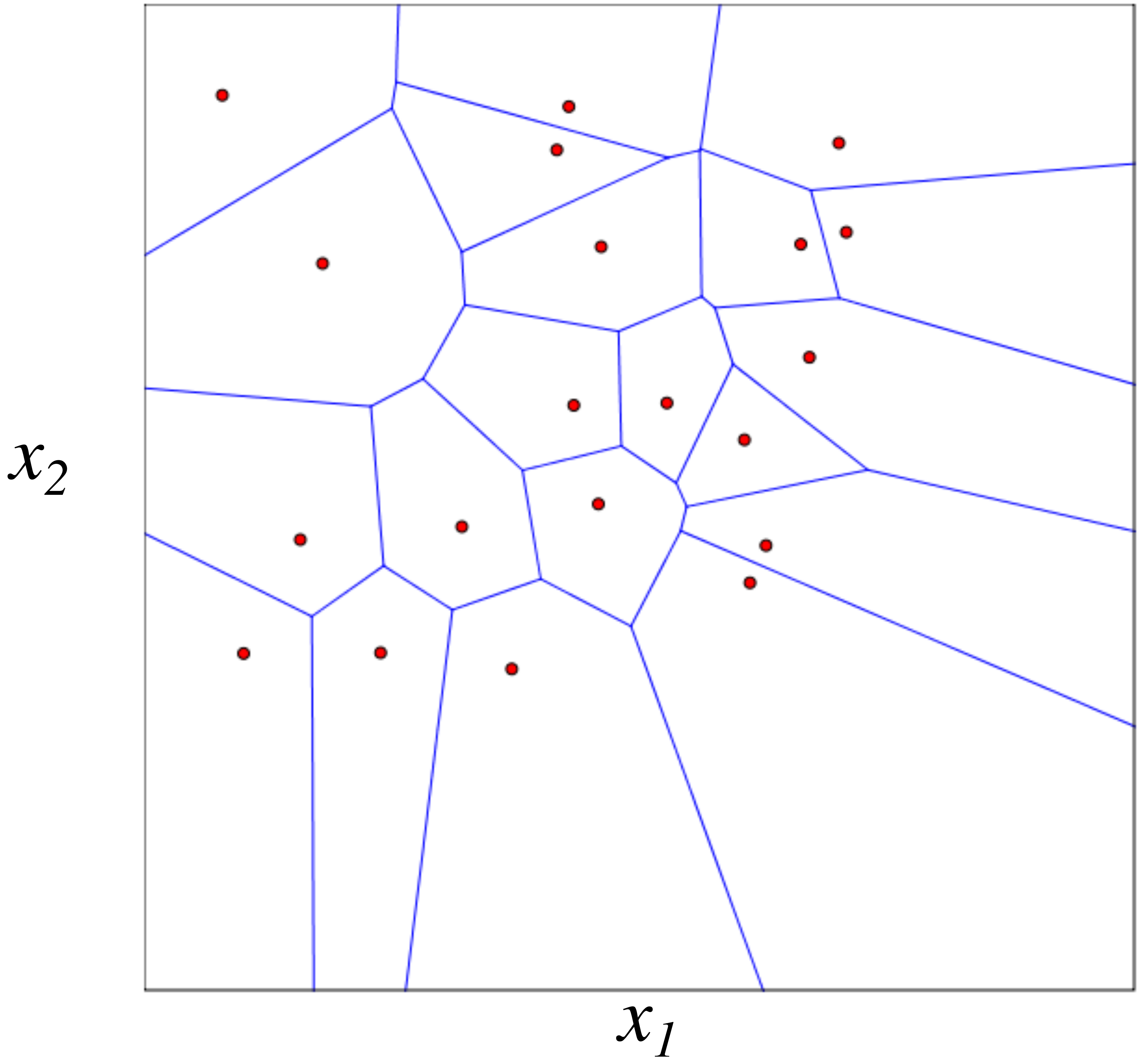


(a) classification by gender

(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 $\frac{1}{k}(y_{i_1} + \ldots + y_{i_k})$

What distance function to use?

- If all features are categorical (discrete and non-numerical): Hamming distance
  - Count the number of features different in the two items

What distance function to use?

