# Introduction to Machine Learning Lecture II

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### Outline

### • Linear models: regression

- Analytic solution
- o (Stochastic) Gradient Descent
- When to stop training?
- (Under) Overtraining and its treatment
- Loss functions & metrics

#### • Linear models: classification

- Binary classifier
- Logistic regression
- Metrics
- Multiclass case

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# Recap — SL fundamentals

### Given:

- Set of objects that forms a training sample  $\{x_1 \dots x_N\} \subset X$
- Set of answers  $y_i = g(x_i), \{y_1 \dots y_N\} \subset Y$

#### Find:

•  $a: X \to Y$  – algorithm a that approximates g on the whole set X

### Define:

- Loss function  $\mathcal{L}(a(x), y)$
- $Q(a, X^N) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(a(x_i), y_i)$

**Then:** 
$$\hat{a} = \arg\min_{a \in A} Q(a, X^N)$$

# Recap — features and answers

# Objects are described by a set of **features** $f_i(x) \in D_i$ :

- $D_i = \{0, 1\} \Rightarrow$  binary feature
- $|D_i| < \infty \Rightarrow$  categorical feature
- $|D_i| < \infty$  + total order  $\Rightarrow$  ordinal feature
- $D_i = \mathbb{R} \Rightarrow$  numerical feature

# Type of answer $y_i \in Y$ generally defines **problem type**:

- $Y = \{0, 1\} \Rightarrow$  binary classification
- $|Y| < \infty \Rightarrow$  multi-class classification
- $|Y| < \infty$  + total order  $\Rightarrow$  ranking
- $Y = \mathbb{R} \Rightarrow$  regression

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# Linear models

regression

# Linear regression

- $Y = \mathbb{R}$
- N objects with K real features:  $D = \mathbb{R}^K$

• 
$$a(\mathbf{x}, \boldsymbol{\theta}) = \theta_0 + \sum_{j=1}^{K} f_j(\mathbf{x}) \cdot \theta_j$$

• Extend and reassign:

$$[1,f_1(\mathbf{x}),\ldots,f_K(\mathbf{x})]\equiv\mathbf{x}$$

$$[\theta_0,\ldots,\theta_K] \equiv \boldsymbol{\theta}$$

• Then  $a(x, \theta) = \langle x, \theta \rangle$ 

• Minimization problem:

$$\circ \ \mathcal{L}(\boldsymbol{\theta}) = (\langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - \boldsymbol{y})^2$$

$$\circ Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} (\langle x_i, \boldsymbol{\theta} \rangle - y_i)^2$$

• Then we need to minimize  $Q(\theta)$  by varying  $\theta$ :

$$\circ \ \hat{a} = \arg\min_{\boldsymbol{\theta} \in \Theta} Q(\boldsymbol{\theta})$$

# Solution can be found analytically

After defining feature matrix as:

$$F = \begin{bmatrix} f_1(\mathbf{x_1}) & \cdots & f_K(\mathbf{x_1}) \\ \vdots & \ddots & \vdots \\ f_1(\mathbf{x_N}) & \cdots & f_K(\mathbf{x_N}) \end{bmatrix}$$

Minimization problem for linear regression:

• 
$$Q(\theta) = \frac{1}{N} (F\theta - y)^T (F\theta - y) =$$
  
 $= \theta^T F^T F\theta - 2y^T F\theta + y^T y$   
•  $\frac{\partial Q}{\partial \theta^T} = 2F^T F\theta - 2F^T y = 0$ 

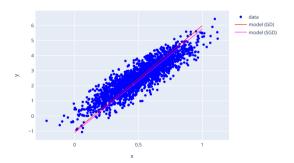
$$\hat{\boldsymbol{\theta}} = (F^T F)^{-1} F^T \boldsymbol{\nu}$$

Problem 1: calculation of  $(F^TF)^{-1}$  has **complexity of**  $O(K^5N) \Rightarrow$  computationally-intensive for large number of features

Problem 2: F is often **ill-conditioned**  $\Rightarrow$  computational errors causes instabilities and extremely large solutions

# Better approach? — example

- Let's consider a problem where objects have only one feature:  $x = [1, f_1(x)]$
- Then  $\boldsymbol{\theta} = [\theta_0, \theta_1]$
- How can we find minimum of  $Q(\theta)$  without solving matrix equation?



