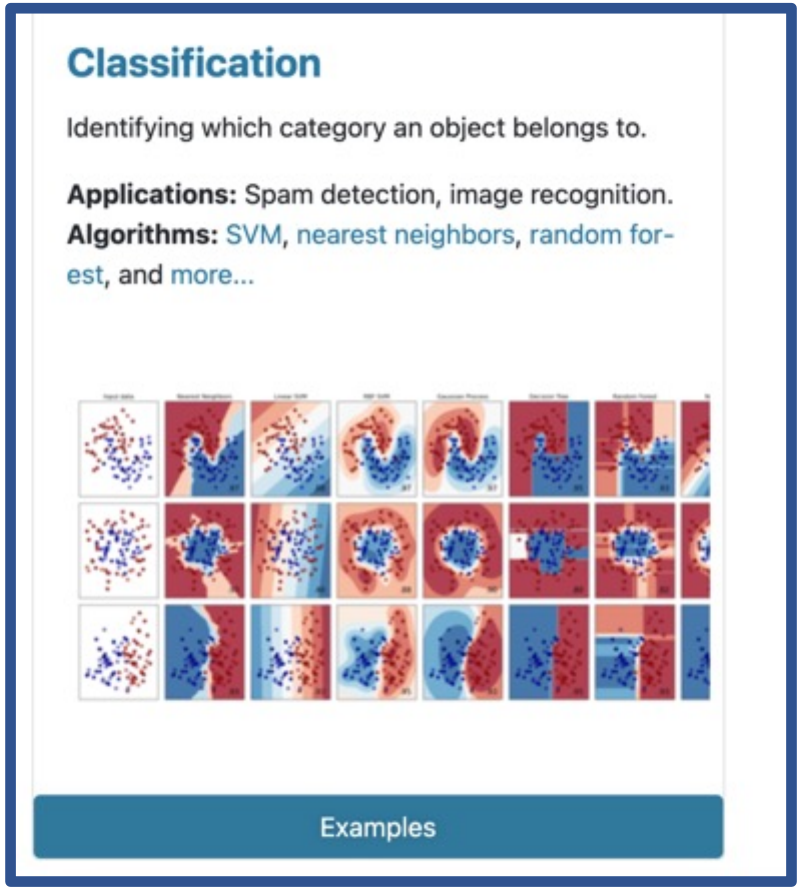
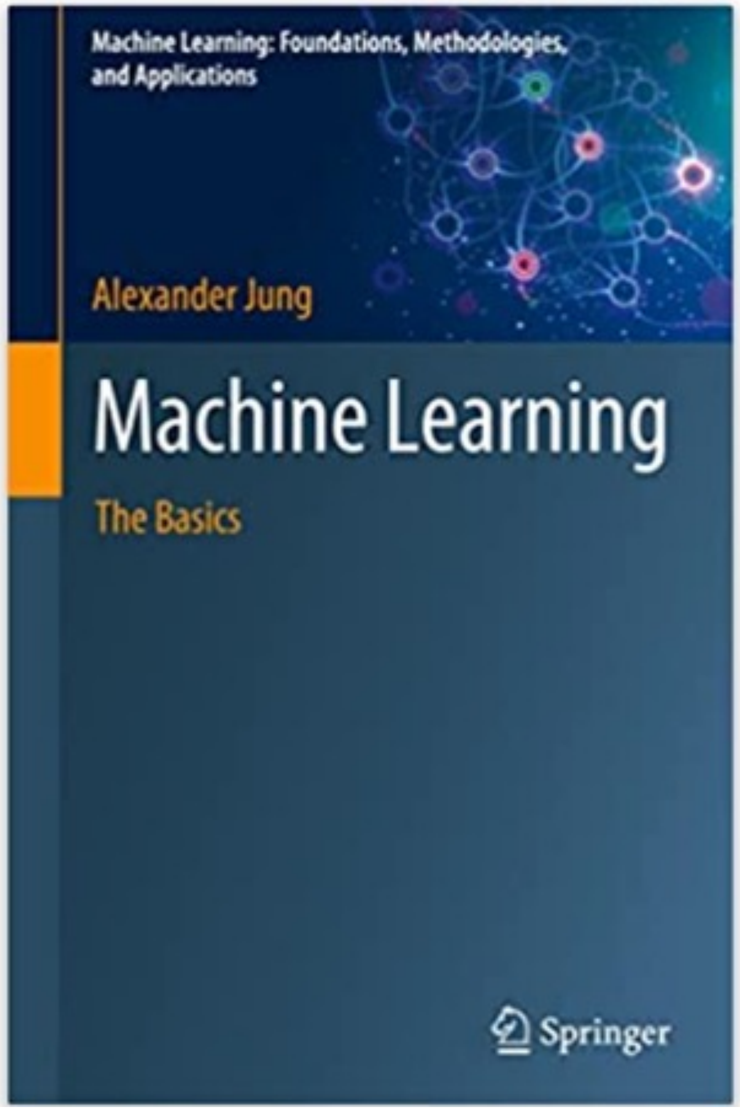
Classification

Alex(ander) Jung
Assistant Professor for Machine Learning
Department of Computer Science
Aalto University

Reading.

- Ch. 2.3, 3.6 of MLBook





https://scikit-learn.org/stable/index.html

Learning Goals:

- be able to recognize classification problems
- know binary, multi-class and multi-label problems
- know design choices of basic classif. methods
- know stat./comp. trade-offs in classif. methods

What is ML About ?

fit models to data to make

predictions or forecasts !

Data. Model. Loss.

data: set of datapoints (x,y)

model: set of hypothesis maps h(.)

loss: quality measure L((x,y),h)

Machine Learning.

find hypothesis in model that incurs smallest loss when predicting label of any datapoint

Expected Loss or Risk

$$\mathbb{E}\{L((\mathbf{x}, y), h)\} := \int_{\mathbf{x},y} L((\mathbf{x}, y), h) dp(\mathbf{x}, y). \qquad (2.14)$$

note: to compute this expectation
we need to know the probability distribution
p(x,y) of datapoints (x,y)

Empirical Risk

IDEA: approximate expected loss by average loss on some datapoints (training set)

$$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})\}.$$

$$\mathbb{E}\{L((\mathbf{x}, y), h)\} \approx (1/m) \sum_{i=1}^{m} L((\mathbf{x}^{(i)}, y^{(i)}), h) \text{ for sufficiently large sample size } m. \tag{2.17}$$

with the average loss or empirical risk

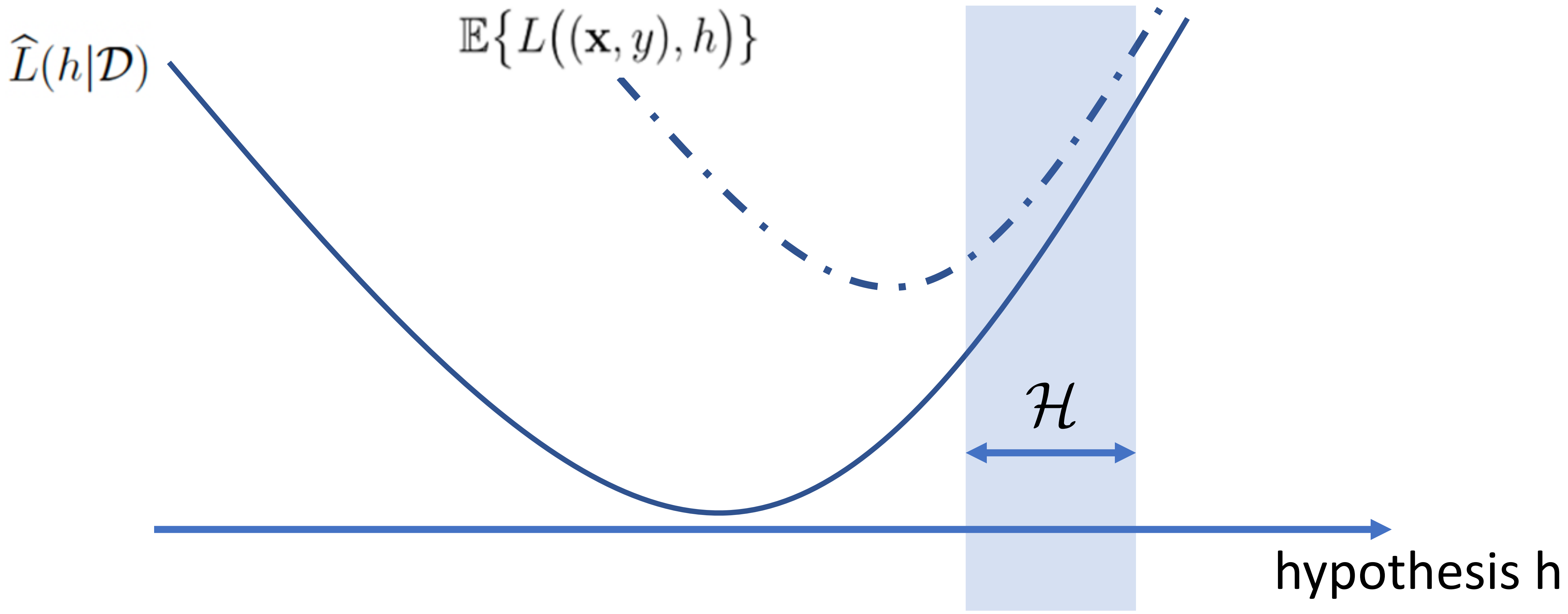
$$\widehat{L}(h|\mathcal{D}) = (1/m) \sum_{i=1}^{m} L((\mathbf{x}^{(i)}, y^{(i)}), h). \tag{2.16}$$

Empirical Risk Minimization

$$\hat{h} \in \underset{h \in \mathcal{H}}{\operatorname{argmin}} \widehat{L}(h|\mathcal{D})$$

$$\overset{(\boxed{2.16})}{=} \underset{h \in \mathcal{H}}{\operatorname{argmin}} (1/m) \sum_{i=1}^{m} L\big((\mathbf{x}^{(i)}, y^{(i)}), h\big).$$

