Geo Data Science

Logistic Regression

Prof. Dr. Martin Kada

Chair Methods of Geoinformation Science (GIS)
Institute of Geodesy and Geoinformation Science

Technische Universität Berlin

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Content of this Lecture

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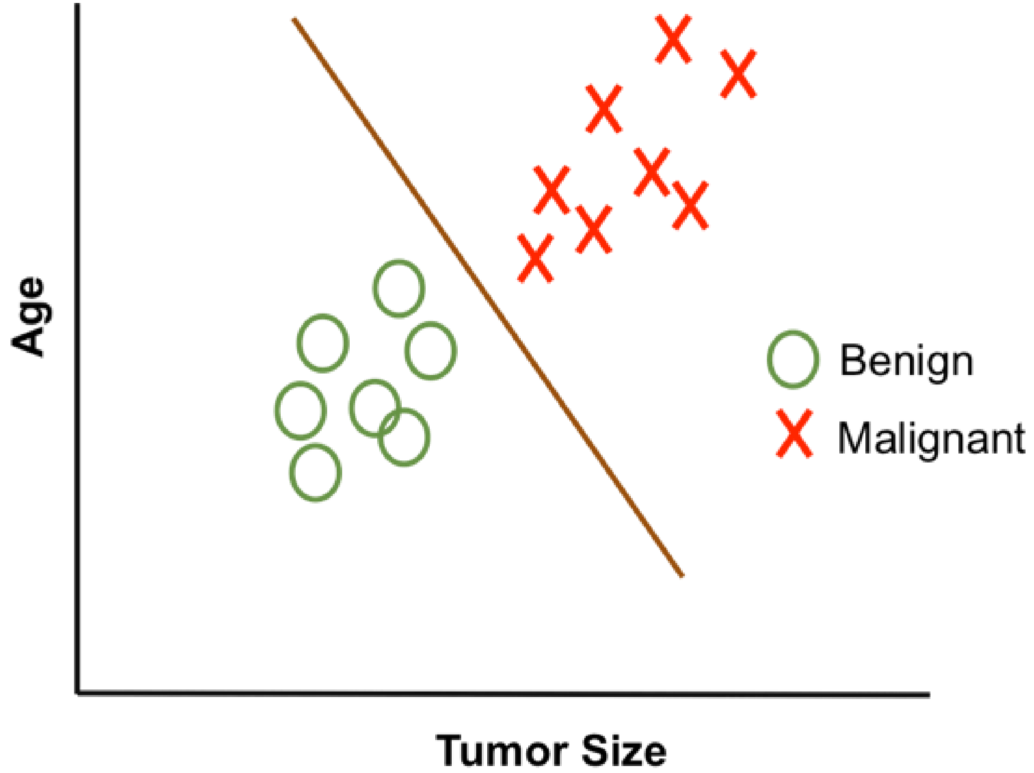
- Linear Regression
- Polynomial Regression
- Regularized Linear Models

regression

- Logistic Regression
- Multinomial Regression

classification: binary, multi-class

Content of this Lecture



- Learn a model by finding a (straight) line that separates the (two) classes
- Predict the class by determining in which region your unseen input dataset lies