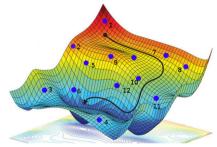
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# Better approach? — o random search

- Start with some vector  $\theta^0$
- Initialize  $\hat{\theta} = \theta^0$
- $\downarrow$  Take randomly another vector  $\theta'$
- $\downarrow$  Compare  $Q(\theta')$  and  $Q(\hat{\theta})$
- $\downarrow \ \hat{\boldsymbol{\theta}} = \arg\min_{\hat{\boldsymbol{\theta}}, \boldsymbol{\theta'}} \left( Q(\hat{\boldsymbol{\theta}}), Q(\boldsymbol{\theta'}) \right)$
- ↓ Repeat until convergence

Problem: random search of  $\hat{\theta}$  is not effective for practical use in high dimensional  $\Theta$  space



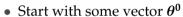
Q as a function of  $\theta_0$  and  $\theta_1$ . Blue dots represent Q values for different  $\theta$ 

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Better approach? — gradient descent

Idea: bring up additional information about the direction to the minimum of Q using its **antigradient** 



• 
$$\hat{\theta} \leftarrow \theta^0$$

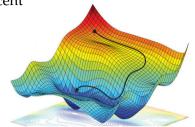
↓ Calculate direction to the minimum:

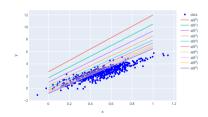
$$-\nabla Q(\hat{\boldsymbol{\theta}}) = -\left[\frac{\partial Q}{\partial \theta_0}, \frac{\partial Q}{\partial \theta_1}\right]_{\hat{\boldsymbol{\theta}}}$$

↓ Move towards the minimum:

$$\hat{\boldsymbol{\theta}} \leftarrow \hat{\boldsymbol{\theta}} - \boldsymbol{\eta} \nabla Q(\hat{\boldsymbol{\theta}})$$

↓ Repeat until convergence



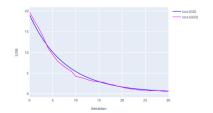


# Better approach? — stochastic gradient descent

### **Gradient descent**

Calculating  $-\nabla Q$  over all objects

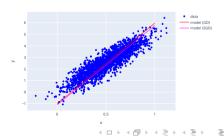
- √ Precise gradient
- X Can be time-consuming for large dataset



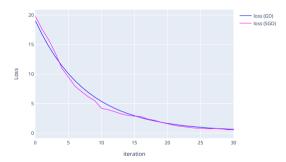
### Stochastic gradient descent

Calculating  $-\nabla Q$  over minibatch

- √ Big data friendly
- × Noisy gradient



### When to stop training?

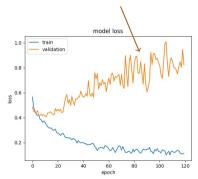


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# When to stop training? — vanilla approaches

- 1 Stop once reached predefined number of iteration
  - ? what if too early? → undertraining
  - ? what if too late? → overtraining
- 2 Stop once training loss is not improving
  - can use  $\mathcal{L}(a(x), y)$  as an error estimator
  - measure it on training data at each iteration
  - stop once  $\mathcal{L}_{\text{train}}$  is not improving by predefined  $\varepsilon$
  - → monitor the progress online throughout the training
  - → can overfit easily

badly overfitted but  $\mathcal{L}_{train}$  is decreasing

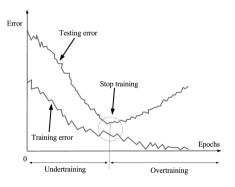


Note: you can use **any metric** instead of  $\mathcal{L}$ 

# When to stop training? — using a test set

- To check model's capability to generalise we apply it to **unseen test data**
- Can do this not only after training is done but throughout
- So check train and test error for each iteration
- And stop once test metric/loss is not improving by  $\varepsilon \rightarrow \text{early stopping}$
- → detect and prevent overfitting before it happens

Note: "test set" and "validation set" are often used interchangeably

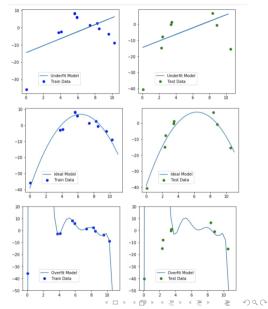


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# Example — measuring model performance

