Empirical Risk Minimization

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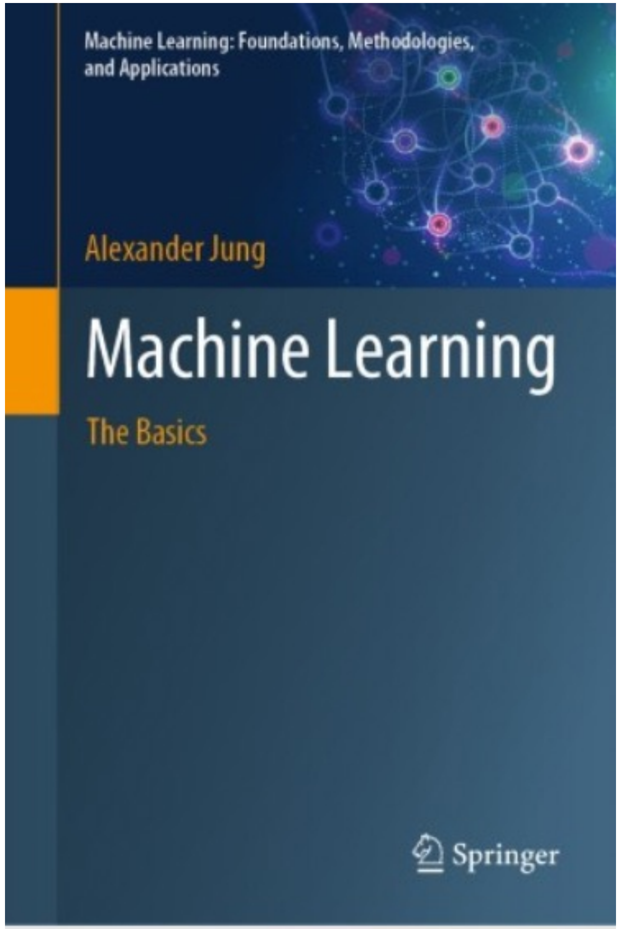
based on Chapter 4 of

preprint: mlbook.cs.aalto.fi



Learning Goals:

- know about notion of expected loss or risk
- know that average loss approximates risk
- know about empirical risk minimization
- be aware of design choices data/model/loss and their effect on ERM 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(.)

$|h(\underline{x}) - y|$

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

Data

	Year	m	d	Time	Time zone	Maximum temperature (degC)	Minimum temperature (degC)
0	2020	2	1	00:00	UTC	3.0	1.9
1	2020	2	2	00:00	UTC	4.9	2.4
2	2020	2	3	00:00	UTC	2.6	-0.4
3	2020	2	4	00:00	UTC	-0.2	-3.7
4	2020	2	5	00:00	UTC	2.5	-4.2
5	2020	2	6	00:00	UTC	2.4	-4.7
6	2020	2	7	00:00	UTC	1.2	-5.5
7	2020	2	8	00:00	UTC	2.7	0.2
8	2020	2	9	00:00	UTC	3.9	2.6

Data.

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

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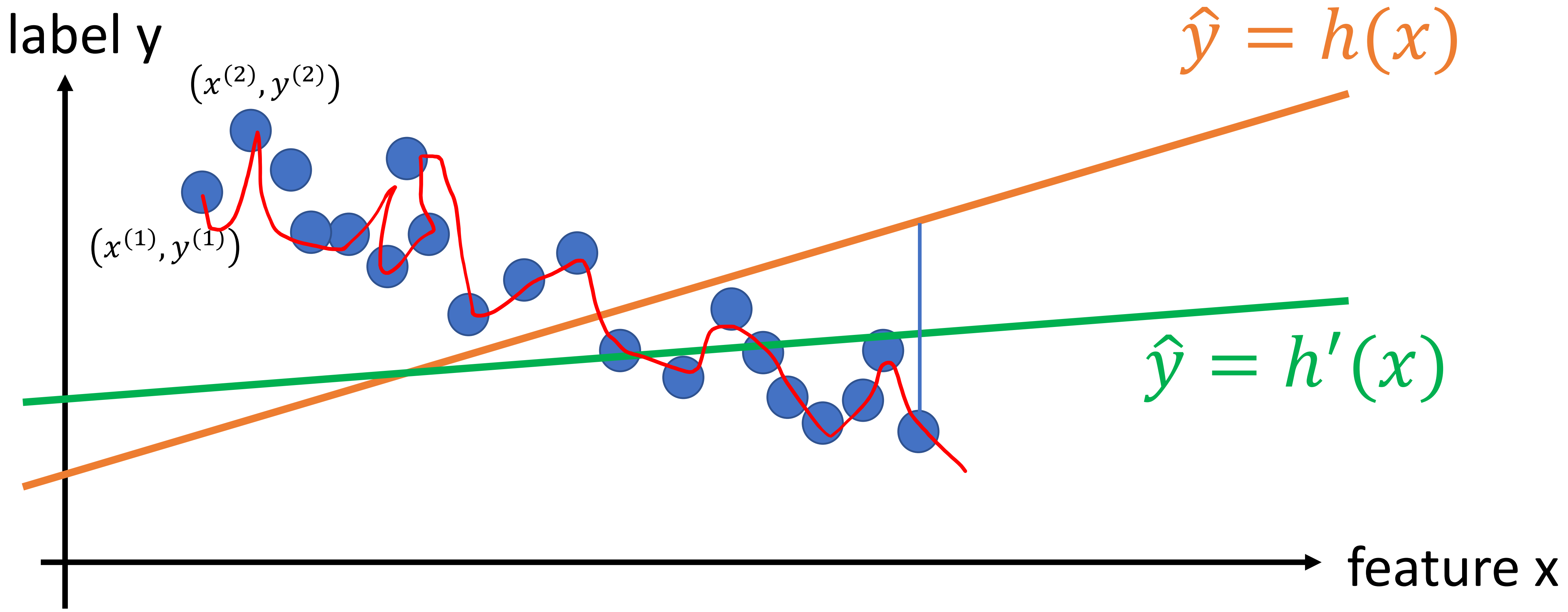
stack feature vecs into matrix

$$\mathbf{X} = \left(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\right)^{T} \in \mathbb{R}^{m \times n}$$