Logistic Regression

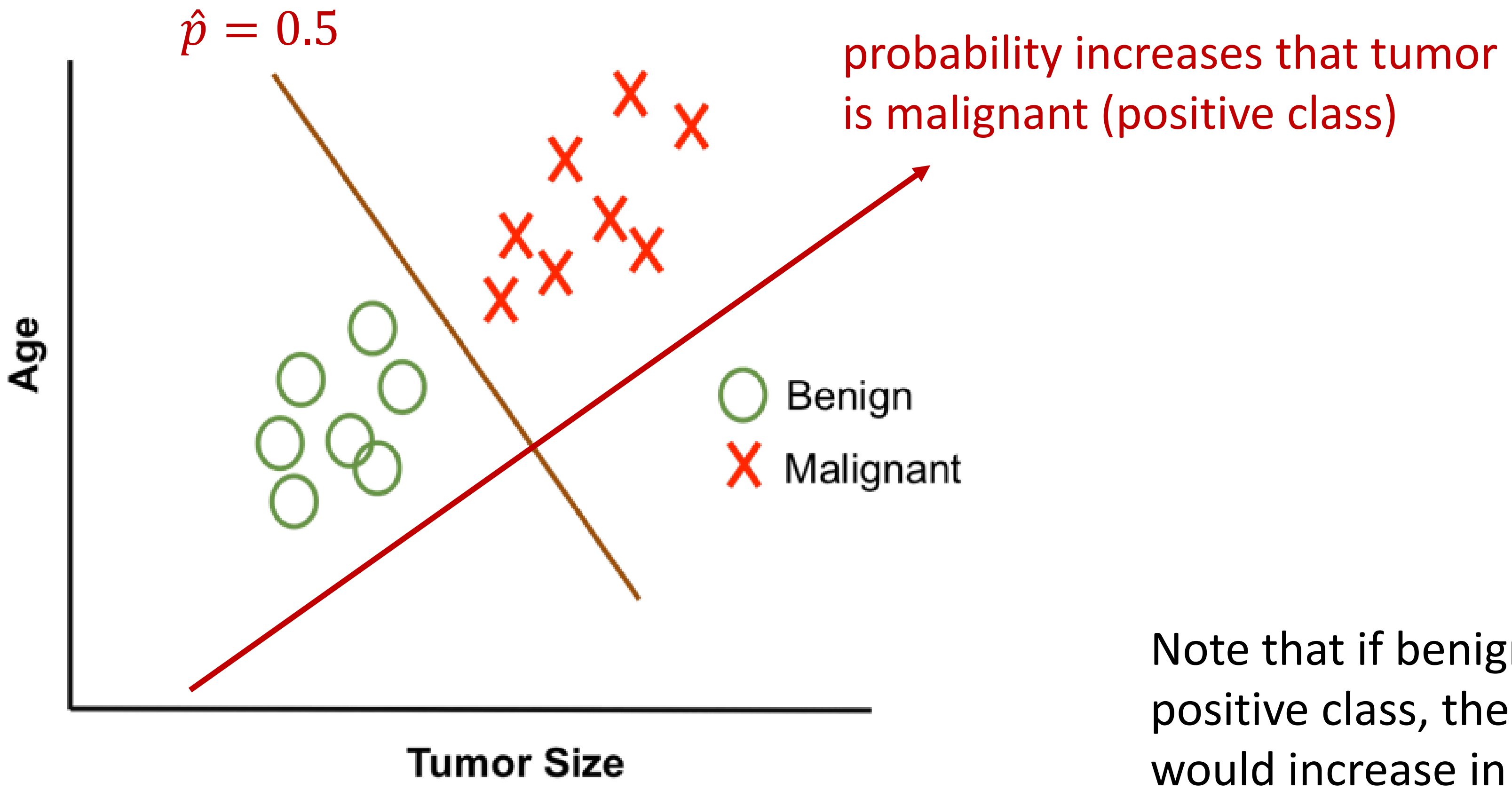
- Logistic Regression (also called Logit Regression) estimates the probability $\hat{p}$ that a data instance belongs to a particular class
  - Estimated probability $\hat{p}$ is greater or equal than 50%
    $\longrightarrow$ instance belongs to this class (positive class, labeled "1")
  - Estimated probability $\hat{p}$ is lesser than 50%
    $\longrightarrow$ instance does not belong to this class (negative class, labeled "0")

$\longrightarrow$ binary classifier

$$\hat{y} = \begin{cases} 1 & \text{if} \quad \hat{p} \geq 0.5 \\ 0 & \text{if} \quad \hat{p} < 0.5 \end{cases}$$

predicted class

Logistic Regression



Note that if benign would be the positive class, then the probabilities would increase in the opposite direction

Estimating Probabilities

- Compute the weighted sum of the input features (plus a bias term) and output the logistic of this result

$$\hat{p} = h_\theta(\mathbf{x}) = \underset{\substack{\uparrow \\ \text{logistic} \\ \text{function}}}{\sigma}(\theta^T \cdot \mathbf{x})$$