- After training is done, we want to measure model's performance by applying it to test (unseen) data
- In this example, upper model performs bad both on train and test sets
- Center model shows acceptable results on train an test sets
- Lower model performs well on train and fails on test

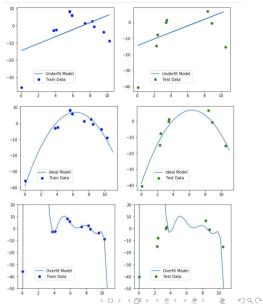


# Example — measuring model performance

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- In this example, upper model performs bad both on train and test sets
- Center model shows acceptable results on train an test sets
- Lower model performs well on train and fails on test



Let's analyze these outcomes



### Possible outcomes

Train - bad Test – bad Undertraining

### Model is too simple

- Model can't capture the underlying structure of data
- Low variance, high bias

# Train - good Test – bad Overtraining

- Model is too complicated
- Model captures noise instead of structure of data
- High variance, low bias

#### What to do?

- Increase model's capacity
- Train longer

- Catch it before it happens (e.g. early stopping)
- Reflect about noise level vs model complexity

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### Possible outcomes

Train – bad Test – bad ↓ Undertraining

# Model is too simple

- Model can't capture the underlying structure of data
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### Train – good Test – bad ↓ **Overtraining**

- Model is too complicated
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#### What to do?

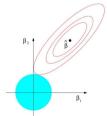
- Increase model's capacity
- Train longer

- Catch it before it happens (e.g. early stopping)
- Reflect about noise level vs model complexity
- Automatically limit algorithm space → regularization

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### L2 regularization (Tikhonov)

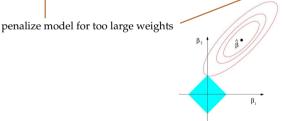
$$Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} (\langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - y_i)^2 + \lambda \sum_{j=1}^{K} \boldsymbol{\theta}_j^2$$



### L1 regularization (LASSO)

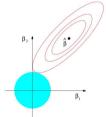
least absolute shrinkage and selection operator

$$Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} (\langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - y_i)^2 + \lambda \sum_{j=1}^{K} |\boldsymbol{\theta}_j|$$



### L2 regularization (Tikhonov)

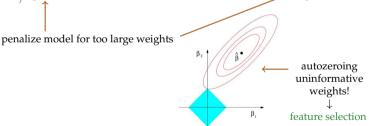
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### L1 regularization (LASSO)

least absolute shrinkage and selection operator

$$Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} (\langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - y_i)^2 + \lambda \sum_{j=1}^{K} |\boldsymbol{\theta}_j|$$



### L2 regularization (Tikhonov)

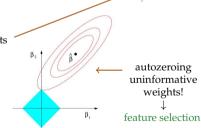
$$Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \left( \langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - y_i \right)^2 + \lambda \sum_{j=1}^{K} \boldsymbol{\theta}_j^2 \qquad \qquad Q(\boldsymbol{\theta}) = \frac{1}{N}$$
penalize model for too large weights

β.

### L1 regularization (LASSO)

least absolute shrinkage and selection operator

$$Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} (\langle \boldsymbol{x}, \boldsymbol{\theta} \rangle - y_i)^2 + \lambda \sum_{j=1}^{K} |\boldsymbol{\theta}_j|$$

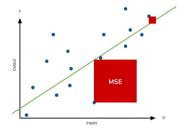


 $\lambda$  is a **hyperparameter**  $\rightarrow$  more in homework

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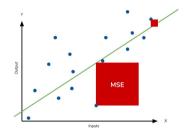
- we chose it because it represents model's error
- which we want to be as small as possible (keeping overfitting in mind)
- and therefore we directly minimize its average over the dataset in training

$$\mathcal{L}_{\text{train}} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(a(x_i), y_i)$$



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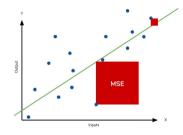
$$\mathcal{L}_{\text{train}} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(a(x_i), y_i) \equiv \mathbb{E}_{p(x,y)}[\mathcal{L}(a(x), y)] \leftarrow \text{expected value}$$

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- we chose it because it represents model's error
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There is something more behind this...