stack labels into vector

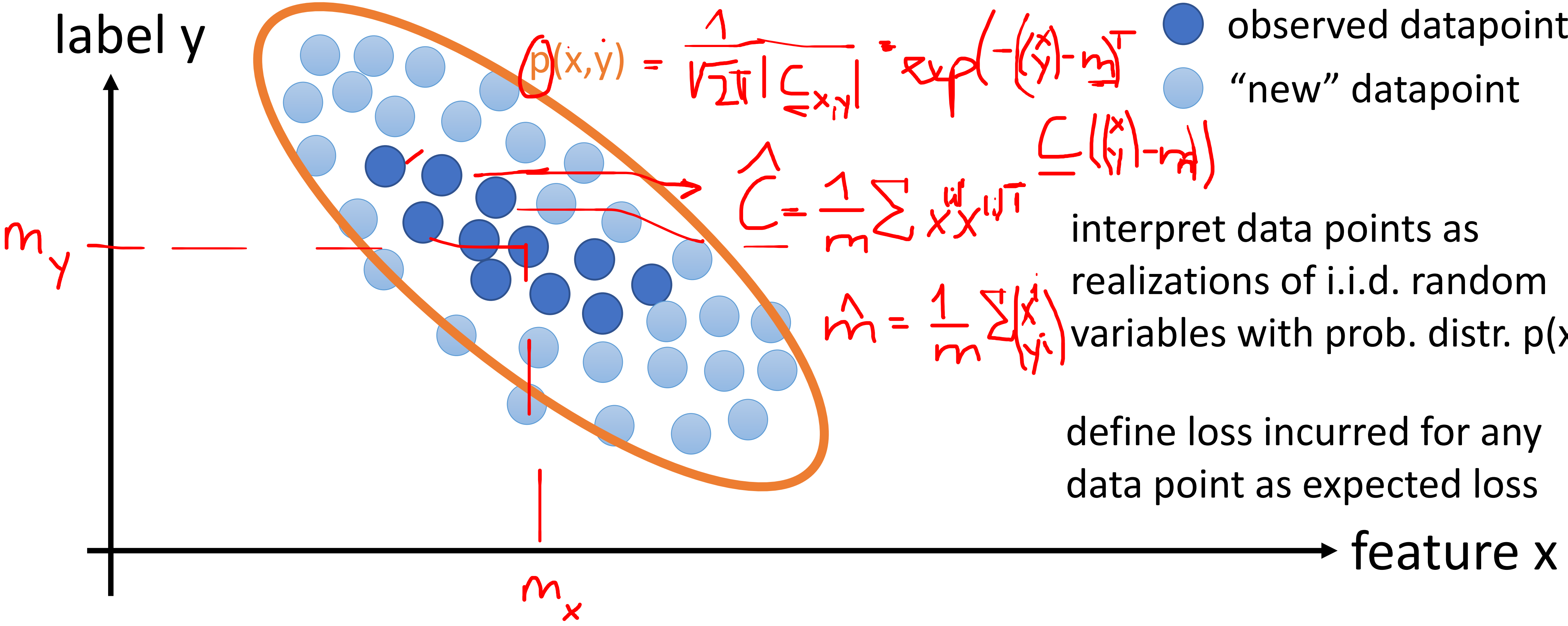
$$\mathbf{y} = (y^{(1)}, \ldots, y^{(m)})^{T} \in \mathbb{R}^{m}$$


label y
$(x^{(2)}, y^{(2)})$
$\hat{y} = h(x)$
$(x^{(1)}, y^{(1)})$
$\hat{y} = h'(x)$
feature x

Machine Learning.

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

What is Any Datapoint?



$$p(x,y) = \frac{1}{\sqrt{2\pi}\,|C_{x,y}|} \exp\left(-\left(\begin{pmatrix}x\\y\end{pmatrix}-m\right)^T C^{-1}\left(\begin{pmatrix}x\\y\end{pmatrix}-m\right)\right)$$

$$\hat{C} = \frac{1}{m}\sum x^{(i)} x^{(i)T}$$

$$\hat{m} = \frac{1}{m}\sum \begin{pmatrix}x^{(i)}\\y^{(i)}\end{pmatrix}$$

interpret data points as realizations of i.i.d. random variables with prob. distr. p(x,y)

define loss incurred for any data point as expected loss

Expected Loss or Risk

w.r.t p(x,y)

$$\min_{h \in \mathcal{H}} \mathbb{E}\{L((\mathbf{x}, y), h)\} := \int_{\mathbf{x},y} L((\mathbf{x}, y), h)\, dp(\mathbf{x}, y). \quad (2.14)$$

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)

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

$\rightarrow \infty$

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

with the average loss or empirical risk

$(h(x)-y)^2$

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

MSE

Empirical Risk Minimization

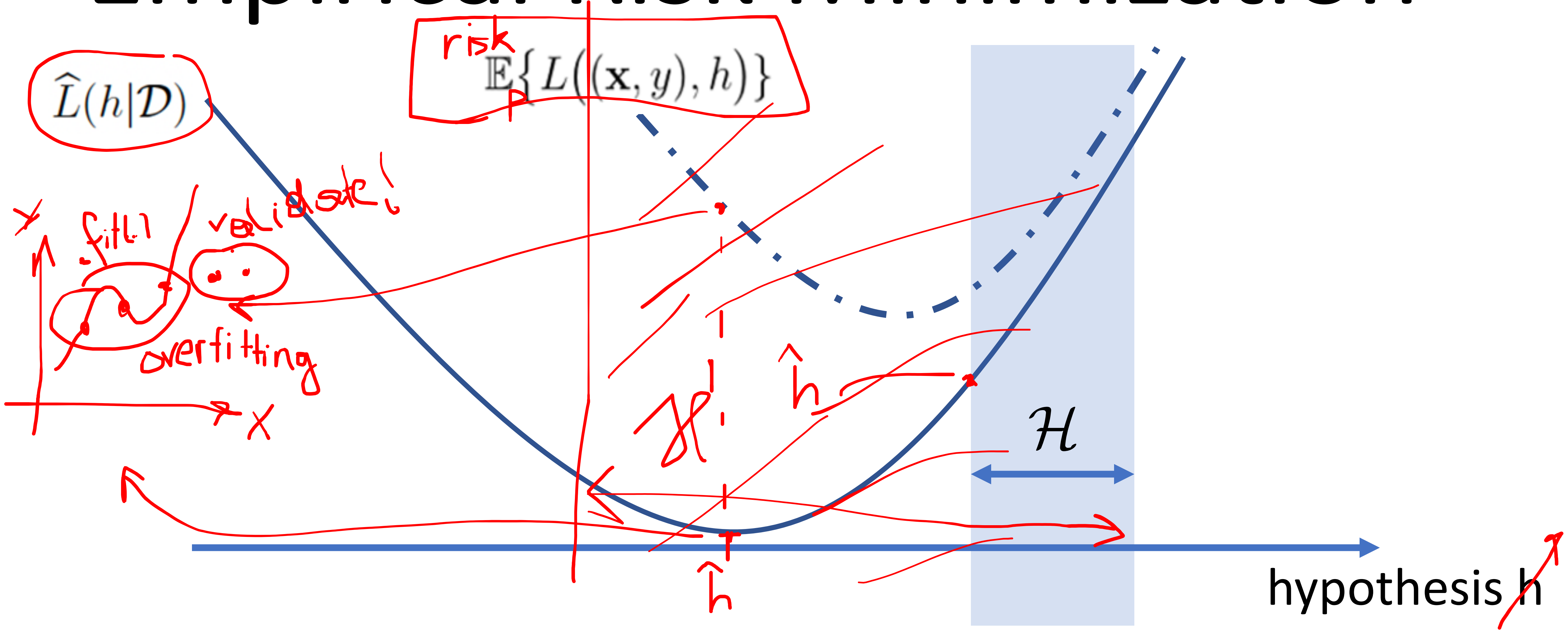
.fit(...)