Estimating Probabilities

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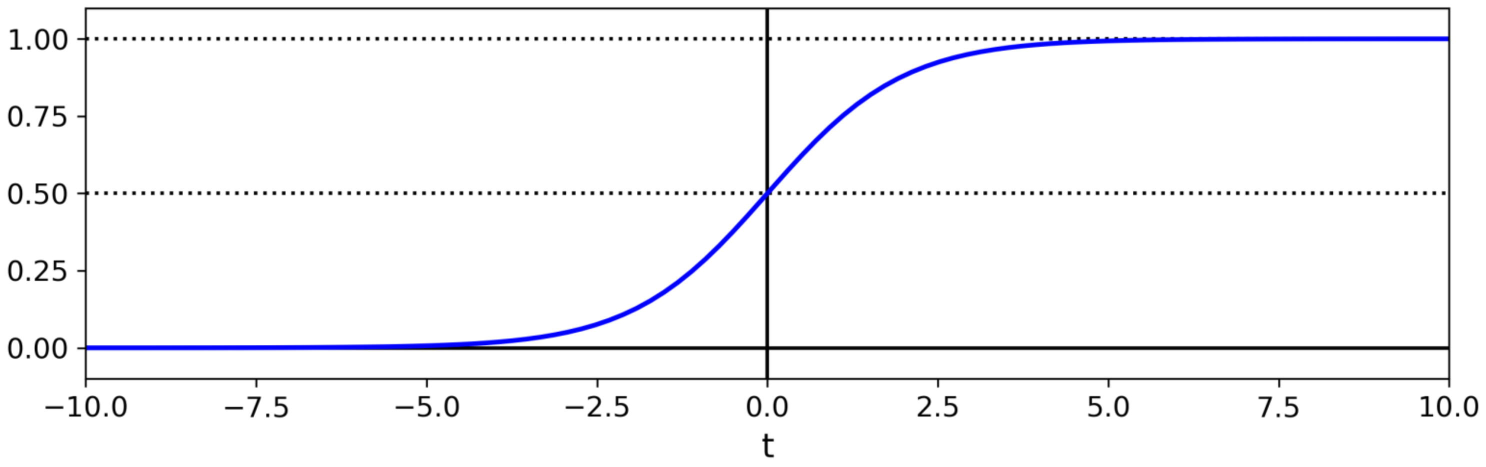
- Logistic function (also called logic) is a sigmoid function that outputs a number between 0 and 1:

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$



Logistic Regression

$$\begin{bmatrix}\theta_0 & \theta_1 & \theta_2 & \dots & \theta_n\end{bmatrix} \begin{bmatrix}1\\ x_1\\ x_2\\ \dots\\ x_n\end{bmatrix} = s \xrightarrow{\sigma(s)} \hat{p} \longrightarrow \hat{y}$$

sometimes called
a score

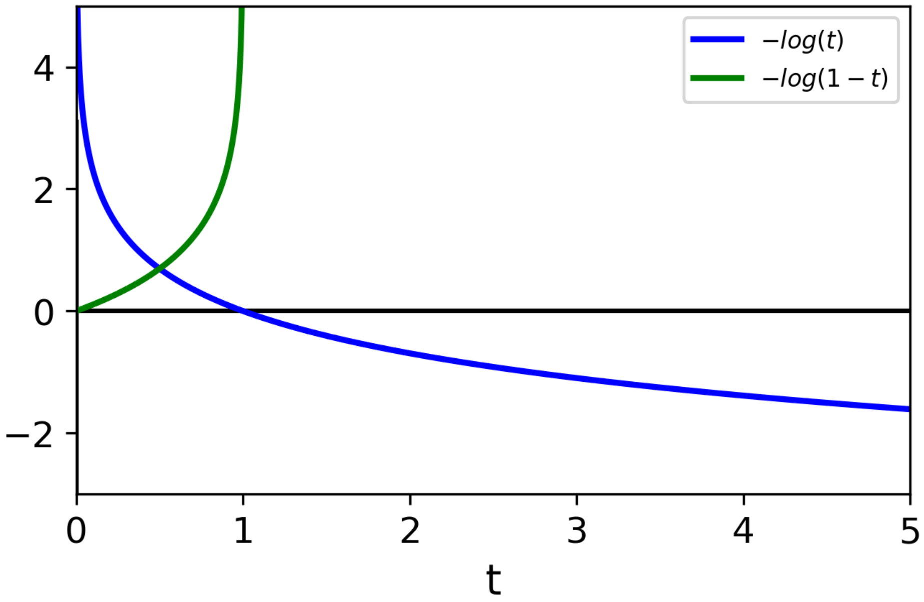
$$\hat{y} = \begin{cases}1 & \text{if } \hat{p} \geq 0.5\\ 0 & \text{if } \hat{p} < 0.5\end{cases}$$