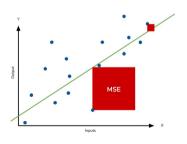
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—○ Mean Squared Error (L2)

$$MSE(a, X, Y) = \mathbb{E}_{p(x,y)} [(a(x) - y)^{2}]$$

- → Grows quadratically with the error ⇒ punish for large mistakes ⇒ sensitive to outliers ("mean-unbiased")
- → **Symmetrical** for under/overestimates
- → **Smooth** ⇒ no problem with finding optimum
- → Doesn't preserve units of measurement ⇒ poorly interpretable
- → Good statistical properties ⇒ might give you BLUE (see Gauss-Markov theorem)



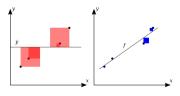
──○ MSE variations

- RMSE =  $\sqrt{MSE}$ 
  - → preserve units of measurement ⇒ interpretable
- MSLE =  $\mathbb{E}_{p(x,y)} [(\log(a(x) + 1) \log(y + 1))^2]$ 
  - → penalize on the "order of magnitude" scale
  - → not symmetric for over/underestimation
- Coeff. of determination

$$R^{2} = 1 - \frac{\mathbb{E}_{\mathbf{p}(x,y)} \left[ \left( a(x) - y \right)^{2} \right]}{\mathbb{E}_{\mathbf{p}(x,y)} \left[ \left( \bar{y} - y \right)^{2} \right]}$$

- → fraction of "explained" variance:  $1 \frac{SS_{\text{res}}}{SS_{\text{tot}}}$
- → "normalised" MSE

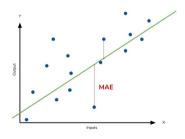
$$MSE = \mathbb{E}_{p(x,y)} [(a(x) - y)^{2}]$$



—○ Mean Absolute Error (L1)

$$MAE(a, X, Y) = \mathbb{E}_{p(x,y)}[|a(x) - y|]$$

- But for example, we could also take absolute value
- \* btw why not  $\mathcal{L} = \mathbb{E}[a(x) y]$ ?
- → Simple to interpret
- → **Symmetrical** for under/overestimates
- → **Robust** to outliers ("median-unbiased")
- → Not smooth
- → Not backed much with statistics



• MAPE = 
$$\mathbb{E}_{p(x,y)} \left[ \left| \frac{y - a(x)}{y} \right| \right]$$

→ "normalised" MAE

• SMAPE = 
$$100\% \cdot \mathbb{E}_{p(x,y)} \left[ \frac{|y - a(x)|}{|y| + |a(x)|} \right]$$

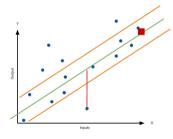
- → symmetrized MAPE
- → not really symmetrized for over/underestimation

$$MAE = \mathbb{E}_{p(x,y)}[|a(x) - y|]$$

→ Huber Loss

$$\operatorname{HL}(a,X,Y) = \mathbb{E}_{\mathrm{p}(x,y)} \left\{ \frac{1}{2} (a(x) - y)^2, & |a(x) - y| < \delta \\ \delta |a(x) - y| - \frac{1}{2} \delta^2, & \text{otherwise} \right\}$$

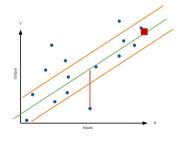
- Or we could also combine them altogether
- → **Robust** to outliers in tails
- → Better performance near minimum (smaller variance)
- $\rightarrow \delta$  is a **hyperparameter**  $\Rightarrow$  should be tuned



→ Huber Loss

$$\operatorname{HL}(a,X,Y) = \mathbb{E}_{\mathrm{p}(x,y)} \left\{ \frac{1}{2} (a(x) - y)^2, & |a(x) - y| < \delta \\ \delta |a(x) - y| - \frac{1}{2} \delta^2, & \text{otherwise} \right\}$$

- Or we could also combine them altogether
- → **Robust** to outliers in tails
- → **Better performance** near minimum (smaller variance)
- $\rightarrow \delta$  is a **hyperparameter**  $\Rightarrow$  should be tuned



All of the above losses can (and should) be used as metrics!