Empirical Risk Minimization



ERM for Parametrized Models

learnt (optimal) parameter vector

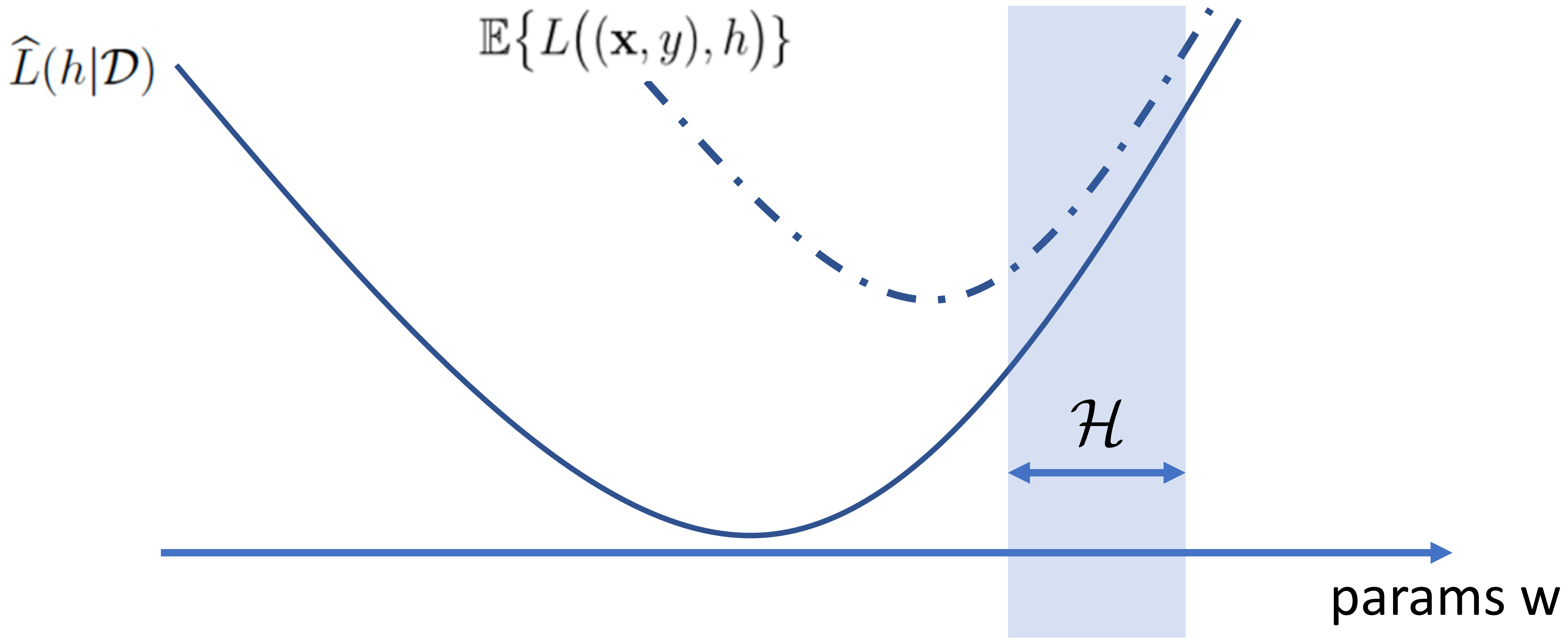
loss incurred by h(.) for i-th data point

$$\widehat{\mathbf{w}} = \operatorname*{argmin}_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w})$$

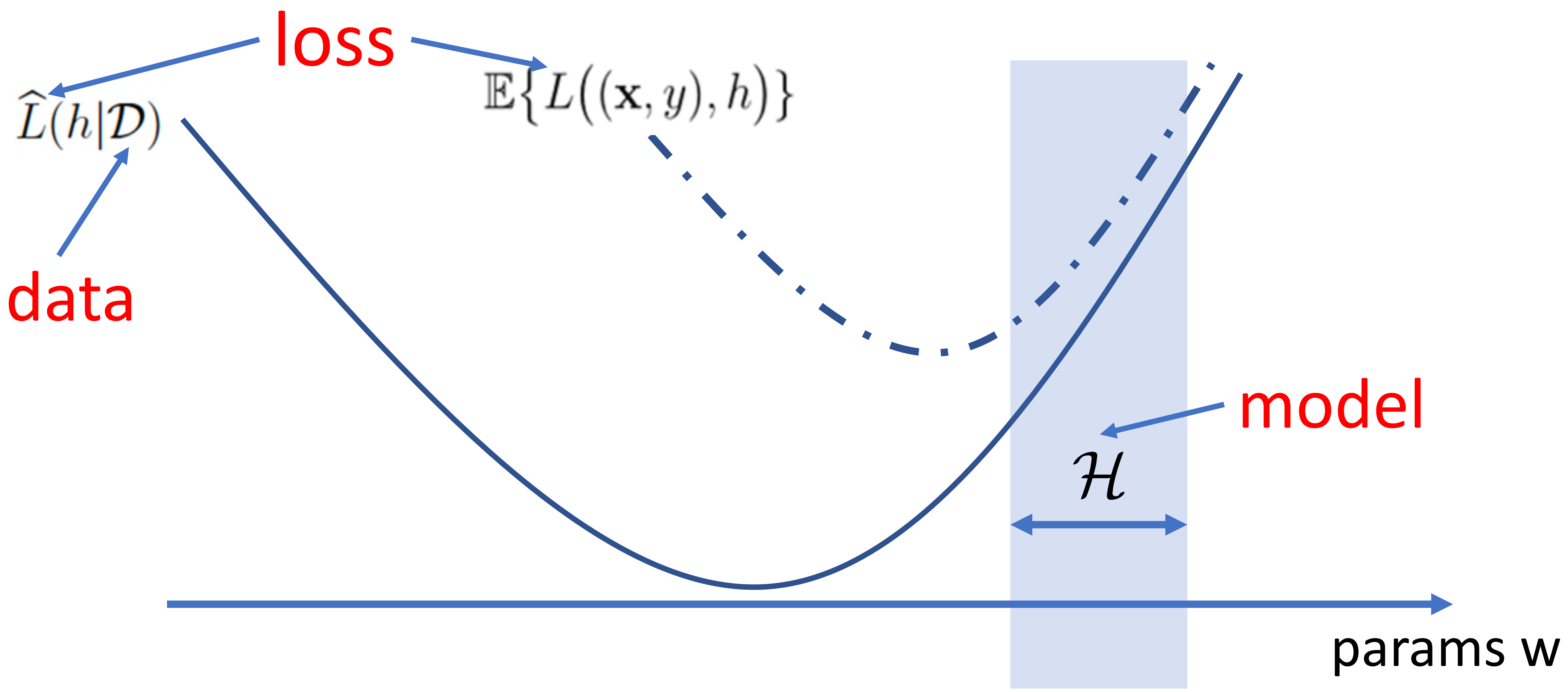
$$\text{with } f(\mathbf{w}) := \underbrace{(1/m) \sum_{i=1}^{m} L\big((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})}\big)}_{\widehat{L}\left(h^{(\mathbf{w})}|\mathcal{D}\right)} .$$

average loss or empirical risk

ERM for Param. Models



Design Choices in ERM



yesterday (“Regression”): numeric labels, loss functions obtained from distance between numbers

today (“Classification”): discrete-valued labels, loss functions obtained from “confidence” measures

Logistic Regression [Sec. 3.6., MLBook]

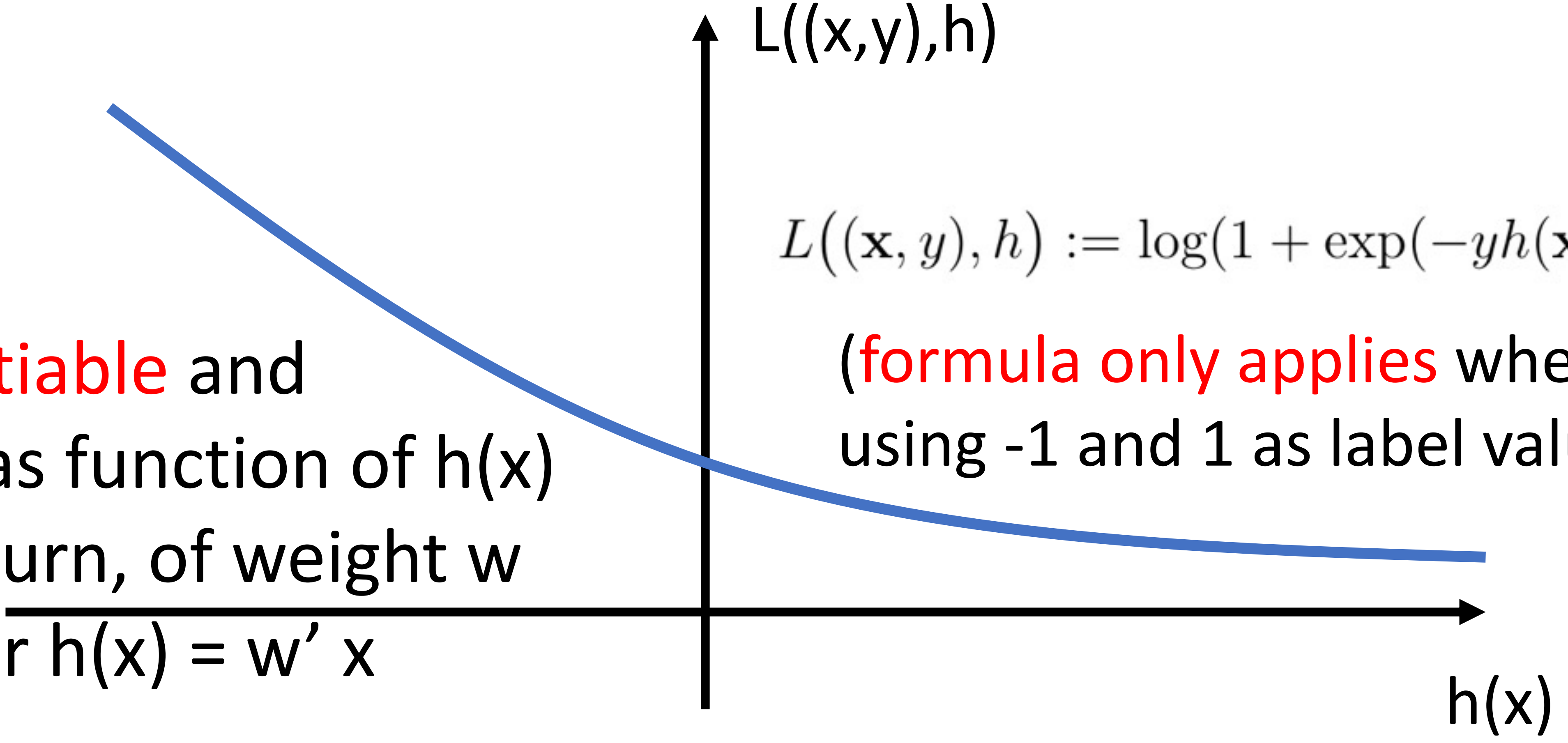
LogReg vs. LinReg

- datapoints with numeric features (same as lin.reg.)
- binary label values, e.g., y=-1 vs. y=1 (diff. from lin.reg.)
- model = space of linear maps (same as lin.reg!)
- logistic loss (different from lin.reg!)