Training and Cost Function

- Learn parameter vector θ so that the model estimates
  - High probabilities for positive instances ($y = 1$)
  - Low probabilities for negative instances ($y = 0$)

- Cost function for a single training instance:

$$c(\theta) = \begin{cases} -\log(\hat{p}) & \text{if } y = 1 \\ -\log(1 - \hat{p}) & \text{if } y = 0 \end{cases}$$



  - By using $-\log(t)$ the cost grows very large if the model estimates a probability close to 0 (or 1) for a positive (or negative) instance
  - $-\log(t)$ is close to 0 for correct estimates

Training and Cost Function

- Cost function over the whole training set (with m data items):

$$J(\theta) = -\underbrace{\frac{1}{m}\sum_{i=1}^{m}}_{\text{average}}\Big[\underbrace{y^{(i)}\log\big(\hat{p}^{(i)}\big)}_{\substack{\text{positive class}\\(y^{(i)}=1)}} + \underbrace{\big(1-y^{(i)}\big)\log\big(1-\hat{p}^{(i)}\big)}_{\substack{\text{negative class}\\(y^{(i)}=0)}}\Big]$$

  - There is no closed-form equation to compute the value of θ that minimizes $J(\theta)$
  - Note that superscript i (e.g. $y^{(i)}$) refers to the i^{th} data item

Training and Cost Function

- Cost function $J(\theta)$ is convex $\longrightarrow$ Gradient Descent finds global optimum

- Partial derivatives of cost function w.r.t. the j^{th} model parameter θ_j:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(\sigma\left(\theta^T \cdot \mathbf{x}^{(i)}\right) - y^{(i)} \right) x_j^{(i)}$$

- Compute the gradient vector that contains all the partial derivatives and use it in the Batch Gradient Descent algorithm

Iris Flower Data Set

- 50 samples from each of three species of Iris
  - Four features: length and width of sepals and petals (in centimeters)