# Linear models

classification

### Classification

- $Y = \{-1, +1\}$
- N objects with K real features:  $D = \mathbb{R}^K$

• 
$$a(\mathbf{x}, \boldsymbol{\theta}) = \theta_0 + \sum_{j=1}^K f_j(\mathbf{x}) \cdot \theta_j$$

• Extend and reassign:  $[1, f_1(\mathbf{x}), \dots, f_K(\mathbf{x})] \equiv [1, x_1, \dots, x_K] \equiv \mathbf{x}$ 

$$[\theta_0,\ldots,\theta_K]\equiv \boldsymbol{\theta}$$

• Then  $a(x, \theta) = \langle x, \theta \rangle$ 

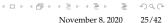
Minimization problem:

$$\circ \ \mathcal{L}(\boldsymbol{\theta}) = \left[ \operatorname{sign} \langle \boldsymbol{x}, \boldsymbol{\theta} \rangle \neq \boldsymbol{y} \right]$$

$$\circ Q(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} [\operatorname{sign}\langle x_i, \boldsymbol{\theta} \rangle \neq y_i]$$

• Then we need to minimize  $Q(\theta)$  by varying  $\theta$ :

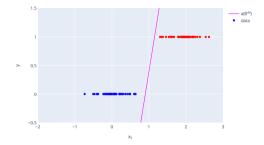
$$\circ \hat{a} = \arg\min_{\boldsymbol{\theta} \in \Theta} Q(\boldsymbol{\theta})$$



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# Example

- Let's consider the problem of two class (red, blue) classification
- We need to find a line\* that provides the best separation of objects from different classes
- Objects have single feature:  $x = [1, x_1]$
- Then  $\theta = [\theta_0, \theta_1]$



\*for a model with multiple features we are looking for hyperplanes

# Minimization problem for classification

- $\mathcal{L}(\theta) = [a(x, \theta) \neq y] = [\operatorname{sign}\langle x, \theta \rangle \neq y]$   $\leftarrow$  step function
- $Q(\theta) = \mathbb{E}_{p(x,y)}[\operatorname{sign}\langle x, \theta \rangle \neq y] \leftarrow \operatorname{accuracy}$
- Then we need to minimize  $Q(a(\theta))$  by varying  $\theta$

Problem 1:  $\mathcal{L}(\theta)$  isn't a smooth function  $\Rightarrow$  gradient methods are not applicable

Problem 2: Discrete  $\{-1, +1\}$  output from the classifier



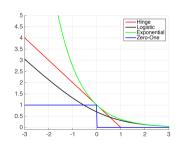
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# From binary classification to logistic regression

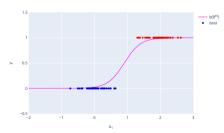
#### Problem 1:

Solution: use smooth approximations



### Problem 2:

Solution: reframe the problem to probabilistic perspective ⇒ logistic regression



• Assume that algorithm  $a(x, \theta)$  returns probability that object  $x_i$  is from positive class  $y_i = +1$ 

- Assume that algorithm  $a(x, \theta)$  returns probability that object  $x_i$  is from positive class  $y_i = +1$
- Probability that  $x_i$  belongs to class  $y_i$ :

$$p_{\boldsymbol{\theta}}(y_i|\mathbf{x}_i) = a(\mathbf{x}_i,\boldsymbol{\theta})^{[y_i=+1]} (1 - a(\mathbf{x}_i,\boldsymbol{\theta}))^{[y_i=-1]}$$

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- Assume that algorithm  $a(x, \theta)$  returns probability that object  $x_i$  is from positive class  $y_i = +1$
- Probability that  $x_i$  belongs to class  $y_i$ :  $p_{\theta}(y_i|x_i) = a(x_i, \theta)^{[y_i = +1]} (1 a(x_i, \theta))^{[y_i = -1]}$
- Function to be optimised:  $\mathcal{L}(\theta) = \prod_{i=1}^{N} p_{\theta}(y_i|x_i)$   $\leftarrow$  maximize probability to observe such data