Linear Classifier

- log.reg. uses linear hypothesis h(x) =w’x
- sign of h(x) used for label prediction
- |h(x)| used as confidence measure
- h(x) = 100000 means very confident in \hat{y}=1
- h(x) = -100000 very confident in \hat{y}=0

Logistic Loss



$$L((\mathbf{x}, y), h) := \log(1 + \exp(-yh(\mathbf{x}))).$$

(formula only applies when using -1 and 1 as label values !)

differentiable and convex as function of h(x) and, in turn, of weight w for linear h(x) = w' x

Logistic Loss Formulas

- label values y = -1 or y= 1
- label values y= 0 or y=1
- label values y=”A” or y=“B”

Value Agnostic Formula

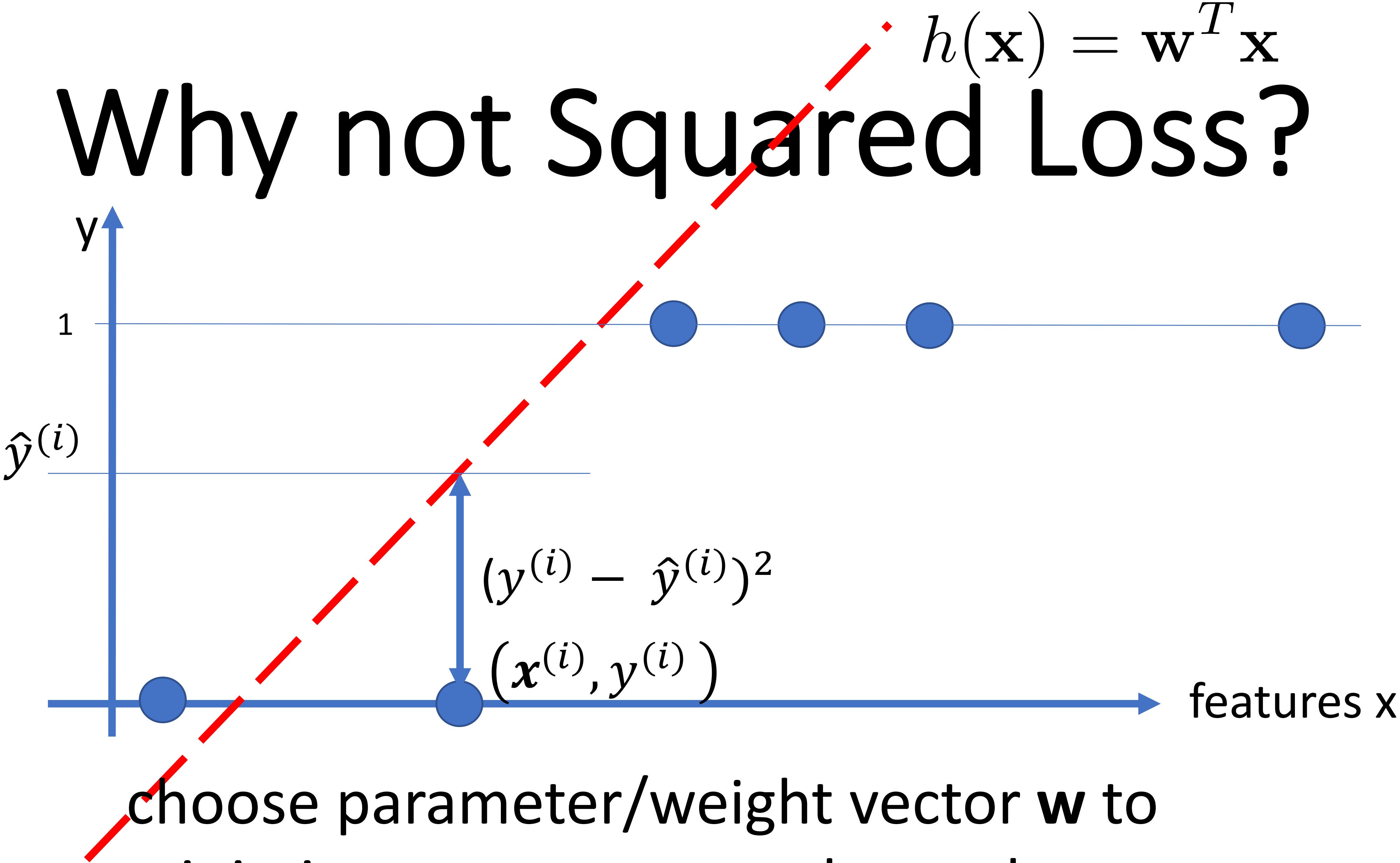
- loss value for correct classification:

$$\log\left(1 + e^{-h(\mathbf{x})}\right)$$

- loss value for wrong classification:

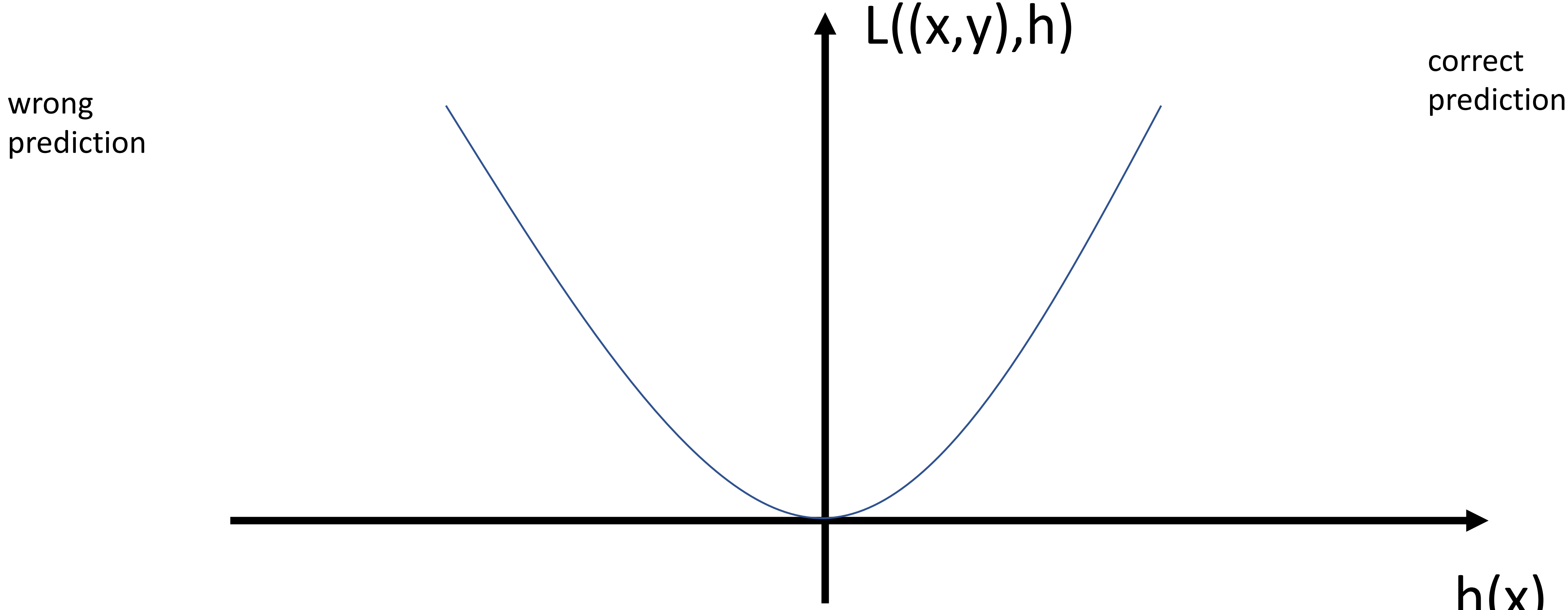
$$\log\left(1 + e^{h(\mathbf{x})}\right)$$

Why not Squared Loss?



choose parameter/weight vector **w** to minimize average squared error loss

Squared Error Loss



Classif. Loss Functions [Sec 2.3.3, MLBook]