Iris versicolor

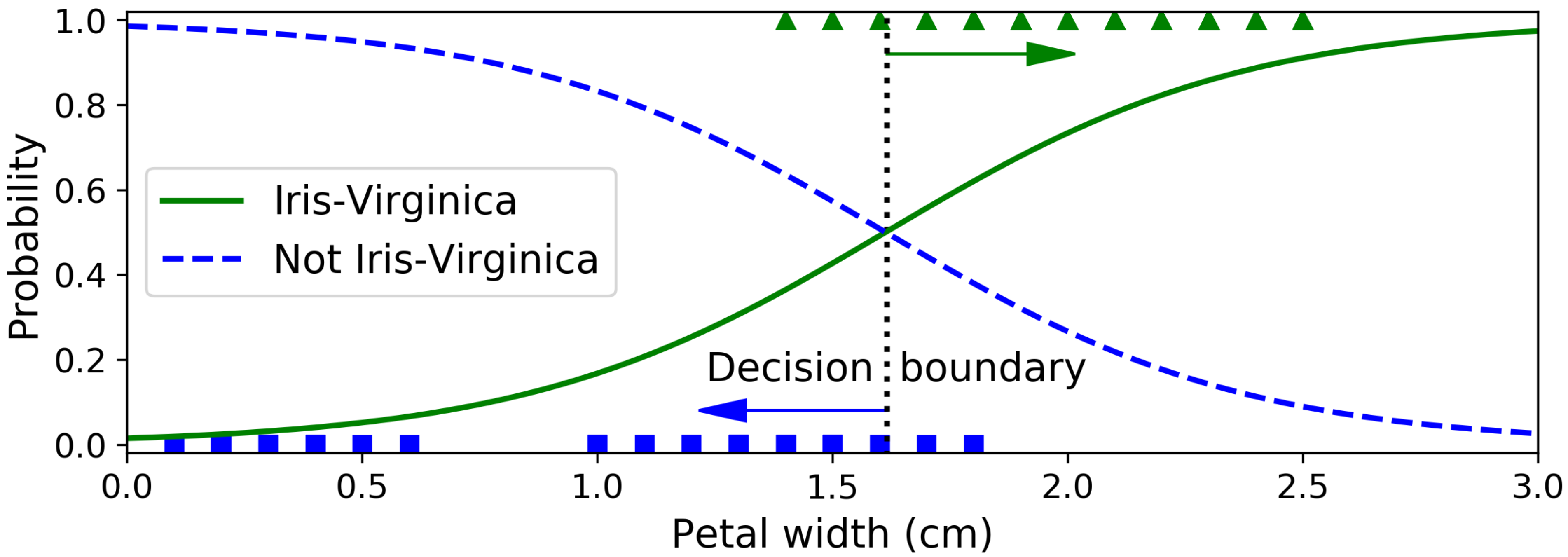
Iris virginica

Iris setosa

  - Ronald Fisher developed 1936 a linear discriminant model to distinguish the species from each other

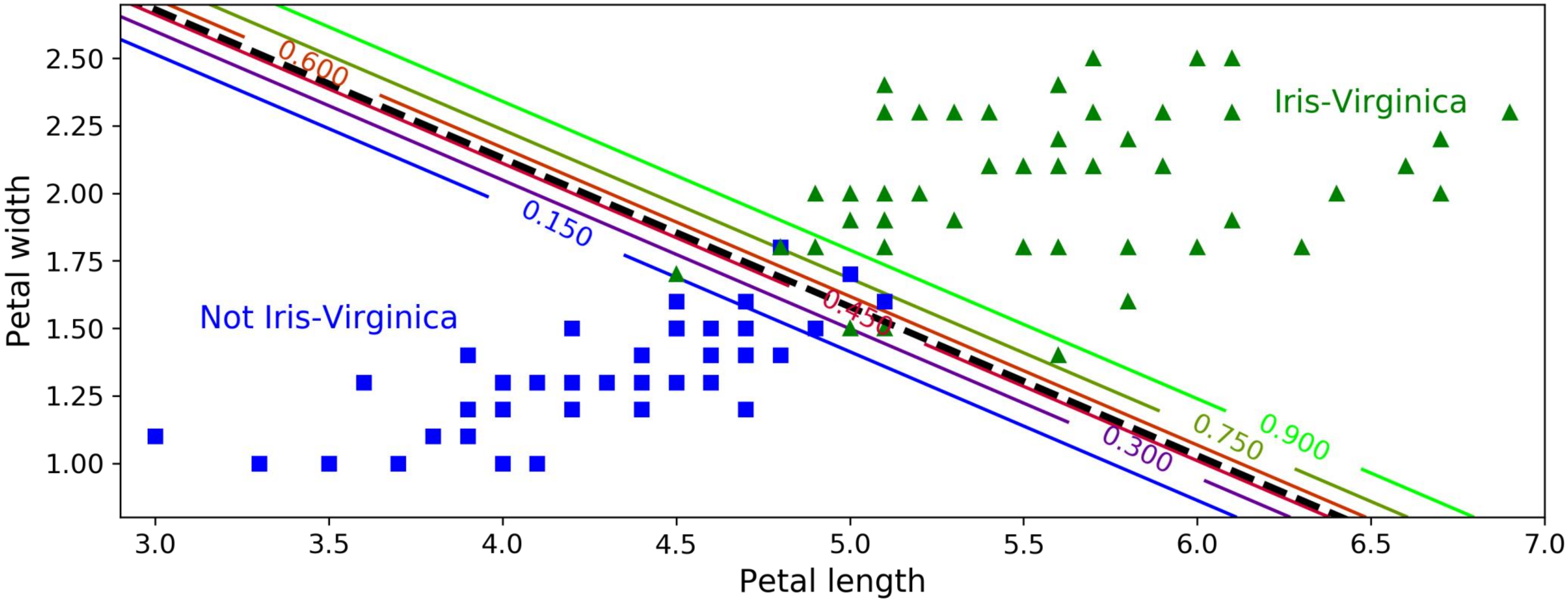
Decision Boundaries

- Decision boundary of model with 1 input feature (petal width)



Linear Decision Boundary

- Decision boundary of model with 2 input features (petal width & length)



Multinomial Logistic Regression

- Multinomial Logistic Regression (also called Softmax Regression)
  - Generalization of Logistic Regression to multiple classes