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- Assume that algorithm  $a(x, \theta)$  returns probability that object  $x_i$  is from positive class  $y_i = +1$
- Probability that  $x_i$  belongs to class  $y_i$ :  $p_{\theta}(y_i|x_i) = a(x_i, \theta)^{[y_i = +1]} (1 a(x_i, \theta))^{[y_i = -1]}$
- Function to be optimised:  $\mathcal{L}(\theta) = \prod_{i=1}^{N} p_{\theta}(y_i|x_i) \leftarrow \text{maximize probability to observe such data}$
- Product is not useful, let's make sum:

$$\log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} [y_i = 1] \log a(\boldsymbol{x}_i, \boldsymbol{\theta}) + [y_i = -1] \log (1 - a(\boldsymbol{x}_i, \boldsymbol{\theta}))$$



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- Assume that algorithm  $a(x, \theta)$  returns probability that object  $x_i$  is from positive class  $y_i = +1$
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- Function to be optimised:  $\mathcal{L}(\theta) = \prod_{i=1}^{N} p_{\theta}(y_i|x_i)$   $\leftarrow$  maximize probability to observe such data
- Product is not useful, let's make sum:

$$\log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} [y_i = 1] \log a(\boldsymbol{x}_i, \boldsymbol{\theta}) + [y_i = -1] \log (1 - a(\boldsymbol{x}_i, \boldsymbol{\theta}))$$

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• Finally:  $\hat{a} = \arg \max_{\theta \in \Theta} \log \mathcal{L}(\theta)$ 

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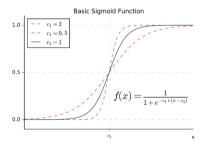
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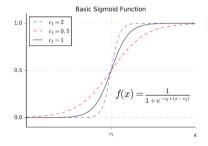
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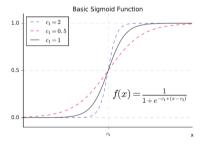
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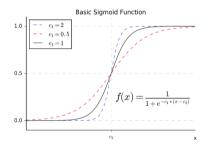
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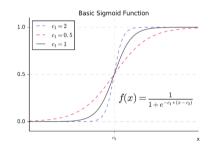


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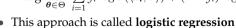
This approach is called logistic regression

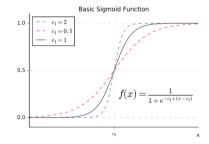


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$$\begin{split} \hat{a} &= \arg\max_{\boldsymbol{\theta} \in \Theta} \ \log \mathcal{L}(\boldsymbol{\theta}) = \\ &= \arg\max_{\boldsymbol{\theta} \in \Theta} \ \sum_{i=1}^{N} y_i \log \sigma(\langle \boldsymbol{x}_i, \boldsymbol{\theta} \rangle) + (1 - y_i) \log \left(1 - \sigma(\langle \boldsymbol{x}_i, \boldsymbol{\theta} \rangle)\right) \end{split}$$





NB: usage of  $\sigma$  and log-likelihood in general does not guarantee probabilistic interpretation

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### Comparison

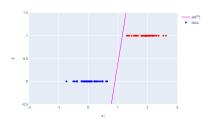
#### Linear classifier

$$Q(\boldsymbol{\theta}) = \sum_{i=1}^{N} [\operatorname{sign}(a(\boldsymbol{x}_i, \boldsymbol{\theta})) \neq y_i]$$

- $a(x, \theta) = \langle x, \theta \rangle$
- $a(x, \theta) : \mathbb{R}^K \times \mathbb{R}^K \mapsto \mathbb{R}$

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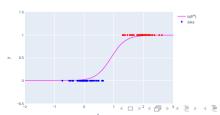
- √ Easy to interpret
- × Gives only yes-no answer



#### Logistic regression

$$\log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} y_i \log a_{\sigma}(\boldsymbol{x}_i, \boldsymbol{\theta}) + (1 - y_i) \log (1 - a_{\sigma}(\boldsymbol{x}_i, \boldsymbol{\theta}))$$

- $a_{\sigma}(\mathbf{x}, \boldsymbol{\theta}) = \sigma[a(\mathbf{x}, \boldsymbol{\theta})] = \sigma[\langle \mathbf{x}, \boldsymbol{\theta} \rangle]$
- $a_{\sigma}(\mathbf{x}, \boldsymbol{\theta}) : \mathbb{R}^{K} \times \mathbb{R}^{K} \mapsto [0, 1]$
- More profound interpretation
- $\checkmark$  Returns probability of positive class y = 1