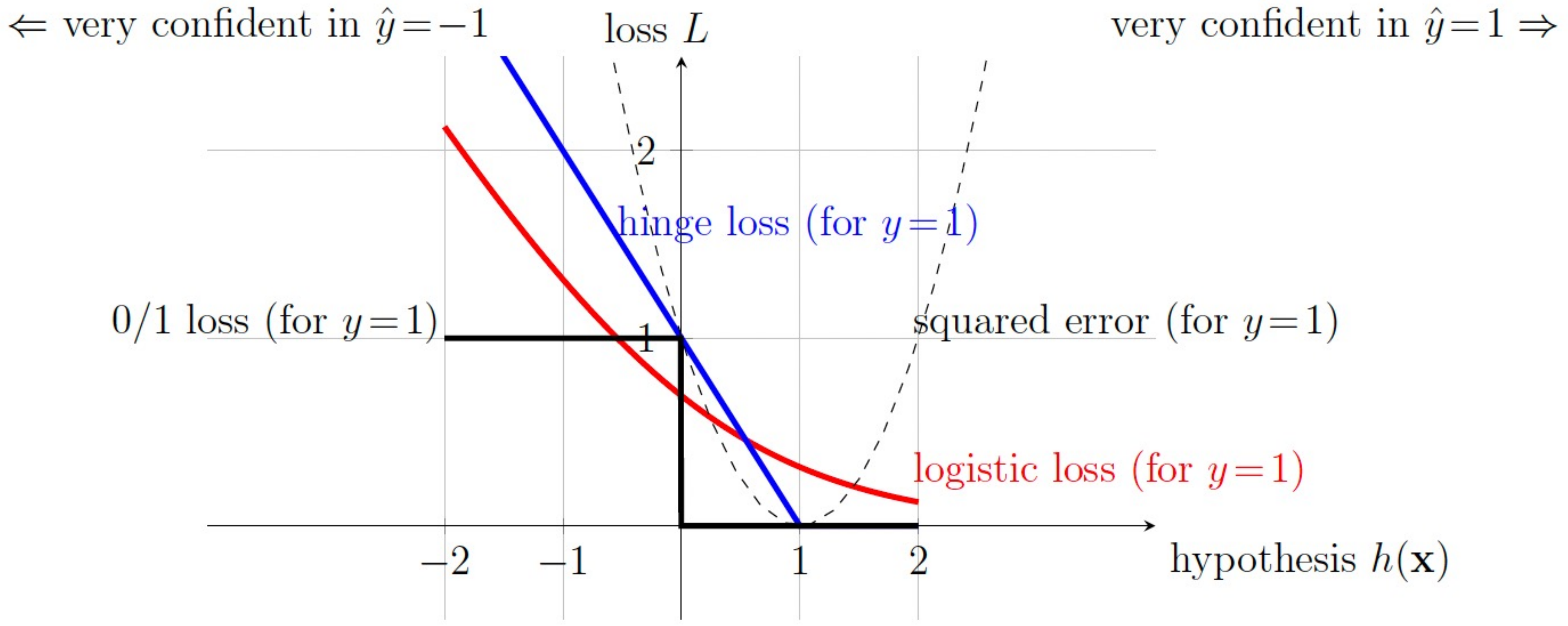


Figure 2.15: The solid curves depict three widely-used loss functions for binary classification.

LogReg. Probabilistic Interpretation

interpret label of data point as realization of binary RV with prob.

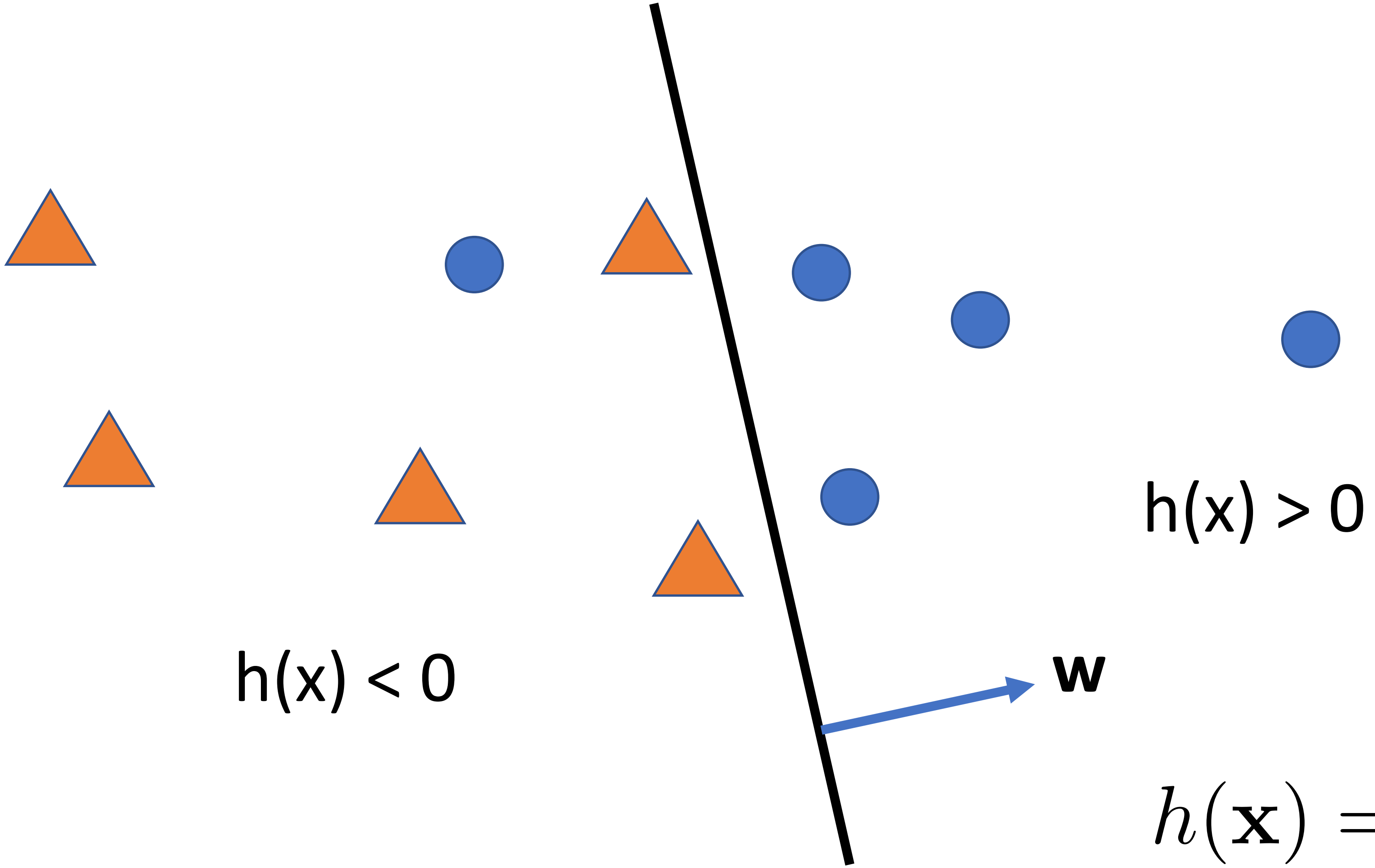
$$p(y=1;\mathbf{w}) = 1/(1+\exp(-\mathbf{w}^T\mathbf{x}))$$

$$\overset{h^{(\mathbf{w})}(\mathbf{x})=\mathbf{w}^T\mathbf{x}}{=} 1/(1+\exp(-h^{(\mathbf{w})}(\mathbf{x})))$$

max. likelihood est. for w equivalent to log.reg.

see Sec. 3.6 of MLBook

Decision Boundary of Log.Reg.



$$h(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

Logistic Regression in Python

sklearn.linear_model.LogisticRegression

class `sklearn.linear_model.LogisticRegression`(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

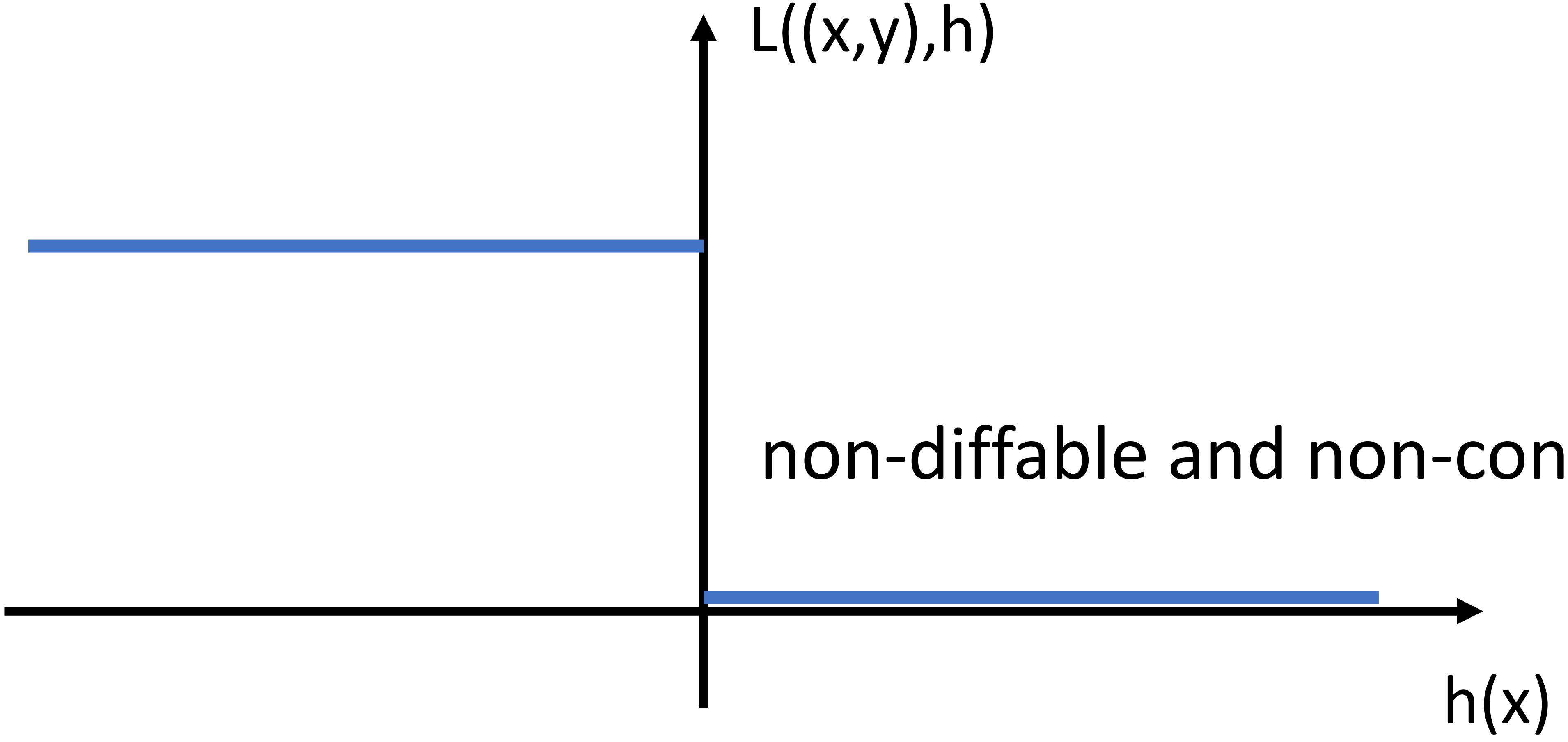
Logistic Regression (aka logit, MaxEnt) classifier.