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

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

model

Empirical Risk Minimization



ERM for Parametrized Models

learnt (optimal) parameter vector

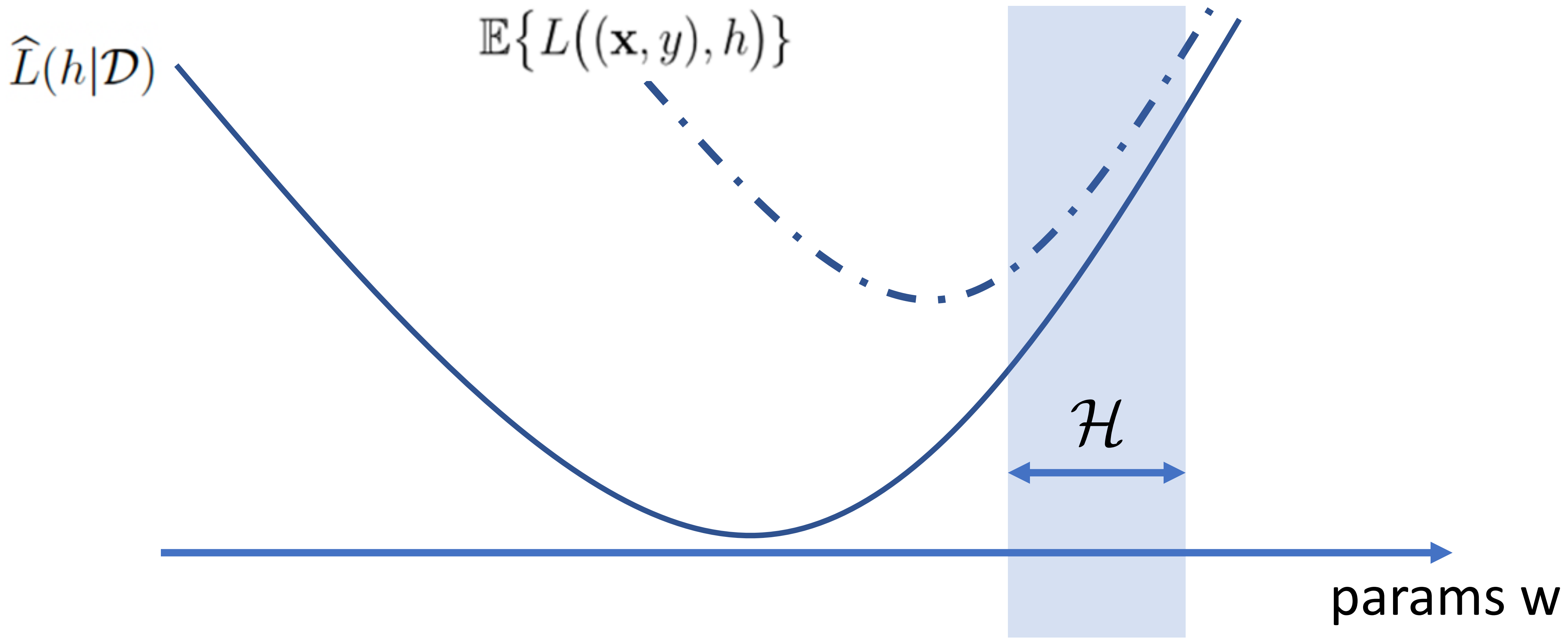
$$\widehat{\mathbf{w}} = \operatorname*{argmin}_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w})$$

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

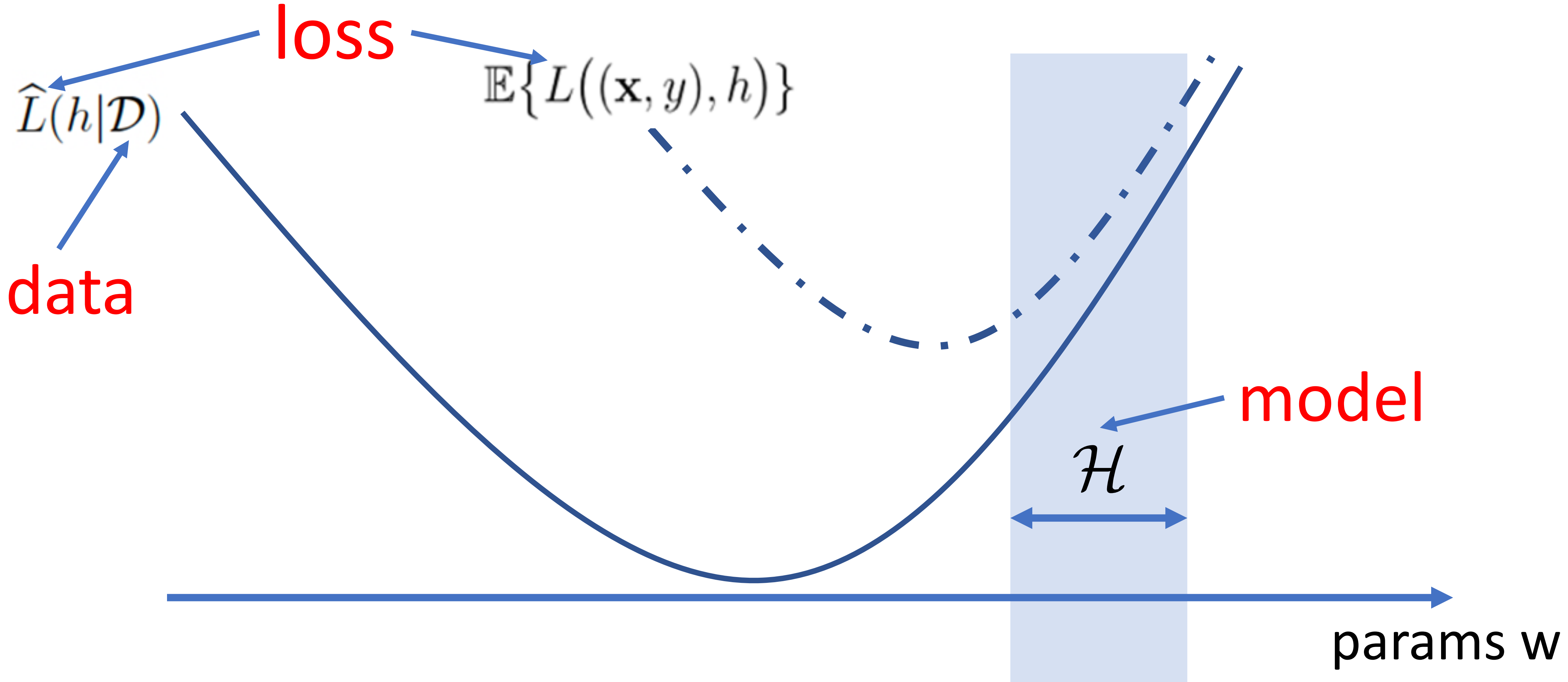
$$\text{with } f(\mathbf{w}) := \underbrace{(1/m) \sum_{i=1}^{m} L\big((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})}\big)}_{\widehat{L}\left(h^{(\mathbf{w})} | \mathcal{D}\right)} .$$

average loss or empirical risk

ERM for Param. Models



Design Choices in ERM

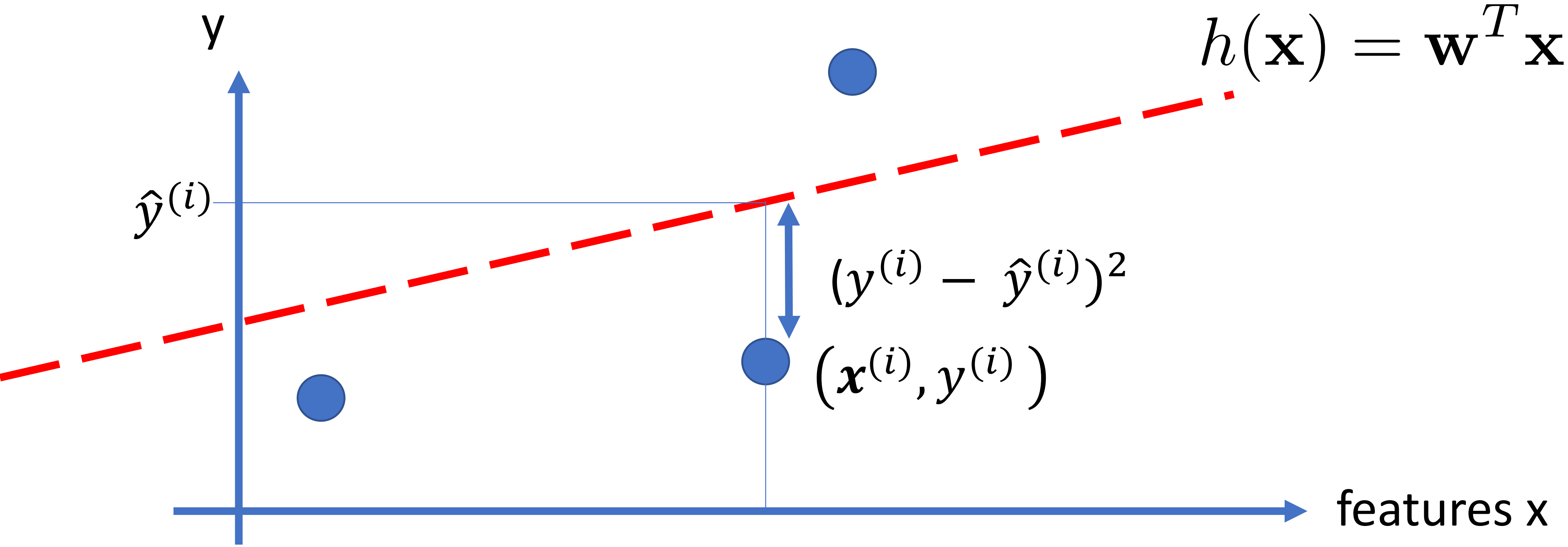


Design Choice: Model and Data

Linear Regression

- datapoints characterized by feature vector and numeric label
- model consists of linear hypothesis maps
- squared error loss