- If all features are numerical: p-norm
  - 2-norm = Euclidean distance

$$d(x, x') = \|x - x'\|_2 = \sqrt{\sum_{i=1}^{d} (x_i - x_i')^2}$$

  - 1-norm = Manhattan distance

$$d(x, x') = \|x - x'\|_1 = \sum_{i=1}^{d} |x_i - x_i'|$$

  - General p-norm $(p \geq 1)$

$$d(x, x') = \|x - x'\|_p = \left(\sum_{i=1}^{d} |x_i - x_i'|^p \right)^{\frac{1}{p}}$$

What distance function to use?

- Be careful with scale
  - Same feature but different units may change relative distance (fixing other features)
  - Some times OK to normalize each feature dimension (z-score)

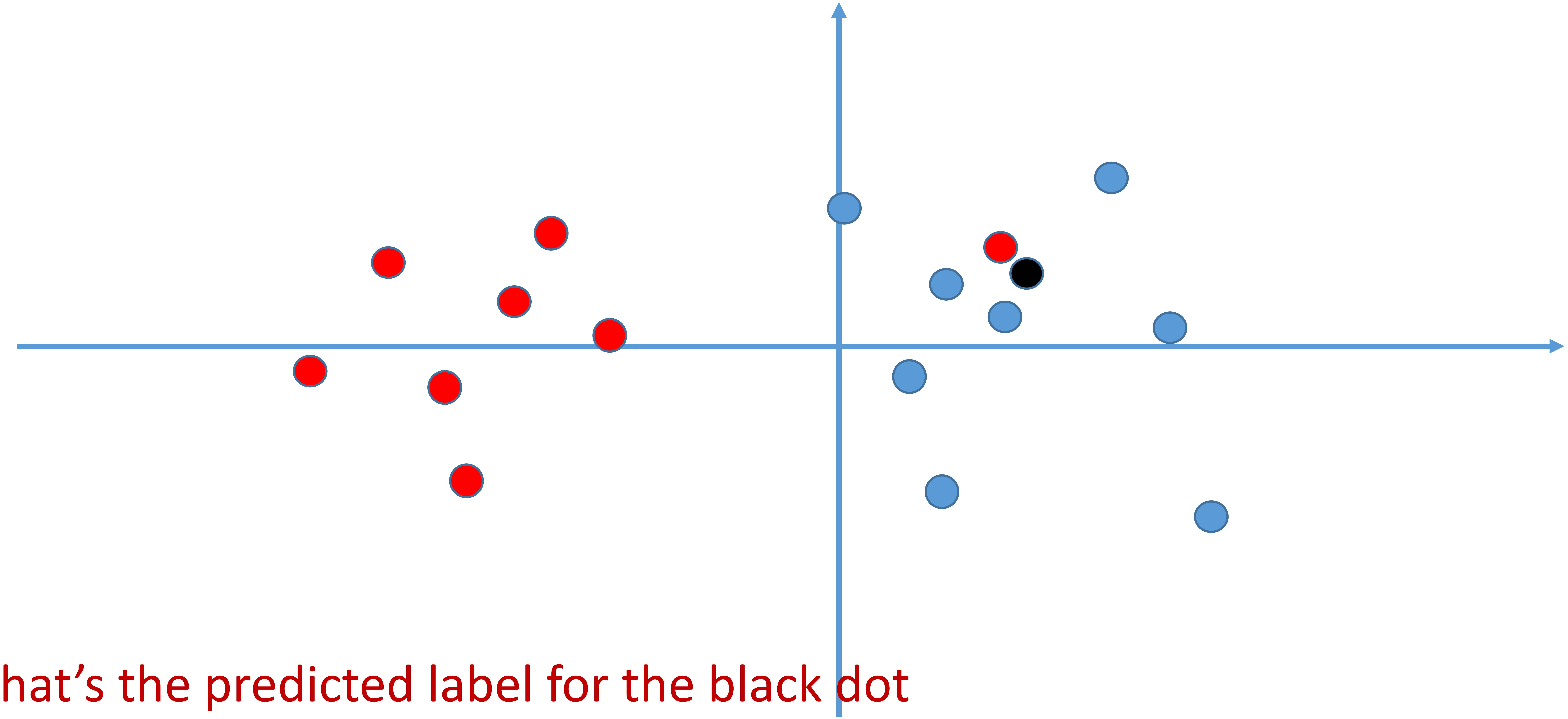
$$x'_{id} = \frac{x_{id} - \mu_d}{\sigma_d}, \forall i = 1 \dots n, \forall d$$