Naïve Bayes’ Classifier (NBClass)

NBClass. – Design Choices

- datapoints with numeric features (same as log.reg.)
- binary label values, e.g., y=-1 vs. y=1 (same as log.reg)
- model = space of linear maps (same as log.reg!)
- 0/1 loss (different from log.reg!)

0/1 Loss

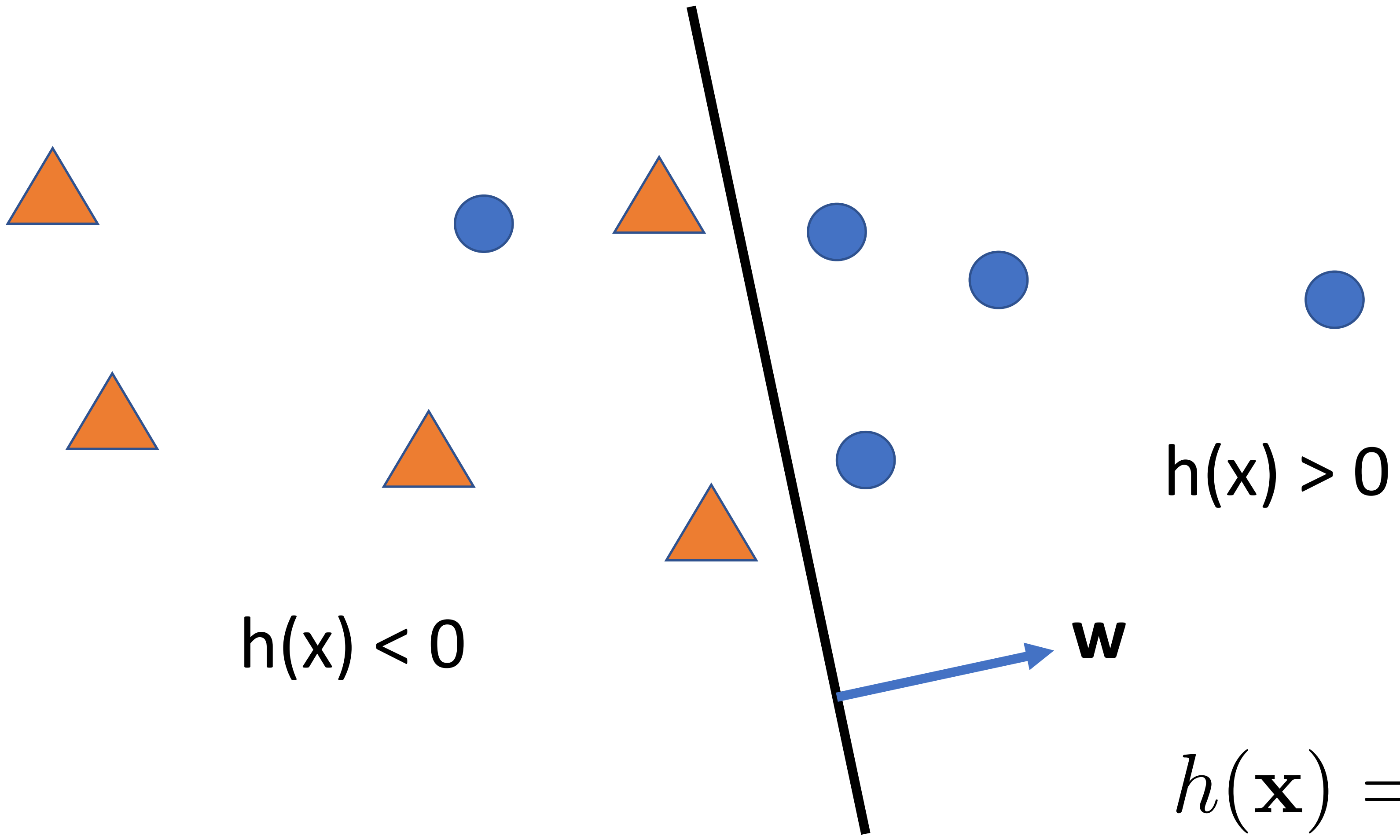


non-diffable and non-convex!

NBClass.

- ERM with 0/1 loss difficult for gradient methods
- ERM aims at minimizing error prob. P($\hat{y} \neq y$)
- Bayes' rule tells that this is equiv. to max. P($\hat{y}|x$)
- assume x is Gaussian with mean depending on y
- P($\hat{y}|x$) maximized by thresholding linear map !

Naïve Bayes' Classifier



$$h(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

Logistic Loss vs. 0/1 Loss

- logistic loss nice for optimization/solving ERM
- 0/1 loss results in (much) longer training duration
- log. loss is not very interpretable
- what does log. loss = 0.3 mean ?
- average 0/1 loss (error rate) is more tangible
- accuracy = 1 – average 0/1 loss

NBClassifier in Python

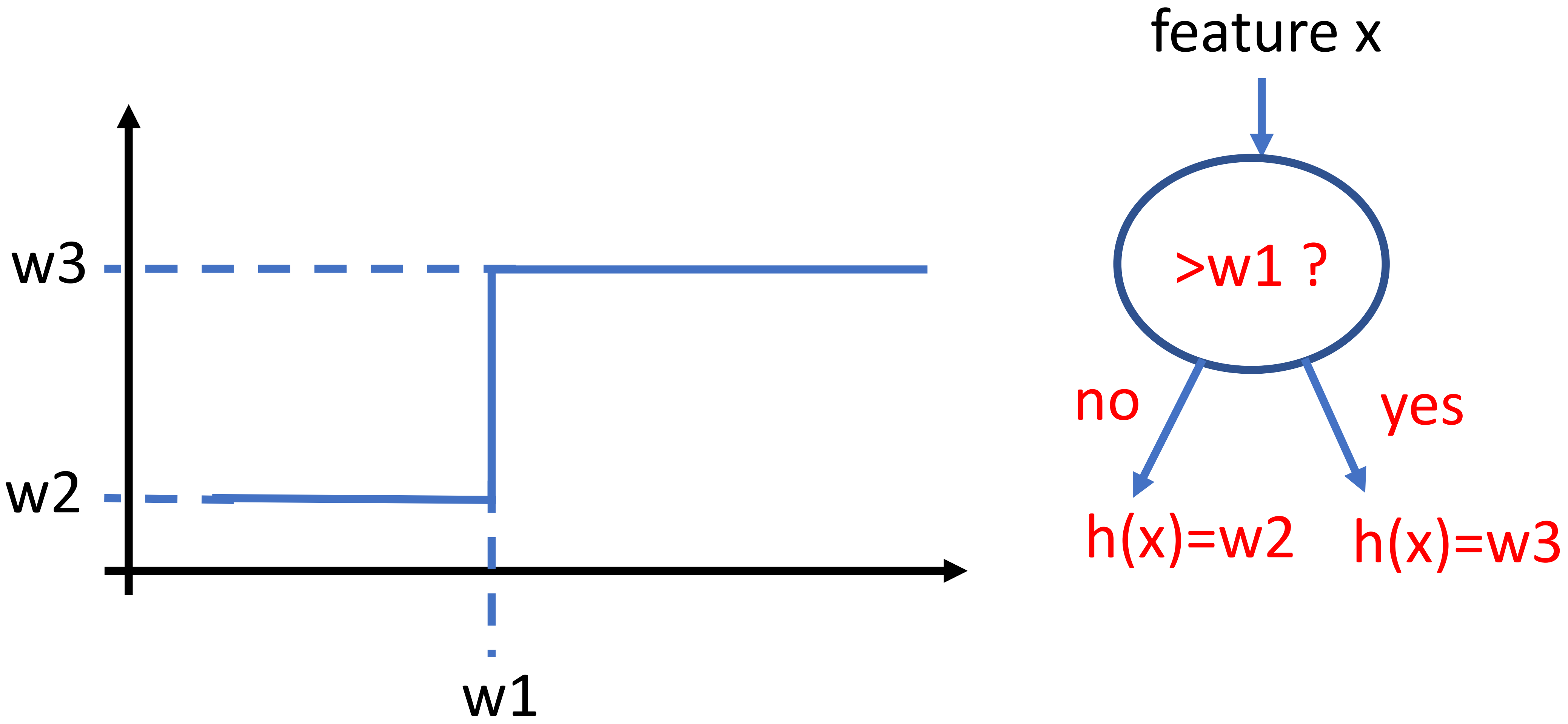
```
>>> from sklearn.datasets import load_iris
>>> from sklearn.model_selection import train_test_split
>>> from sklearn.naive_bayes import GaussianNB
>>> X, y = load_iris(return_X_y=True)
>>> X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_state=0)
>>> gnb = GaussianNB()
>>> y_pred = gnb.fit(X_train, y_train).predict(X_test)
>>> print("Number of mislabeled points out of a total %d points : %d"
...       % (X_test.shape[0], (y_test != y_pred).sum()))
Number of mislabeled points out of a total 75 points : 4
```