Linear Regression

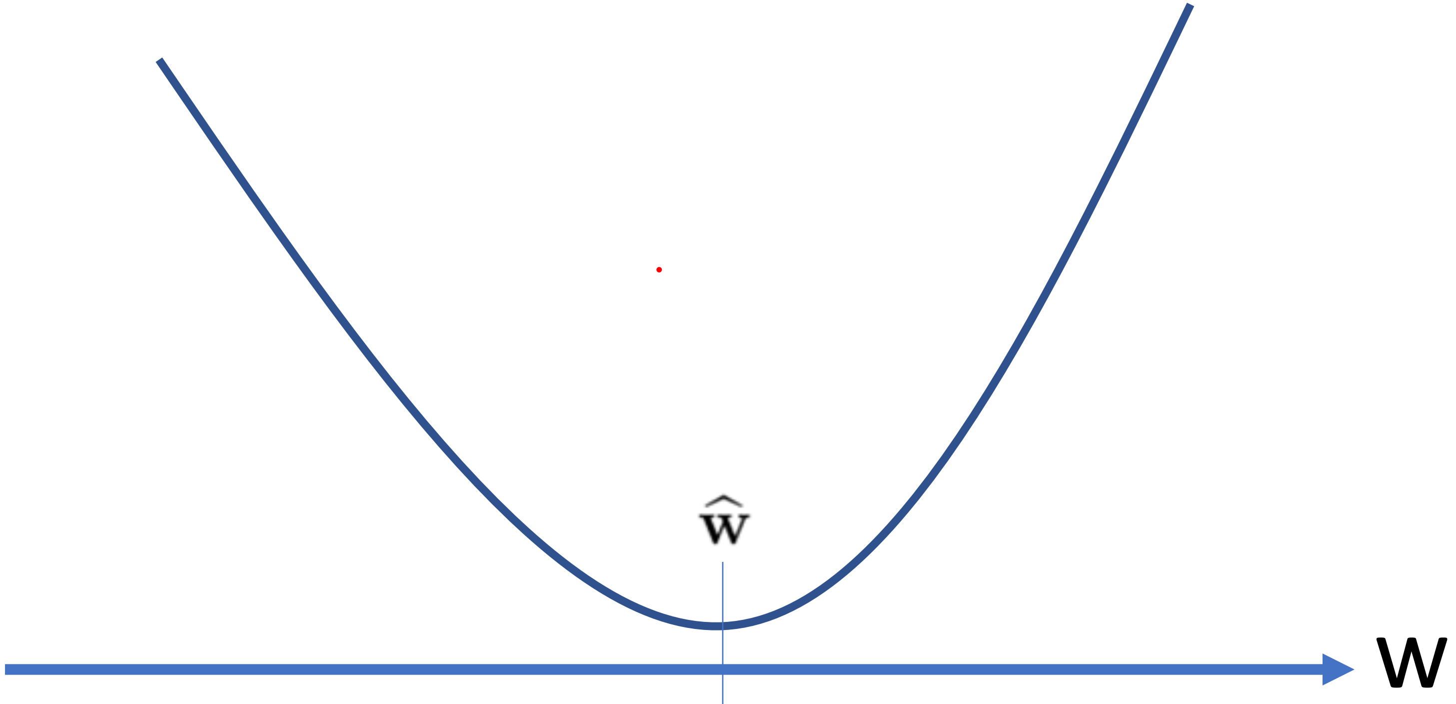


choose parameter/weight vector **w** to minimize average squared error loss

ERM for Linear Regression

$$\widehat{\mathbf{w}} = \underset{\mathbf{w} \in \mathbb{R}^n}{\operatorname{argmin}} (1/m) \sum_{m=1}^{m} \left(y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)} \right)^2. \quad (4.5)$$

$$\underline{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$$



Linear Regression in Python

$$\widehat{\mathbf{w}} = \underbrace{\operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^n} (1/m) \sum_{m=1}^{m} \big(\overset{\in\mathbb{R}}{y^{(i)}} - \mathbf{w}^T\mathbf{x}^{(i)}\big)^2}_{f(w)}. \qquad (4.5)$$

$\nabla f(w) = 0$

$X^T X w = X y$

```
In [81]: # Create a linear regression model
         lr = LinearRegression()
         # Fit the model to our data in order to get
         lr = lr.fit(features, labels)
```

$\to$ lr.coef_

$w =$

$X = | x_1 \; \vdots \; x_n$

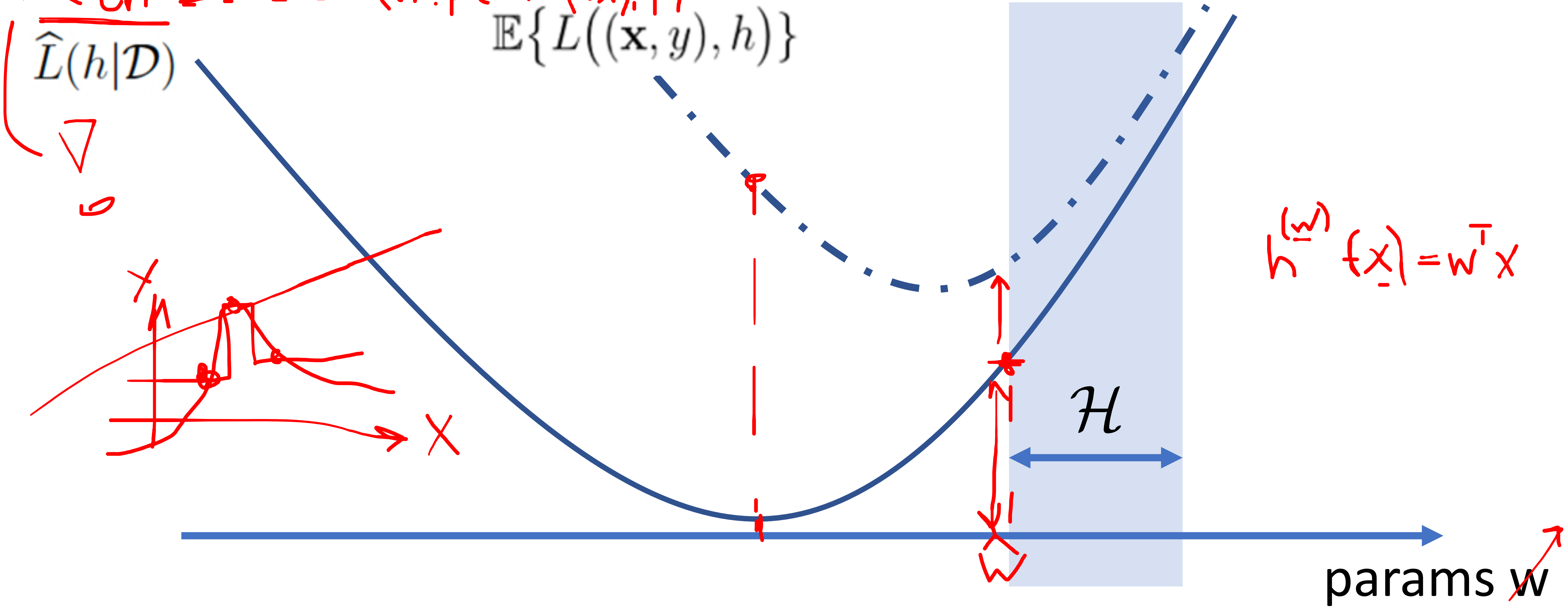
$$\mathbf{X} = \left(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\right)^T \in \mathbb{R}^{m\times n} \qquad \mathbf{y} = \left(y^{(1)}, \ldots, y^{(m)}\right)^T \in \mathbb{R}^m$$

train test split → X, y → X', y'

```python
# create and train a linear model
lr = LinearRegression()
lr = lr.fit(X, y)
w_hat = lr.coef_
trainerr = mean_squared_error(lr.predict(X), y)
```