1. Compute a score $s_k(\mathbf{x})$ for each class k from given feature instance $\mathbf{x}$

$$s_k(\boldsymbol{x}) = \left(\theta^{(k)}\right)^T \cdot \mathbf{x}$$

2. Apply the **softmax function** (also called normalized exponential) to each score to estimate the probability of each class

$$\hat{p}_k = \sigma\big(s(\mathbf{x})\big)_k = \frac{e^{(s_k(\mathbf{x}))}}{\sum_{j=1}^{K} e^{(s_j(\mathbf{x}))}}$$

exponential score

normalization

Multinomial Logistic Regression

- Predicts the class with the highest estimated probability (highest score)

$$\hat{y} = \underset{k}{\operatorname{argmax}}\, \sigma\big(s(\mathbf{x})\big)_k = \underset{k}{\operatorname{argmax}}\, s_k(\mathbf{x}) = \underset{k}{\operatorname{argmax}} \left(\left(\theta^{(k)}\right)^T \cdot \mathbf{x}\right)$$

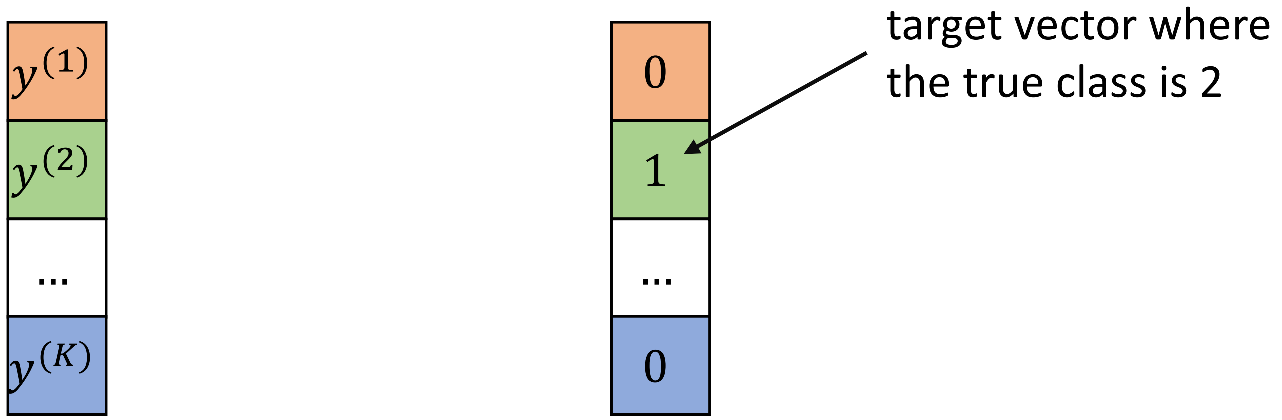
the argmax operator returns the value of the variable k (index) that maximizes the function

Multinomial Logistic Regression

$$\begin{bmatrix} \theta_0^{(1)} & \theta_1^{(1)} & \theta_2^{(1)} & \dots & \theta_n^{(1)} \\ \theta_0^{(2)} & \theta_1^{(2)} & \theta_2^{(2)} & \dots & \theta_n^{(2)} \\ \dots & \dots & \dots & \dots & \dots \\ \theta_0^{(K)} & \theta_1^{(K)} & \theta_2^{(K)} & \dots & \theta_n^{(K)} \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} = \begin{bmatrix} s^{(1)} \\ s^{(2)} \\ \dots \\ s^{(K)} \end{bmatrix} \xrightarrow{\sigma(s(\mathbf{x}))_k} \begin{bmatrix} \hat{p}^{(1)} \\ \hat{p}^{(2)} \\ \dots \\ \hat{p}^{(K)} \end{bmatrix} \xrightarrow[\underset{k}{\operatorname{argmax}}]{} \boxed{\hat{y}}$$

Multinomial Logistic Regression

- A training instance is typically given in one-hot-encoding, where all values are 0 with the exception of the true class, which is given as 1



Multinomial Logistic Regression

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- Careful as the meaning of the superscript changes from here on!
- In previous slides, superscript is used for the class, e.g. $\hat{p}^{(2)}$ for the probability of the second class
- In the following slides, the superscript is used for the training instance, e.g. $\hat{p}^{(3)}$ for the data instance 3 (of the training data)
- And the subscript is now used for the class, e.g. $\hat{p}_2^{(3)}$ for the probability of the second class for the data instance 3