Decision Tree (DT) Classifier

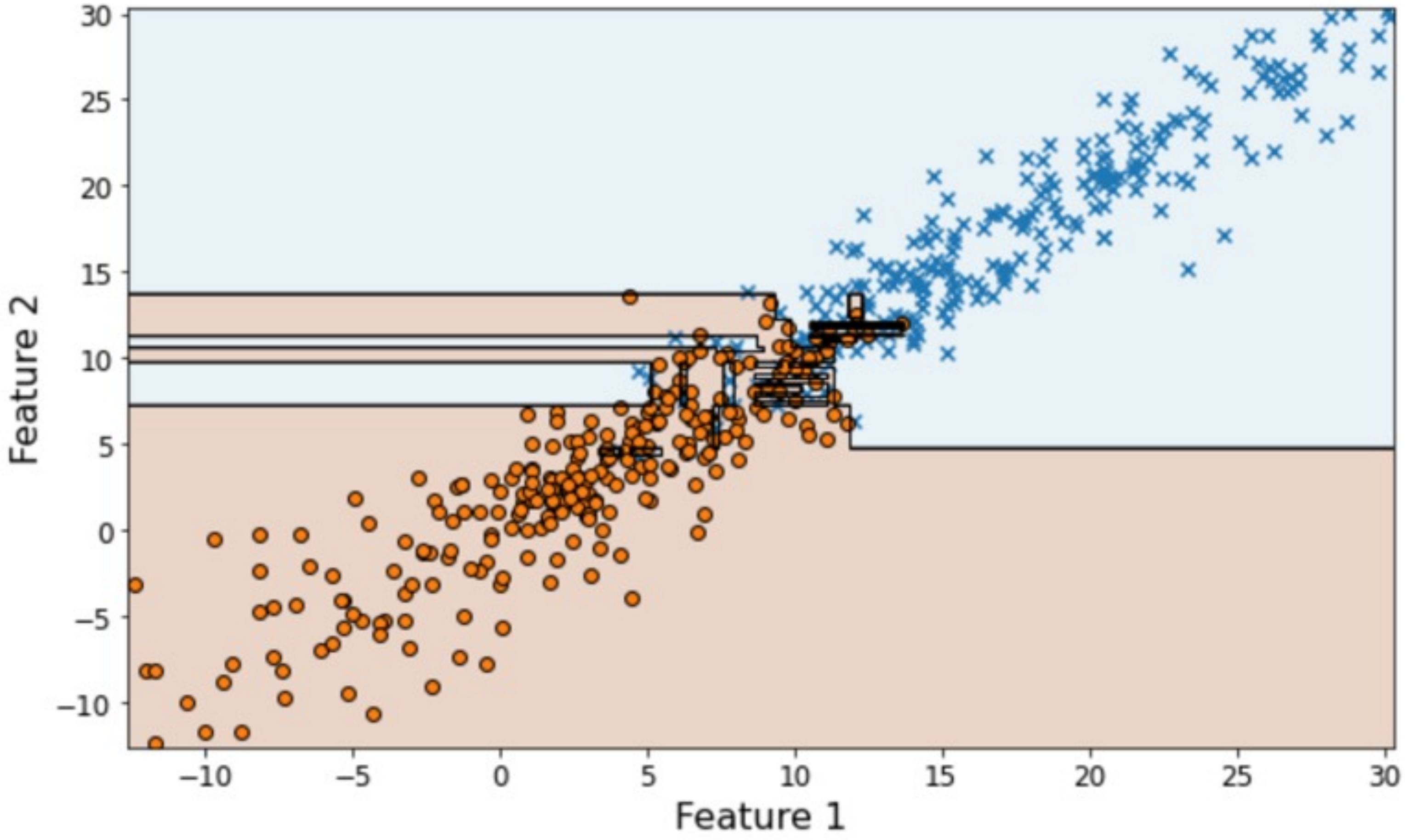
Design Choices

- data points with numeric and categ. features
- label values arbitrary, we use y=-1 vs. y=1
- model = piece-wise constant maps represented by flow chart (“decision tree”)
- different options for loss function

Parametrized DT

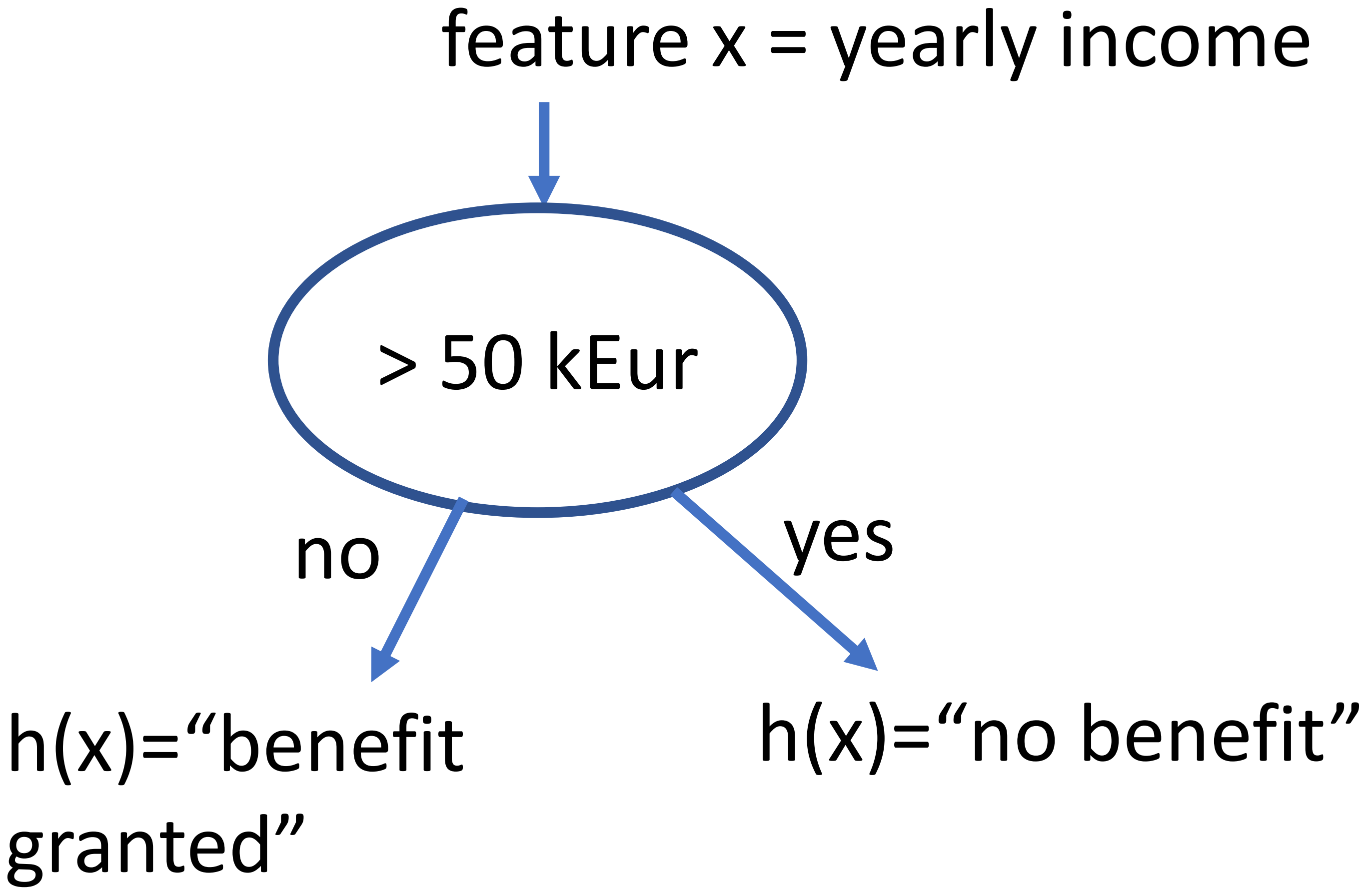


DT - Decision Boundary



piece-wise constant !

DT - Interpretability



DT Pro/Con

- allows for non-linear decision boundary
- computationally expensive
- shallow DT considered interpretable

DT in Python

sklearn.tree.DecisionTreeClassifier

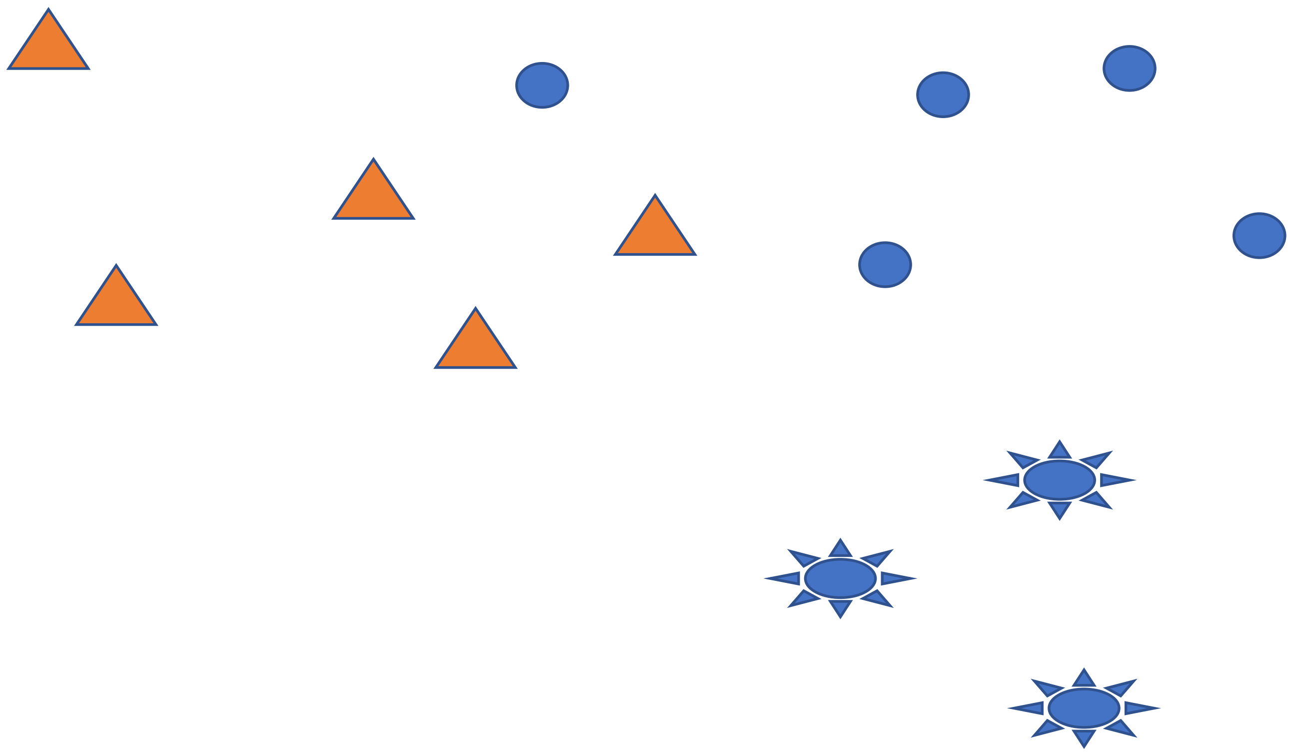
class `sklearn.tree.DecisionTreeClassifier`(*, *criterion='gini'*, *splitter='best'*, *max_depth=None*, *min_samples_split=2*, *min_samples_leaf=1*, *min_weight_fraction_leaf=0.0*, *max_features=None*, *random_state=None*, *max_leaf_nodes=None*, *min_impurity_decrease=0.0*, *class_weight=None*, *ccp_alpha=0.0*) [source]