Training set mean for dimension d

Training set standard deviation for dimension d

  - Other times not OK: e.g. dimension contains small random noise

Effect of k



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

How to pick k the number of neighbors

- Randomly split data into **training**, **tuning**, **test sets**
- Classify tuning set with different k
- Pick k that produces least tuning-set error
- Report test-set error

(Shuffle whole dataset first)

Error and Accuracy for classification

Given training set $(x_1, y_1) \dots (x_n, y_n)$

Training set error = $\frac{1}{n} \sum_{i=1}^{n} 1_{[f(x_i) \neq y_i]}$

Similarly for tuning, test sets.

Accuracy = 1 - error

Quiz break

Q1-1: K-NN algorithms can be used for:

- A Only classification
- B Only regression
- C Both

Quiz break

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Q1-2: Which of the following distance measure do we use in case
categorical variables in k-NN?

- A Hamming distance
- B Euclidean distance
- C Manhattan distance

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Quiz break

Q1-3: Consider binary classification in 2D where the intended label of a point x = (x1, x2) is positive if x1>x2 and negative otherwise. Let the training set be all points of the form x = [4a, 3b] where a,b are integers. Each training item has the correct label that follows the rule above. With a 1NN classifier (Euclidean distance), which ones of the following points are labeled positive? Multiple answers.

- [5.52, 2.41]
- [8.47, 5.84]
- [7,8.17]
- [6.7,8.88]

Quiz break

Q1-3: Consider binary classification in 2D where the intended label of a point x = (x1, x2) is positive if x1>x2 and negative otherwise. Let the training set be all points of the form x = [4a, 3b] where a,b are integers. Each training item has the correct label that follows the rule above. With a 1NN classifier (Euclidean distance), which ones of the following points are labeled positive? Multiple answers.

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- [8.47, 5.84]
- [7,8.17]
- [6.7,8.88]

Nearest neighbors are
[4,3] => positive
[8,6] => positive
[8,9] => negative
[8,9] => negative
Individually.

Part II: Maximum Likelihood Estimation

Supervised Machine Learning

Non-parametric (e.g., KNN)	vs.	**Parametric**

Supervised Machine Learning

Statistical modeling approach

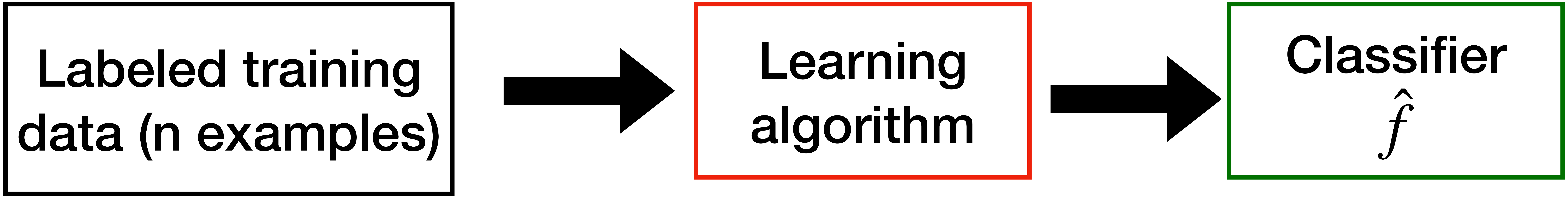
Labeled training data (n examples)

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

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)