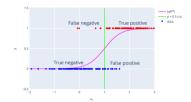


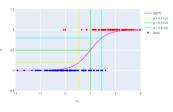
### Output of binary classifier

Let red correspond to a positive class (1) and blue – to a negative (0)

- 1 classified as  $1 \Rightarrow$  True positive (TP)
- 0 classified as  $0 \Rightarrow$  True negative (TN)
- 1 classified as  $0 \Rightarrow$  False negative (FN)
- 0 classified as  $1 \Rightarrow$  False positive (FP)

NB: in case of logistic regression you need to specify a cut on the model's output to get deterministic prediction





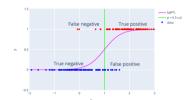
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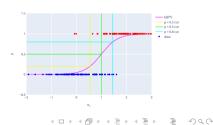
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→ Then how do we measure model's performance?





### Metrics

Using these output for binary classifier we can construct several quality metrics:

• 
$$accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

→ fraction of correct answers

• precision = 
$$\frac{TP}{TP + FP}$$

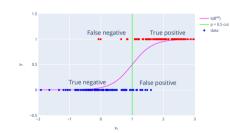
→ fraction of correct positive answers in all positive answers

• recall = 
$$\frac{TP}{TP + FN}$$

→ fraction of correctly classified positive objects

• **F1-score** = 
$$\frac{2 \cdot \text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

→ harmonic mean of precision and recall



### **Metrics**

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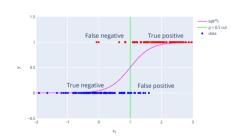
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choose metrics wisely!

• Consider a dataset with 10000 negative and 10 positive objects

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- Hence, you could've assumed that the model is really good (but it's not)
- → Always take imbalance into account! (e.g. up-/downsampling, reweighting)
- → Be careful when interpreting your metrics!

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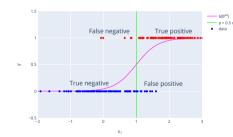
### Choosing the right threshold

- As was mentioned before, classifier decision (thus performance) depends on the threshold
- How can we estimate its performance for all cuts in general?

$$\circ$$
 define true positive rate: TPR =  $\frac{TP}{TP + FN}$ 

and false positive rate: FPR = 
$$\frac{FP}{FP + TN}$$

- move the green line on the plot
- moving to the left results in TP↑ and FN↓ (sensitive, but not specific)
- moving to the right results in TP↓ and FN↑ (specific, but not sensitive)



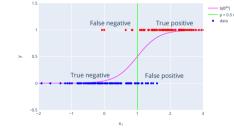
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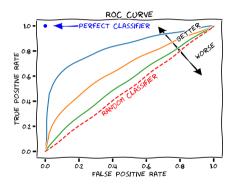
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Idea: plot jointly values of TPR and FPR for different values of threshold

# Receiver Operating Characteristic —o curve

- Scanning through thresholds we can calculate for each of them TPR and FPR and plot them
- This will give a **ROC curve**
- → Random classifier diagonal line at ROC
- → Perfect classifier step function
- → Something-went-wrong classifier curve below diagonal line



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# Receiver Operating Characteristic

area under curve

The power of a classifier can be represented by the **area under ROC curve**:

$$ROC AUC = \int_{0}^{1} TPR(FPR)d(FPR)$$

- → aggregated measure of performance across all possible thresholds ⇒ threshold-invariant
- $\rightarrow$  1  $\Rightarrow$  predictions are 100% correct
- $\rightarrow 0.5 \Rightarrow$  random classifier
- $\rightarrow 0 \Rightarrow$  predictions are 100% wrong
- → probability that a random positive (green) example is positioned to the right of a random negative (red) example  $\Rightarrow$  scale-invariant



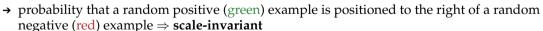
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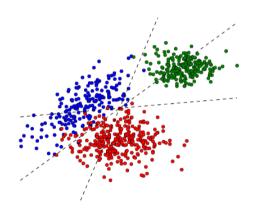
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Nice moment to show this animation

### Multiclass classification

- If the number of classes > 2, then we need to modify classification approach
- $|Y| < \infty = \{1, ..., L\} \Rightarrow$  impossible to use single model