Multi-Class Classification

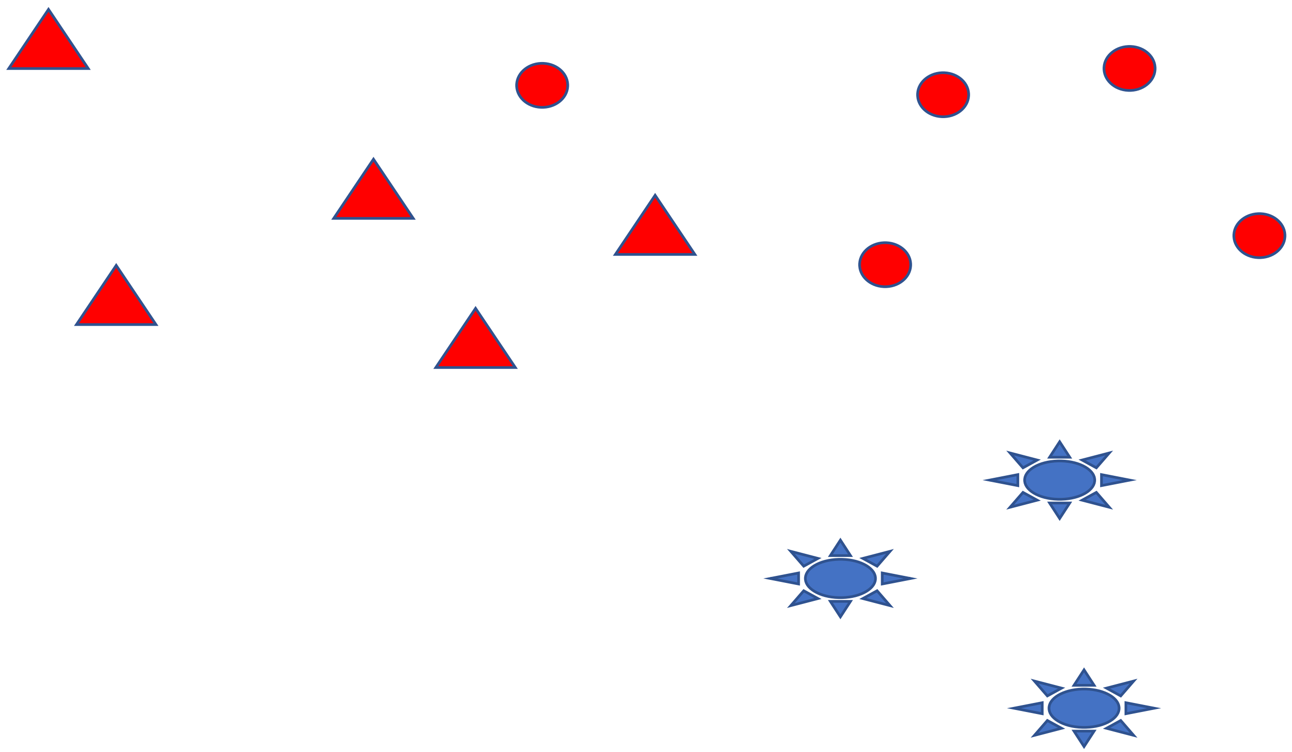
One-vs-Rest Trick

- data points with label values ”1”, “2”, “3”
- break into 3 binary class. problems
  - Problem 1: label values “1” ,“either 2 or 3”
  - Problem 2: label values “2”, “either 1 or 3”
  - Problem 3: label values ”3”, “either 2 or 3”

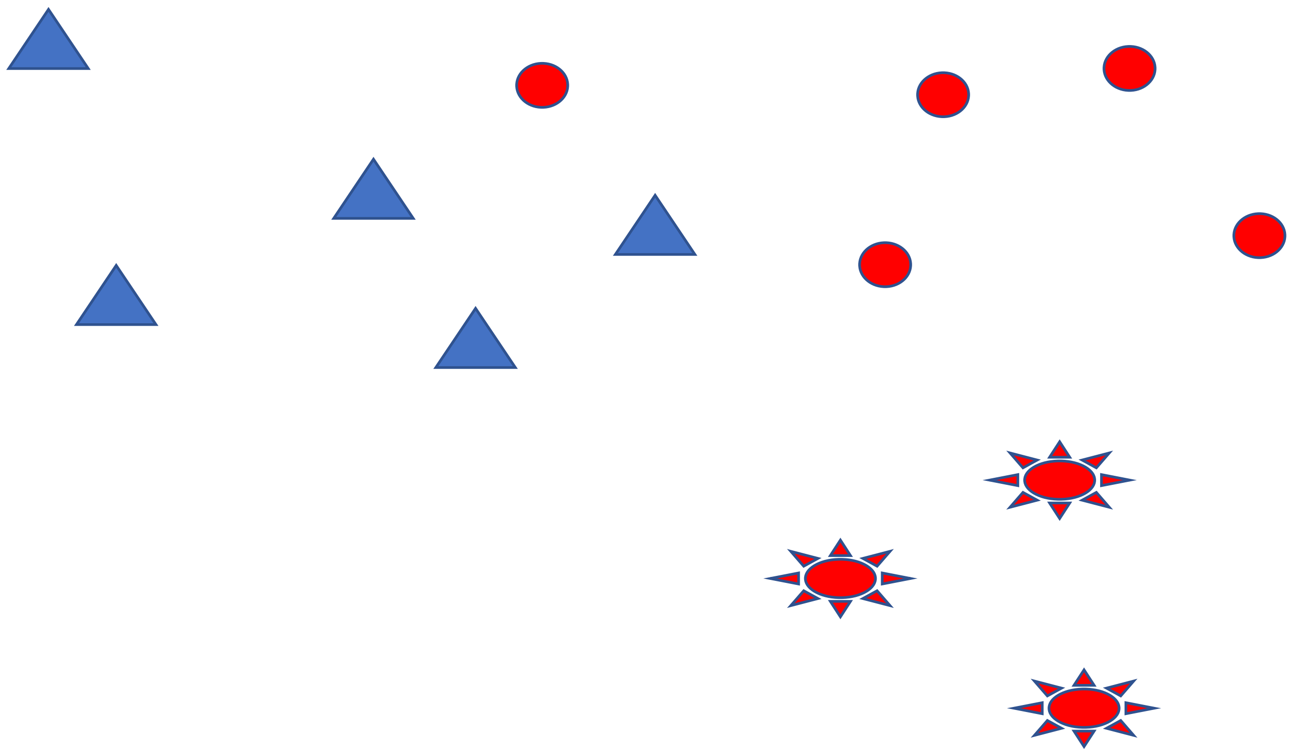
One-vs-Rest Trick



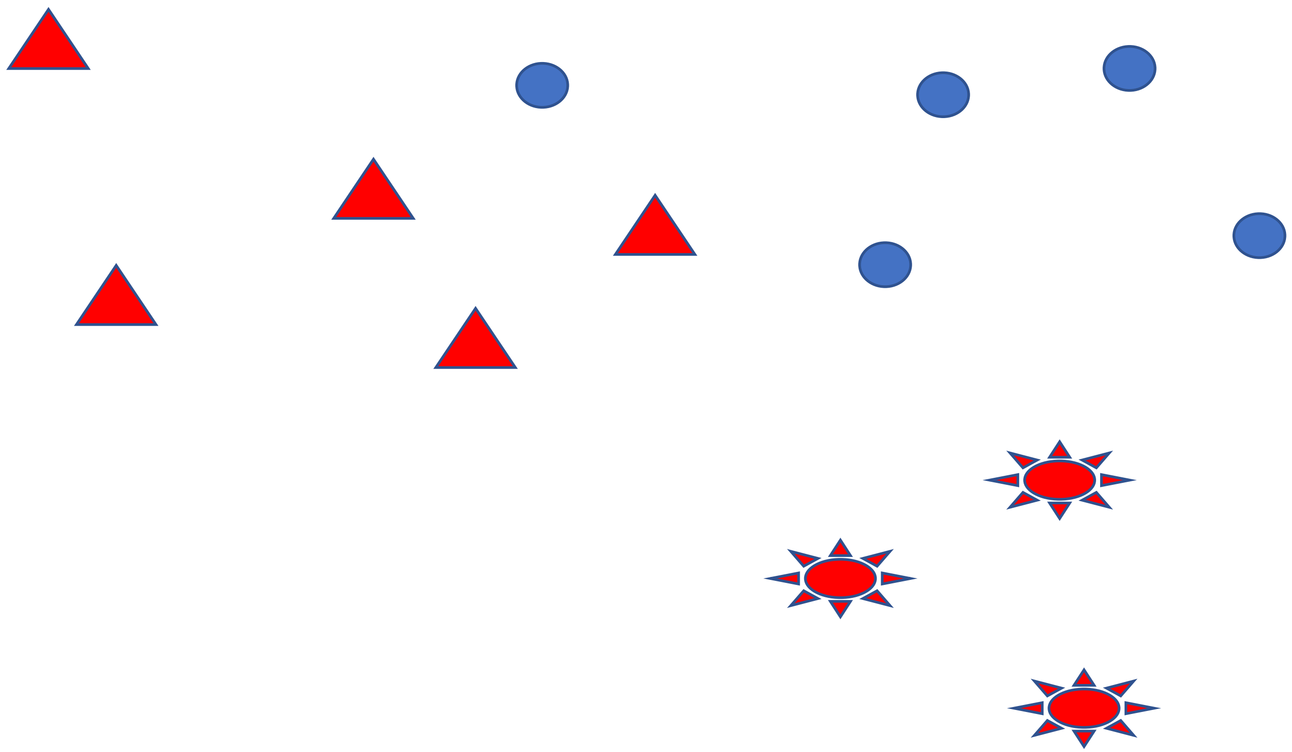
Sub-Problem 1 (red/blue)