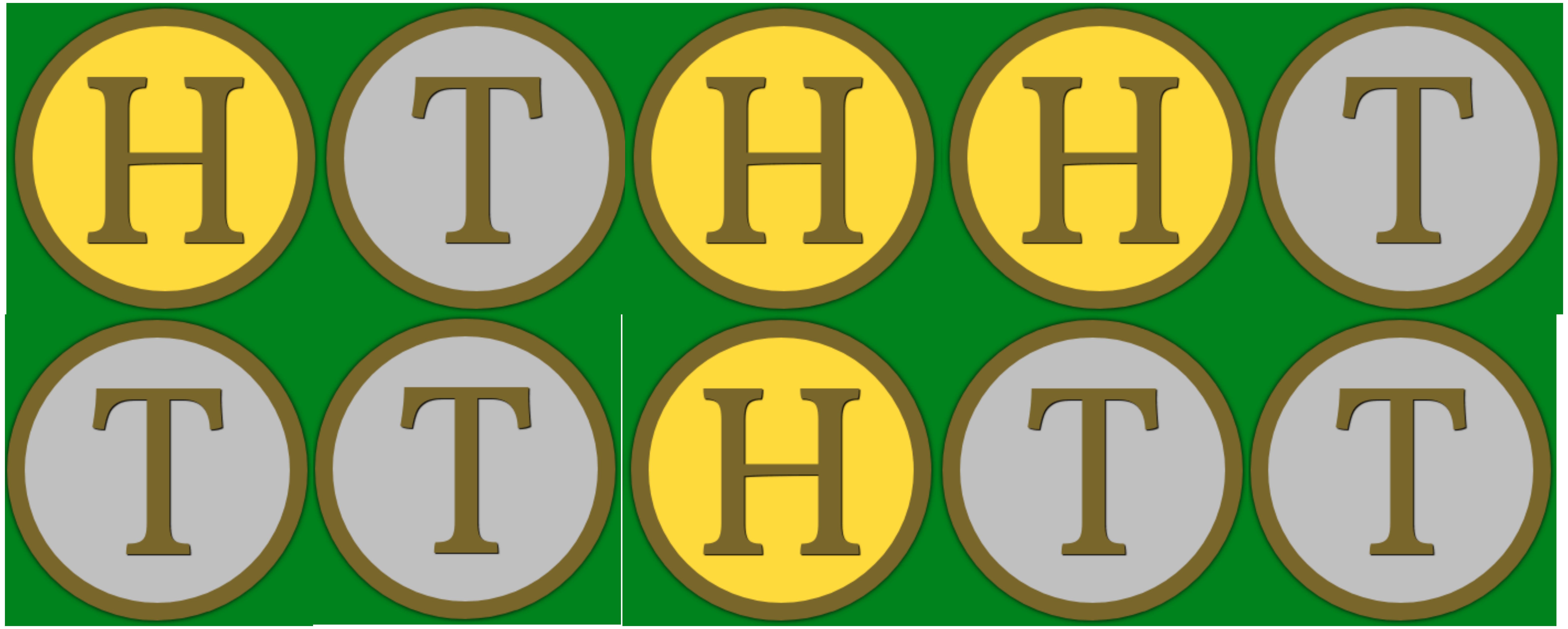
select $\hat{f}(\theta)$ from a pool of models $\mathcal{F}$
that **best describe the data observed**

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

- **Maximum likelihood (best fits the data)**
- Maximum a posteriori (best fits the data AND 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 $L(\theta) = \Pi_i p(\mathbf{x}_i \,|\, \theta)$

↑

Under i.i.d assumption

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

How good is θ?