"training error"

valerr = - - - (lr.predict(X'), y')

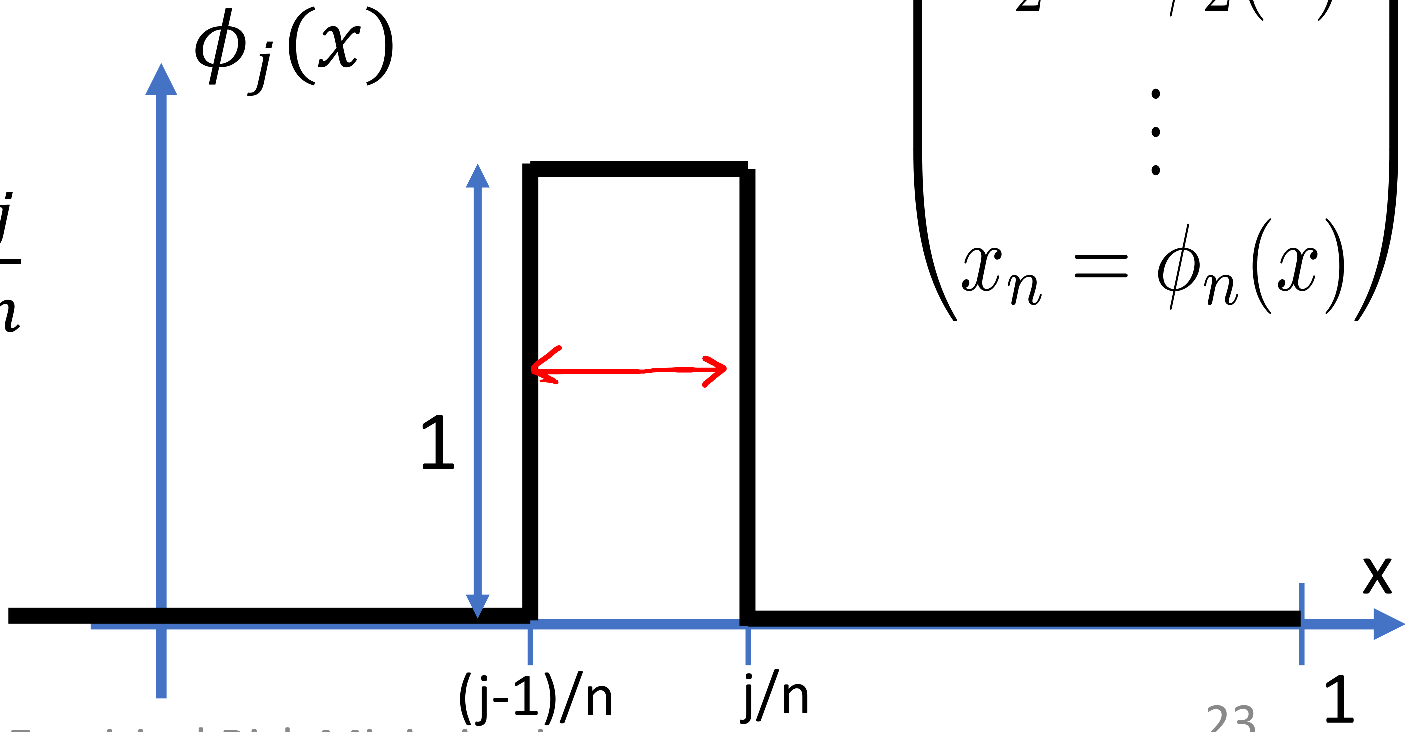


Upgrade Linear Model with new Features !

- consider data points with single numeric feature x
- construct new features $x_1, \ldots, x_n$

$$\begin{pmatrix} x_1 = \phi_1(x) \\ x_2 = \phi_2(x) \\ \vdots \\ x_n = \phi_n(x) \end{pmatrix}$$

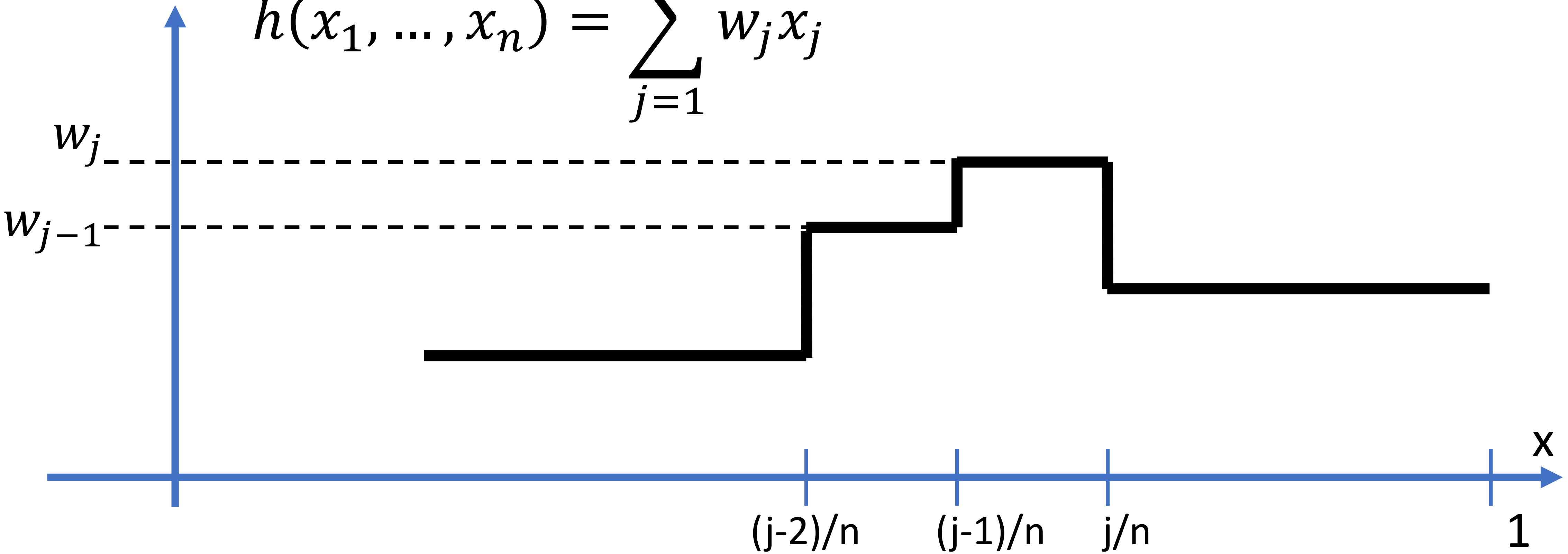
- $x_j = \begin{cases} 1 \; for \;\; \frac{j-1}{n} \leq x \leq \frac{j}{n} \\ 0 \; for \; all \; other \; x. \end{cases}$



You Can Do Anything with Linear Predictors!