Sub-Problem 2 (red/blue)



Sub-Problem 3 (red/blue)



One-vs-Rest Summary

- one sub-problem for each label value c
- sub-problem c: “label = c or not”
- learn hypothesis hc for each sub-problem
- predict c with highest confidence/prob. |hc|

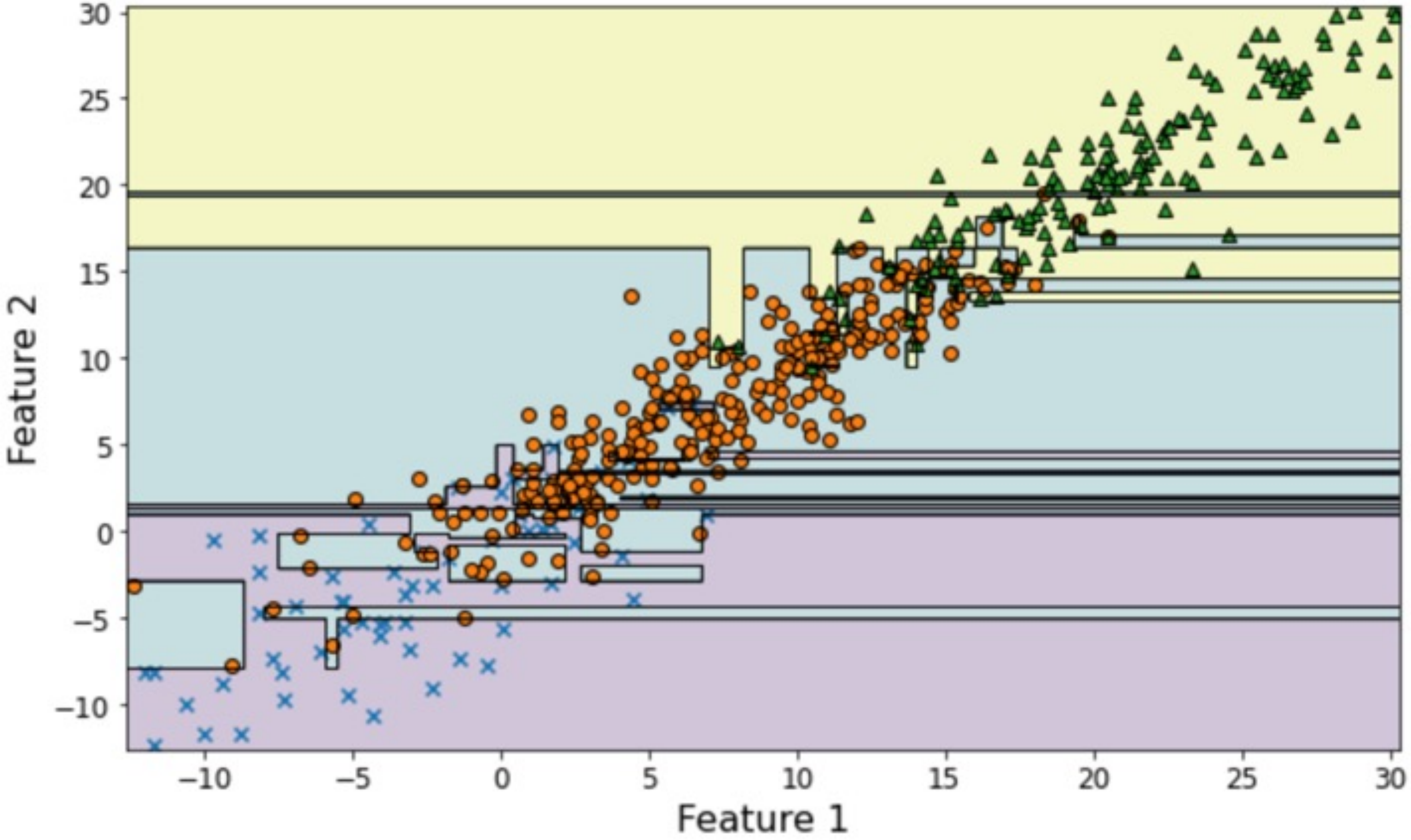
Multi-Class LogReg

- specific loss functions for multi-class data
- 0/1 loss also works for > 2 label values (classes)
- but how to encode confidence in predictions?
- soft-max (extending log-loss to more classes):

$$P(y=j \mid \mathbf{x}) = \frac{e^{\mathbf{x}^{\mathsf{T}}\mathbf{w}_j}}{\sum_{k=1}^{K} e^{\mathbf{x}^{\mathsf{T}}\mathbf{w}_k}}$$

source: https://en.wikipedia.org/wiki/Softmax_function

DT Multi-Class



Multi-Label Classification

label y1 = contains tree ? yes/no
label y2 = contains house ? yes/no
label y3 = taken during leisure? yes/no
label y4 = taken during office? yes/no
label y5 = location in Finland? yes/no
label y6 = location in Sweden? yes/no

Bonsai - Diverse and Shallow Trees for Extreme Multi-label Classification

Sujay Khandagale[1], Han Xiao[2] and Rohit Babbar[2]

[1]Indian Institute of Technology Mandi, India
[2]Aalto University, Helsinki, Finland

"…benchmark Amazon-3M dataset with 3 million labels,..

Ignorant Approach

- consider each label separately
- solve binary/multi-class problem for each label
- ignores correlations among different labels

label y1 = contains tree ? yes/no

label y2 = contains house ? yes/no

label y6 = location in Sweden? yes/no

Multi-Class Approach

- each combination of label values defines category
- obtain a multi-class problem with many classes
- huge number of resulting categories

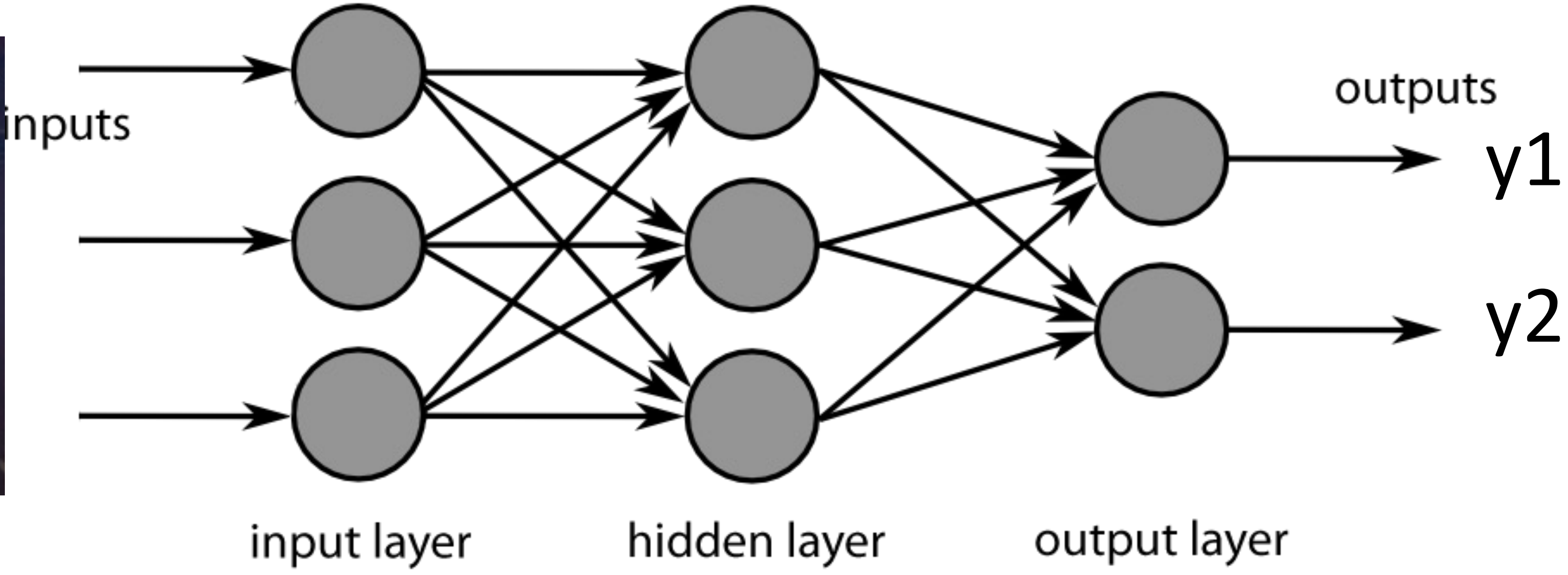
	y1	y2
cat. 1	0	0
cat. 2	0	1
cat. 3	1	0
cat. 4	1	1

Multi-Task Learning

- each individual label results in separate learning task
- use similarities between learning tasks
- similarities inform regularization techniques
- more in Lecture "Regularization"

Y. Huang, W. Wang, L. Wang and T. Tan, "Multi-task deep neural network for multi-label learning," *2013 IEEE International Conference on Image Processing*, 2013, pp. 2897-2900, doi: 10.1109/ICIP.2013.6738596.

Multi-Head Deep Net



share lower-level feature maps/layers across hypotheses

source: https://commons.wikimedia.org/wiki/File:MultiLayerNeuralNetwork_english.png

Summary

- classif. using finite label values
- loss obtained from “confidence” measures
- binary, multi-class and multi-label classif.
- classif. methods use same models as regr. methods
- comput./statist./interpretability trade off

What’s Next ?

- lecture “Model Validation and Selection”, tmrw morning
- lecture “SVM” [MLBook, Sec. 3.7.], tmrw afternoon