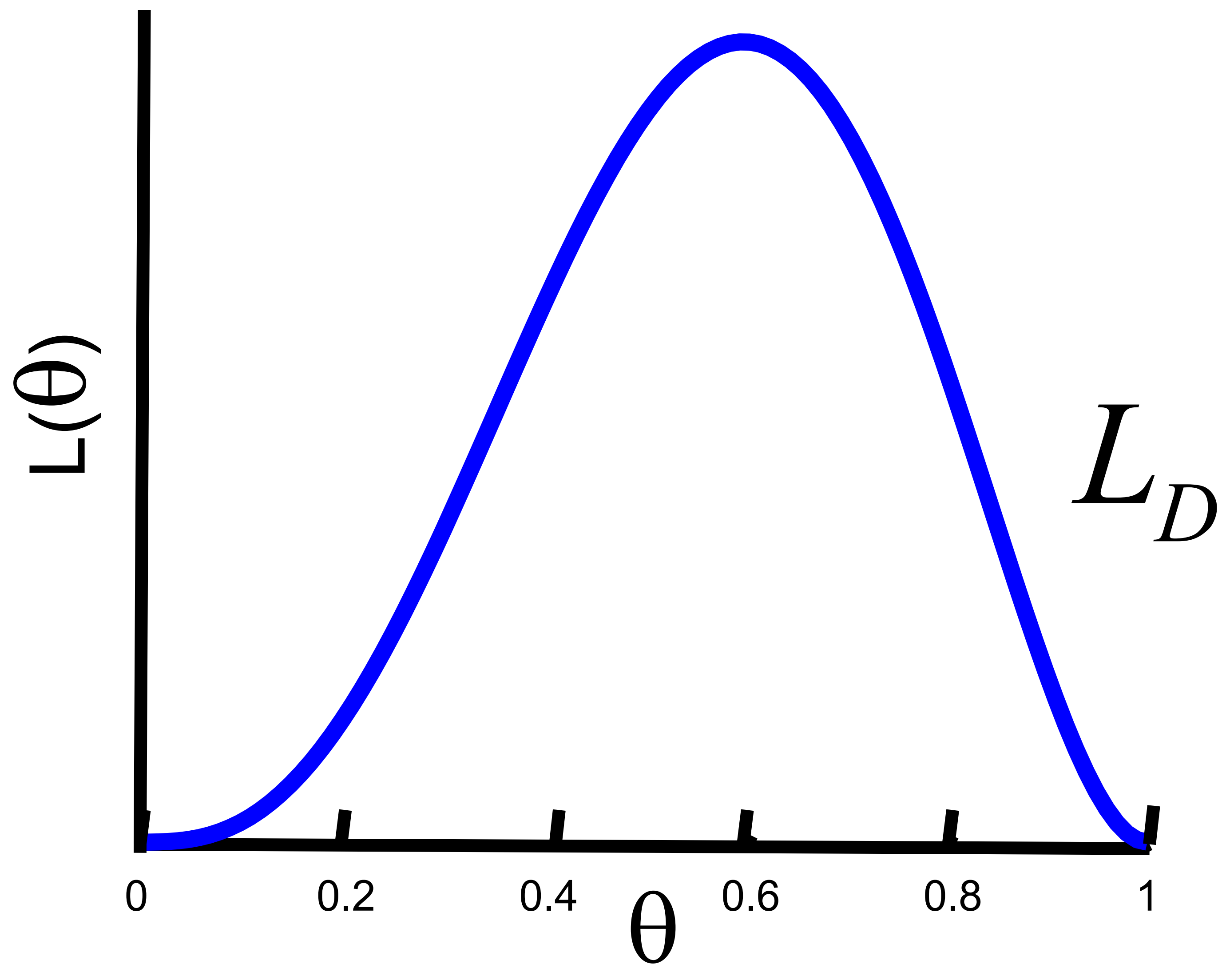
It depends on how likely it is to generate the observed data

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

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

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

which confirms your intuition!

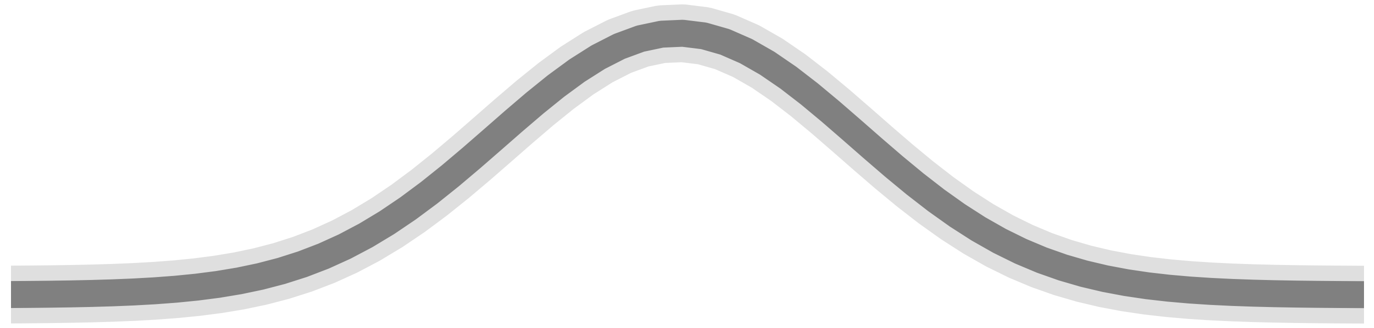
Maximum Likelihood Estimation: Gaussian Model