- h(x) is linear in new features but non-linear in raw feature x!

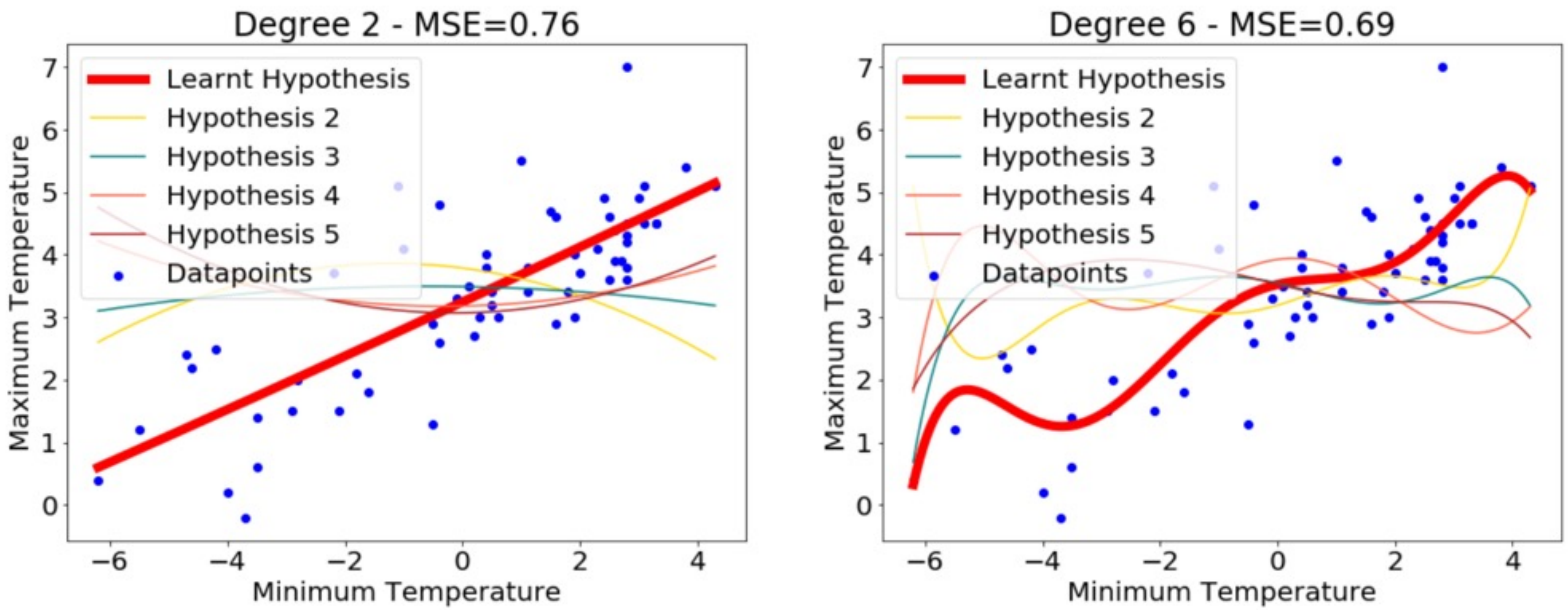
$$h(x_1, \ldots, x_n) = \sum_{j=1}^{n} w_j x_j$$



Polynomial Regression

$$\mathcal{H}^{(n)}_{\text{poly}} = \{h^{(\mathbf{w})} : \mathbb{R} \rightarrow \mathbb{R} : h^{(\mathbf{w})}(x) = \sum_{j=1}^{n} w_j x^{j-1}, \\ \text{with some } \mathbf{w} = (w_1, \ldots, w_n)^T \in \mathbb{R}^n\}. \quad (3.4)$$

Polynomial Regression



from notebook of TA George
https://github.com/alexjungaalto/cs-c3240spring2022/blob/main/George_Demo_PolynomialRegression.ipynb

Polynomial Regression= Lin. Reg. with Feature Transform.

linear map

$$\mathbf{w}^T\mathbf{x} = \sum_{j=1}^{n} w_j x_j$$

feature map

single feature x

$$\begin{pmatrix} x_1 = \phi_1(x) \\ x_2 = \phi_2(x) \\ \vdots \\ x_n = \phi_n(x) \end{pmatrix}$$

$$h(x) = \sum_{j=1}^{n} w_j \phi_j(x)$$

sklearn.preprocessing.PolynomialFeatures

.preprocessing.PolynomialFeatures(*degree=2*, *, *interaction_only=False*, *include_bias=Tru*

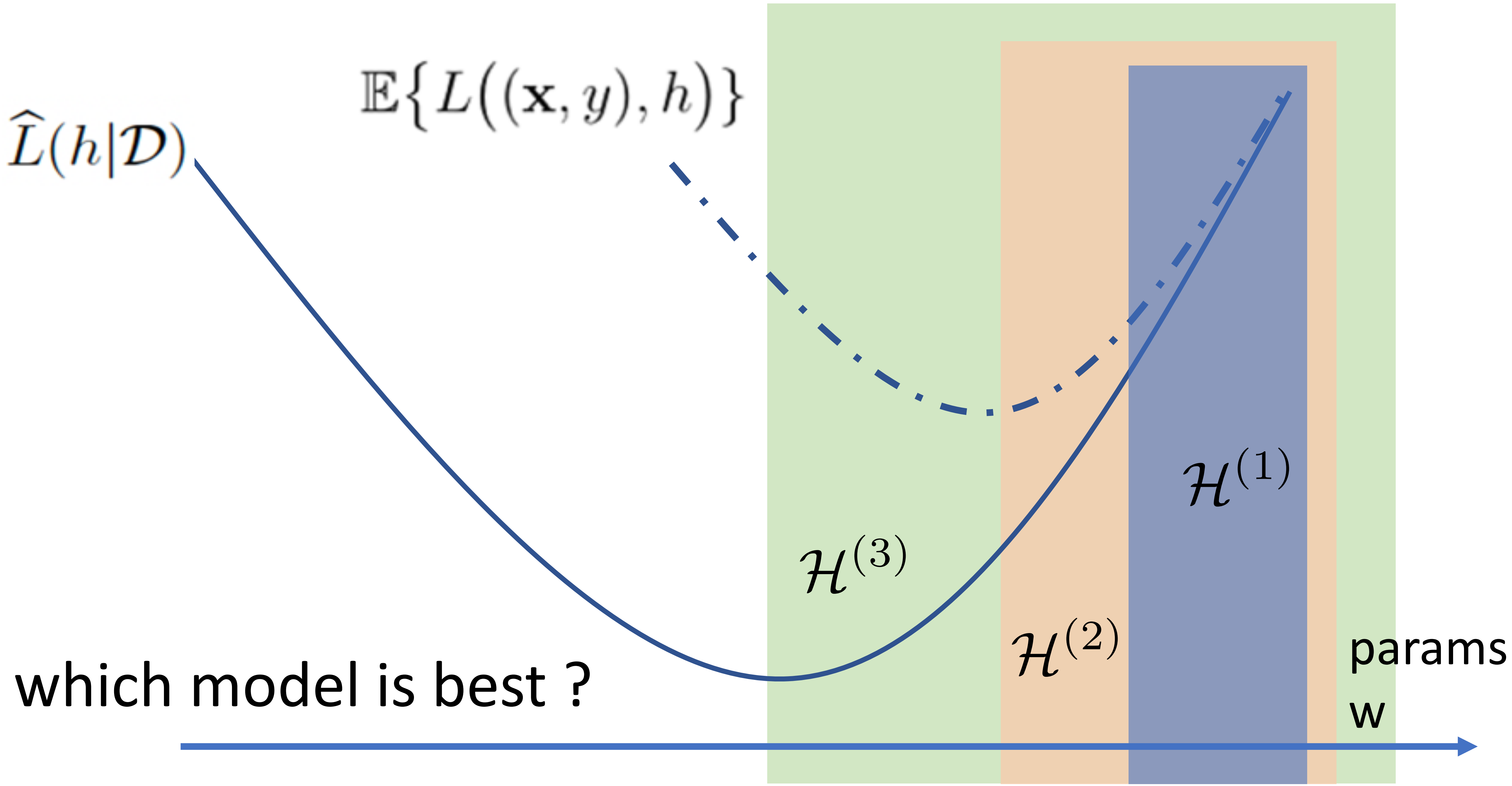
sklearn.linear_model.LinearRegression

class sklearn.linear_model.LinearRegression(*, *fit_intercept=True*, *normalize='deprecated'*, *copy_X=True*, *n_*
positive=False)

Polynomial Features

we can use anything as features that can be computed or measured easily !