Multinomial Logistic Regression

- Objective of training:
  - A model that estimates a high probability for the target (correct) class and low probabilities for the other classes

- **Cross entropy** cost function:

$y_k^{(i)}$ is equal to 1 if the target class for the ith instance is k; otherwise 0

$$J(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log\left(\hat{p}_k^{(i)}\right)$$

  - Measures how well a set of estimated class probabilities match the target class
    - Penalizes the model when it estimates a low probability for the target class
  - Is equivalent to the Logistic Regression's cost function (log loss) for $K = 2$

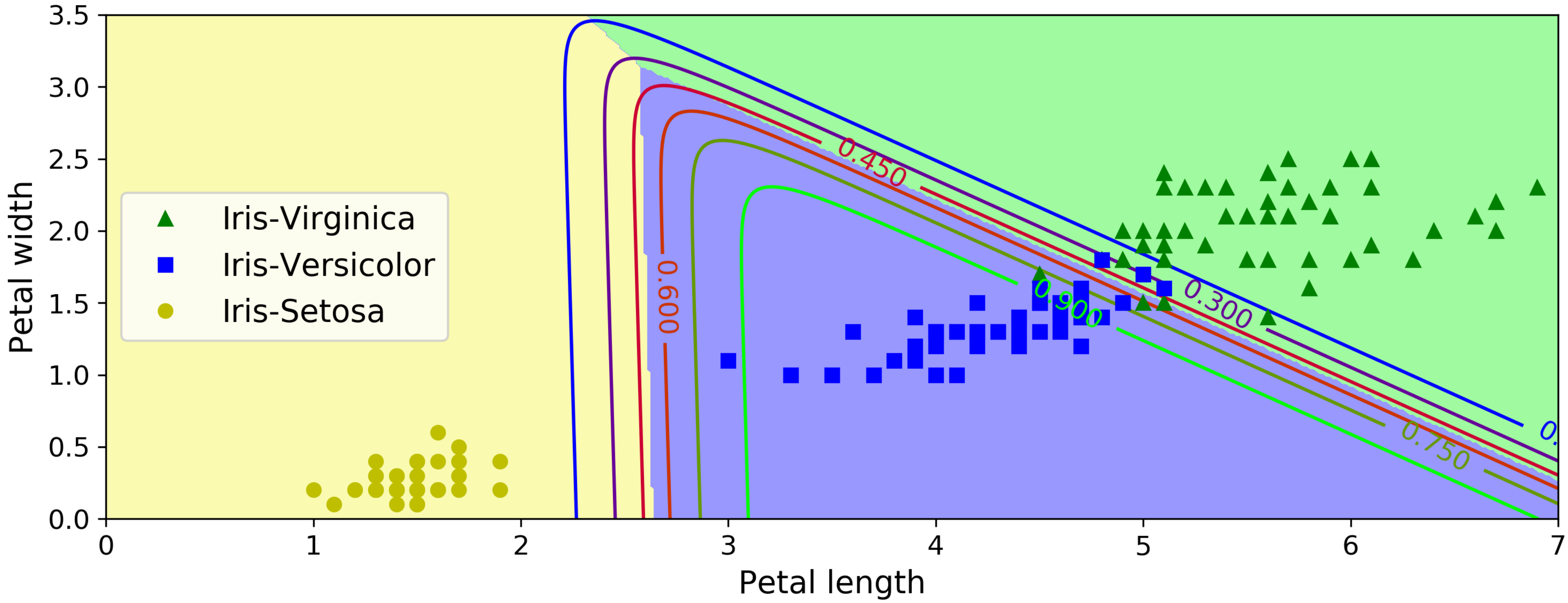
Multinomial Logistic Regression

- Cross entropy gradient vector for class k

$$\nabla_{\theta^{(k)}} J(\Theta) = \frac{1}{m} \sum_{i=1}^{m} \left(\hat{p}_k^{(i)} - y_k^{(i)} \right) \mathbf{x}^{(i)}$$

- Training:
  - Compute the gradient vector for every class, then use Gradient Descent to find the parameter matrix Θ that minimizes the cost function

Softmax Regression Decision Boundaries



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Thank you for your attention!