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**

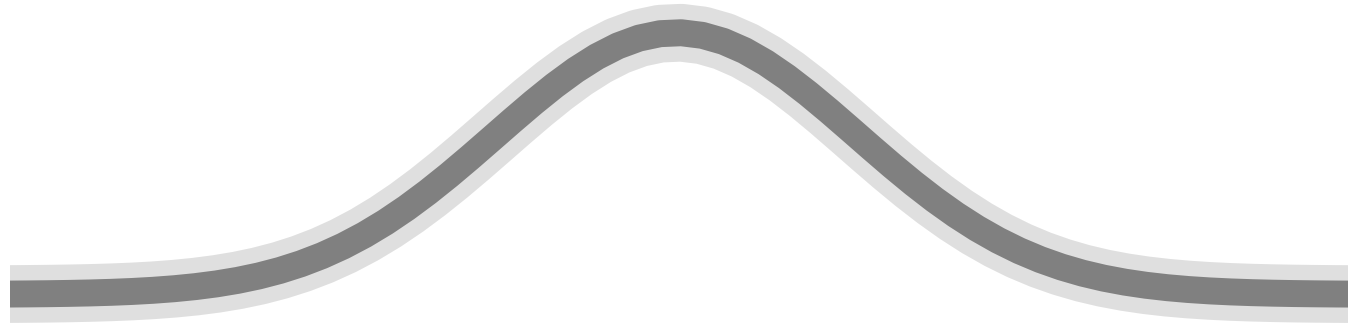
$$\sigma^2 = \mathbf{E}\left[(x-\mu)^2\right] \text{ hence } \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n} (x_i - \hat{\mu})^2$$

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

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

- **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

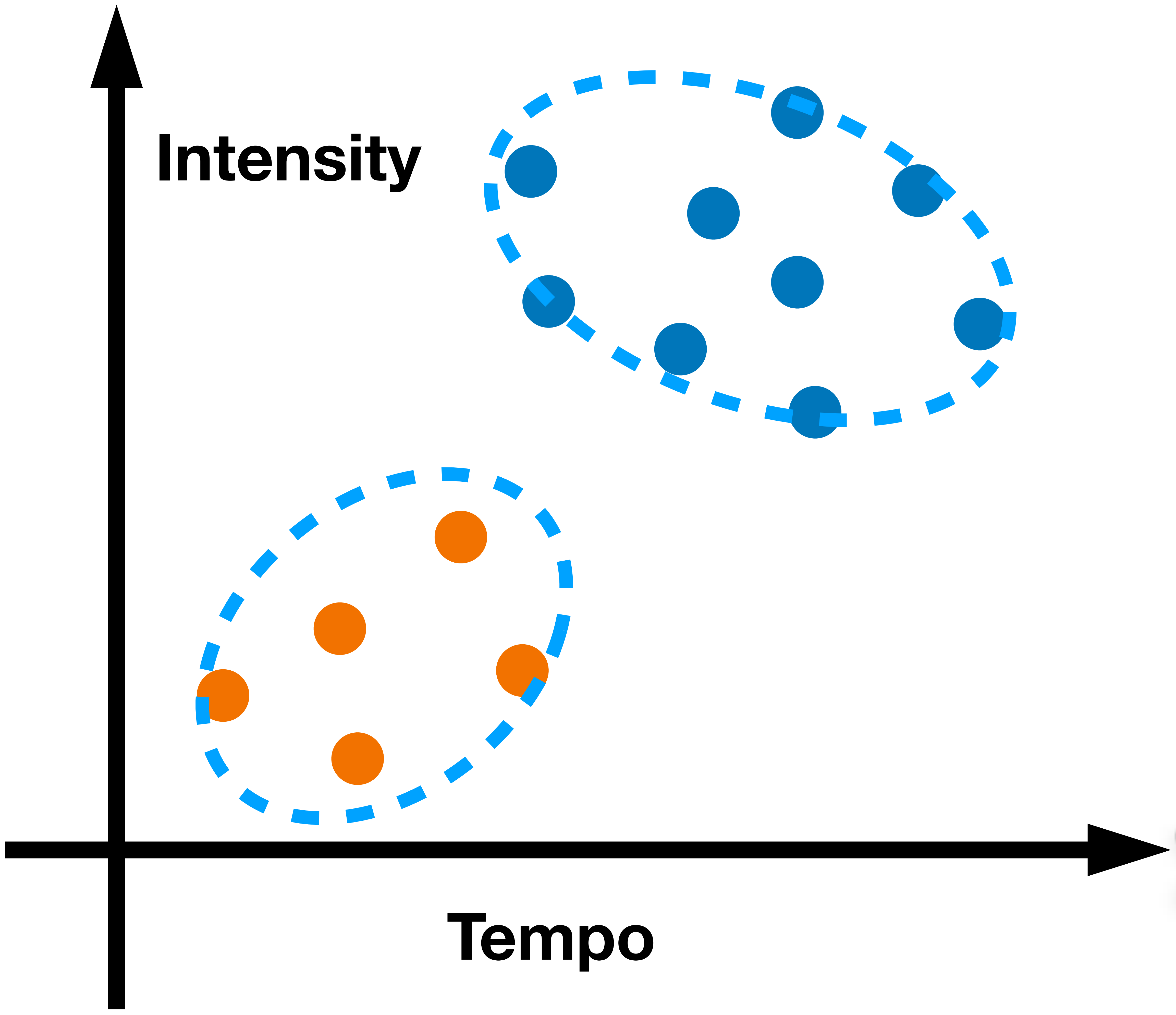
$$\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$