	Date	Max temp	Min temp	(Min temp)^2
0	2020-2-1	3.0	1.9	3.61
1	2020-2-2	4.9	2.4	5.76
2	2020-2-3	2.6	-0.4	0.16
3	2020-2-4	-0.2	-3.7	13.69
4	2020-2-5	2.5	-4.2	17.64

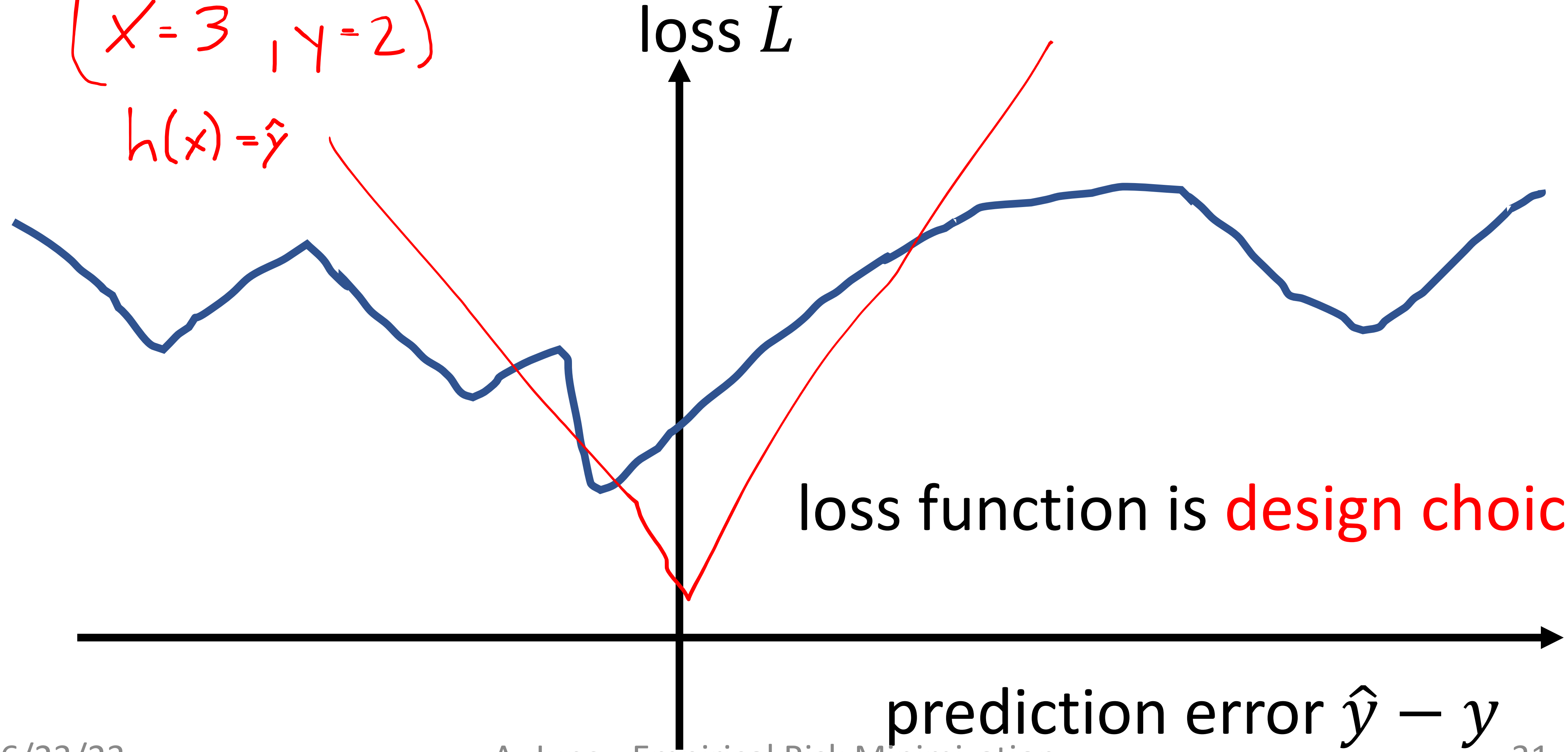

$\widehat{L}(h|\mathcal{D})$
$\mathbb{E}\{L((\mathbf{x},y),h)\}$
$\mathcal{H}^{(1)}$
$\mathcal{H}^{(3)}$
$\mathcal{H}^{(2)}$
params
w
which model is best ?