### From multiclass problem to a set of binary problems

#### "One vs all"

- Train *L* binary classifiers:  $b_{\ell}(\boldsymbol{x},\boldsymbol{\theta}), \ell \in \{1,\ldots,L\}$
- Each  $a_{\ell}(x, \theta)$  is trained to separate between  $\ell$ -th class and all the rest
- The most confident classifier gives the final separation:

$$a(\mathbf{x}, \boldsymbol{\theta}) = \underset{\ell \in \{1, \dots, L\}}{\operatorname{arg max}} b_{\ell}(\mathbf{x}, \boldsymbol{\theta})$$

#### "All vs all"

- Train  $C_I^2$  binary classifiers to separate every two classes:  $a_{i,j}(\boldsymbol{x},\boldsymbol{\theta}), i,j \in 1,\ldots,L, i \neq j$
- In this case each classifier decides only between two classes
- $\hat{y} = \arg\max \sum_{i=1}^{L} \sum_{j=1}^{L} [b_{i,j}(x, \theta) = \ell]$  $\ell \in \{1,...,L\}$  i=1  $i\neq i$
- Class with the highest vote over  $C_L^2$ classifiers wins!

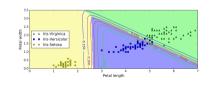


# Multiclass logistic regression

- Suppose we trained  $a_{\ell}(\mathbf{x}, \boldsymbol{\theta}) = \langle \mathbf{x}, \boldsymbol{\theta} \rangle, \ell = 1, \dots, L$  each separating its individual class
- Now we need to turn their output into probabilities
- Reminder:  $a_{\ell}(x, \theta)$  has a range  $\mathbb{R}$
- We need to convert vector  $[a_1(x, \theta), \dots, a_L(x, \theta)]$  into a vector of probabilities
- We can put **softmax** on top:

$$\left[a_1(\boldsymbol{x},\boldsymbol{\theta}),\ldots,a_L(\boldsymbol{x},\boldsymbol{\theta})\right] \mapsto \left[\frac{\exp[a_1(\boldsymbol{x},\boldsymbol{\theta})]}{\sum\limits_{\ell=1}^L \exp[a_\ell(\boldsymbol{x},\boldsymbol{\theta})]},\ldots,\frac{\exp[a_L(\boldsymbol{x},\boldsymbol{\theta})]}{\sum\limits_{\ell=1}^L \exp[a_\ell(\boldsymbol{x},\boldsymbol{\theta})]}\right]$$

 Then components sum up to 1 and each component represents\* probability that object x belongs to a correspondent class



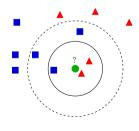
#### Final note

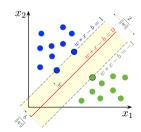
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We didn't have time to describe them, but in the family of "classical algorithms" there are also these guys – and they are cool enough to be studied and tried out:

- **kNN** *k*-nearest neighbors algorithm
- **SVM** Support Vector Machine
- Naive Bayes Naive Bayes classifier

$$\hat{y} = \arg\max_{y} P(y) \prod_{i=1}^{n} P(x_i \mid y)$$







### Summary

- Linear models are the simplest example of models used for SL
- Solution of optimization problem can be found analytically, but (stochastic) gradient descent is a more general approach to training
- During the process of training model's performance is checked throughout to control under- and overtraining
- Model regularization prevents overtraining thanks to additional term in the loss function
- Several variations to MSE and MAE loss functions exist, each with its unique properties all can be used both as losses and as metrics

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- Linear models are the simplest example of models used for SL
- Solution of optimization problem can be found analytically, but (**stochastic**) **gradient descent** is a more general approach to training
- During the process of training model's performance is checked throughout to control under- and overtraining
- Model regularization prevents overtraining thanks to additional term in the loss function
- Several variations to MSE and MAE loss functions exist, each with its unique properties all can be used both as losses and as metrics
- Classification problem has pretty the same pipeline as the regression. Furthermore, it can be
  converted into logistic regression that estimates probability of belonging to a class
- **Dedicated classification metrics** exist, all being specific/sensitive to its own thing, both threshold dependent (e.g. accuracy) and not (e.g. ROC AUC)
- Multiclass clasification can be also performed using "one-vs-all" and "all-vs-all" methods, or in case of log.regression with applying softmax function

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