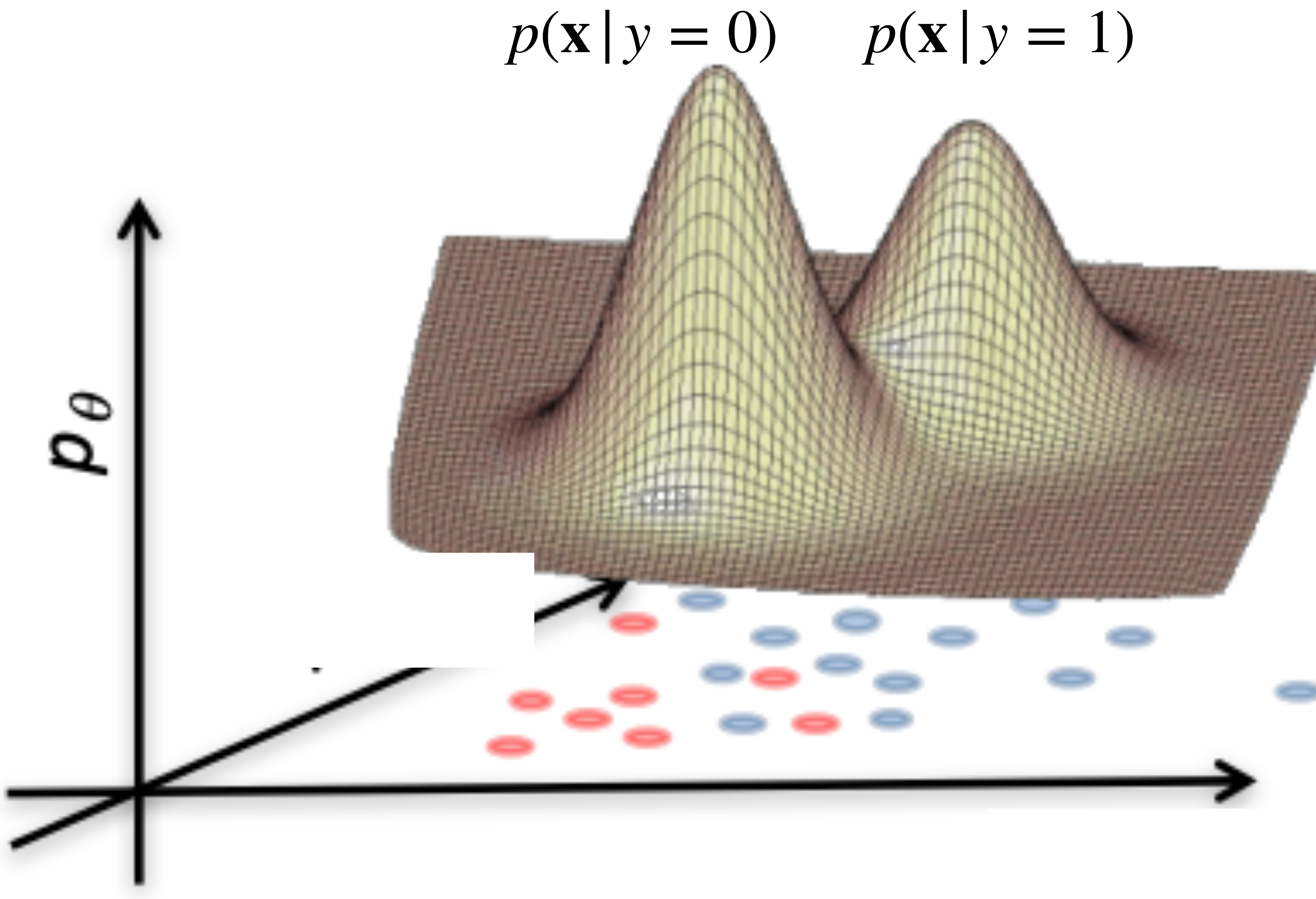
- Take derivatives with respect to it

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

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

Classification via Bayes rule and MLE





Classification via Bayes rule and MLE

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

(Posterior)

(Prediction)

Classification via MLE

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

(Prediction)

$$= \arg\max_{y} \frac{p(\mathbf{x} \,|\, y) \cdot p(y)}{p(\mathbf{x})}$$ (by Bayes' rule)

$$= \arg\max_{y} \; p(\mathbf{x} \,|\, y) p(y)$$

Using labelled training data, learn MLE **class priors** and **class conditionals, plug in to above**

Quiz break

Q2-2: True or False
Maximum likelihood estimation is the same regardless of whether we maximize the likelihood or log-likelihood function.

- A True
- B False

Quiz break

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- A True
- B False

Quiz break

Q2-3: Suppose the weights of randomly selected American female college students are normally distributed with unknown mean μ and standard deviation σ. A random sample of 10 American female college students yielded the following weights in pounds: 115 122 130 127 149 160 152 138 149 180. Find a maximum likelihood estimate of μ.

- A 132.2
- B 142.2
- C 152.2
- D 162.2

Quiz break

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Part III: 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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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}
- Play = {Yes, No}
- Observed data {Weather, play on day *m*}, m={1,2,…,N}

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!

Classification via Bayes rule

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

(Prediction)

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

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

Classification via Bayes rule

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 $\mathbf{x} = \{X_1, \ldots, X_k\}$

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

(Prediction)

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

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

Class conditional likelihood

Class prior

Naïve Bayes Assumption

Assume 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!)

Quiz break

Q3-1: Which of the following about Naive Bayes is incorrect?

- A Attributes can be nominal or numeric
- B Attributes are equally important
- C Attributes are statistically dependent of one another given the class value
- D Attributes are statistically independent of one another given the class value
- E All of above

Quiz break

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Quiz break

Q3-2: Consider a classification problem with two binary features, $x_1, x_2 \in \{0,1\}$. Suppose $P(Y = y) = 1/32$, $P(x_1 = 1 | Y = y) = y/46$, $P(x_2 = 1 | Y = y) = y/62$. Which class will naive Bayes classifier produce on a test item with $x_1 = 1$ and $x_2 = 0$?

- A 16
- B 26
- C 31
- D 32

Quiz break

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Quiz break

Q3-3: Consider the following dataset showing the result whether a person has passed or failed the exam based on various factors. Suppose the factors are independent to each other. We want to classify a new instance with Confident=Yes, Studied=Yes, and Sick=No.

Confident	Studied	Sick	Result
Yes	No	No	Fail
Yes	No	Yes	Pass
No	Yes	Yes	Fail
No	Yes	No	Pass
Yes	Yes	Yes	Pass

- A Pass
- B Fail

Quiz break

Q3-3: Consider the following dataset showing the result whether a person has passed or failed the exam based on various factors. Suppose the factors are independent to each other. We want to classify a new instance with Confident=Yes, Studied=Yes, and Sick=No.

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Yes	No	No	Fail
Yes	No	Yes	Pass
No	Yes	Yes	Fail
No	Yes	No	Pass
Yes	Yes	Yes	Pass

- A Pass
- B Fail

What we’ve learned today…

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