Design Choice: Loss Function

Measuring Error Size via Loss Functions

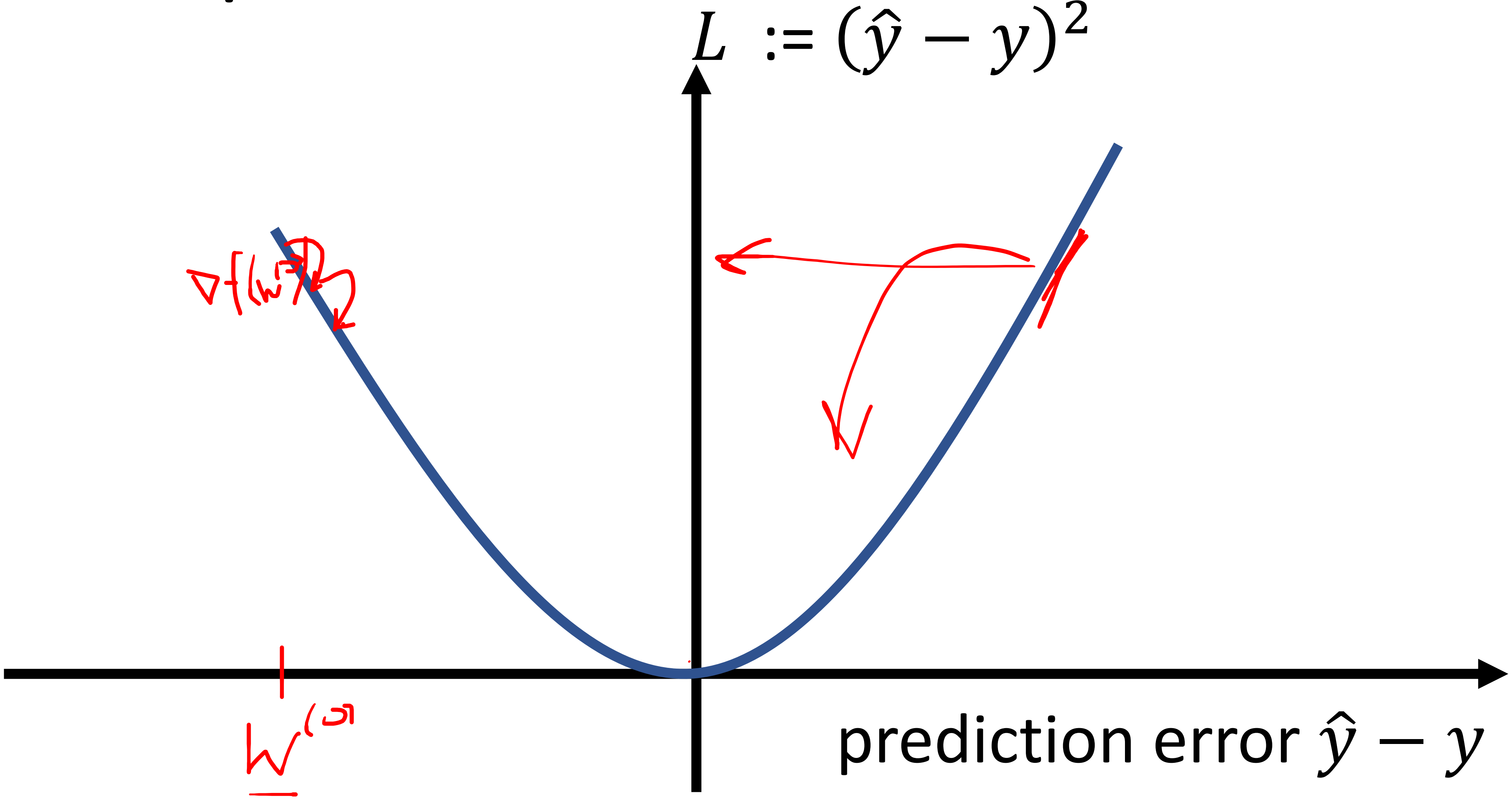
$(x=3, y=2)$

$h(x)=\hat{y}$

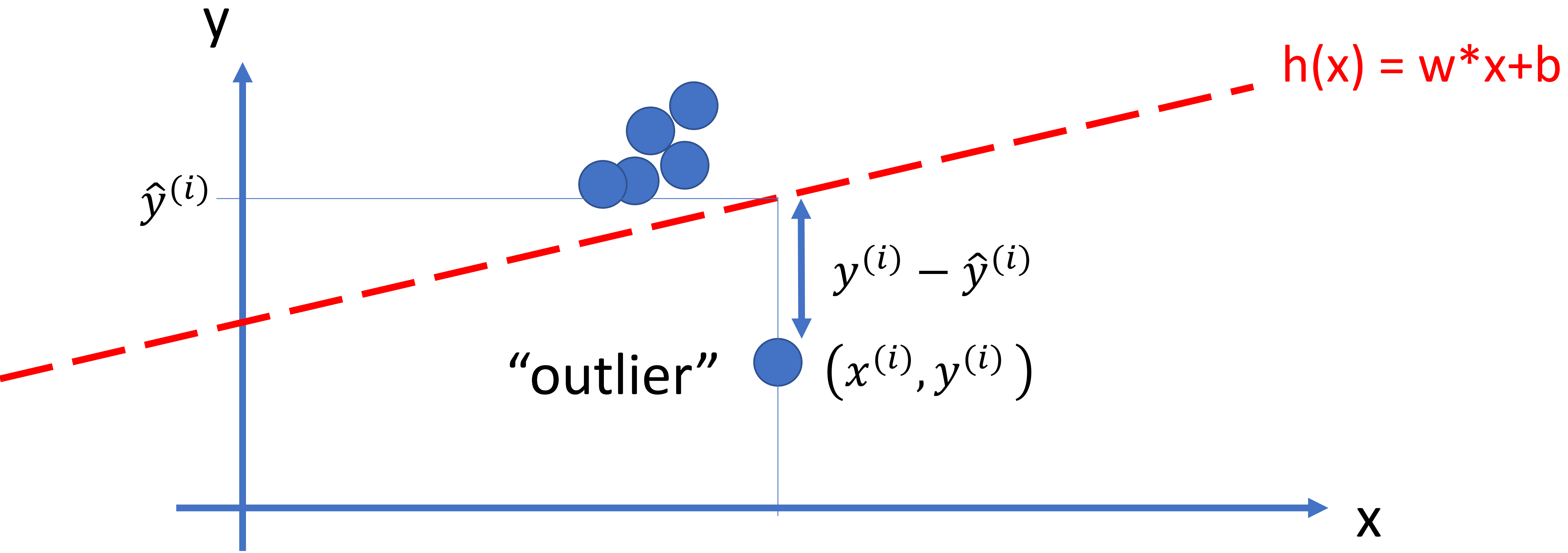


loss function is design choice !

The Squared Error Loss

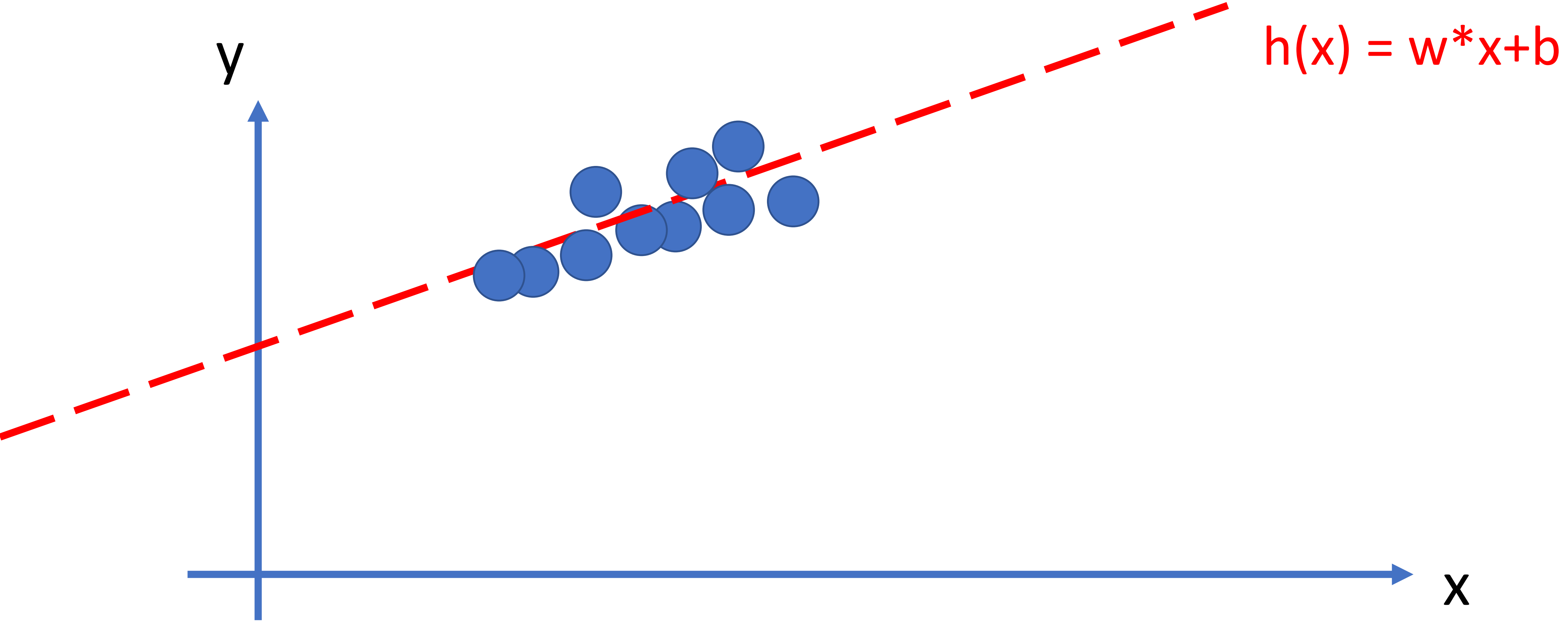


Squared Error Loss Sensitive to Outliers

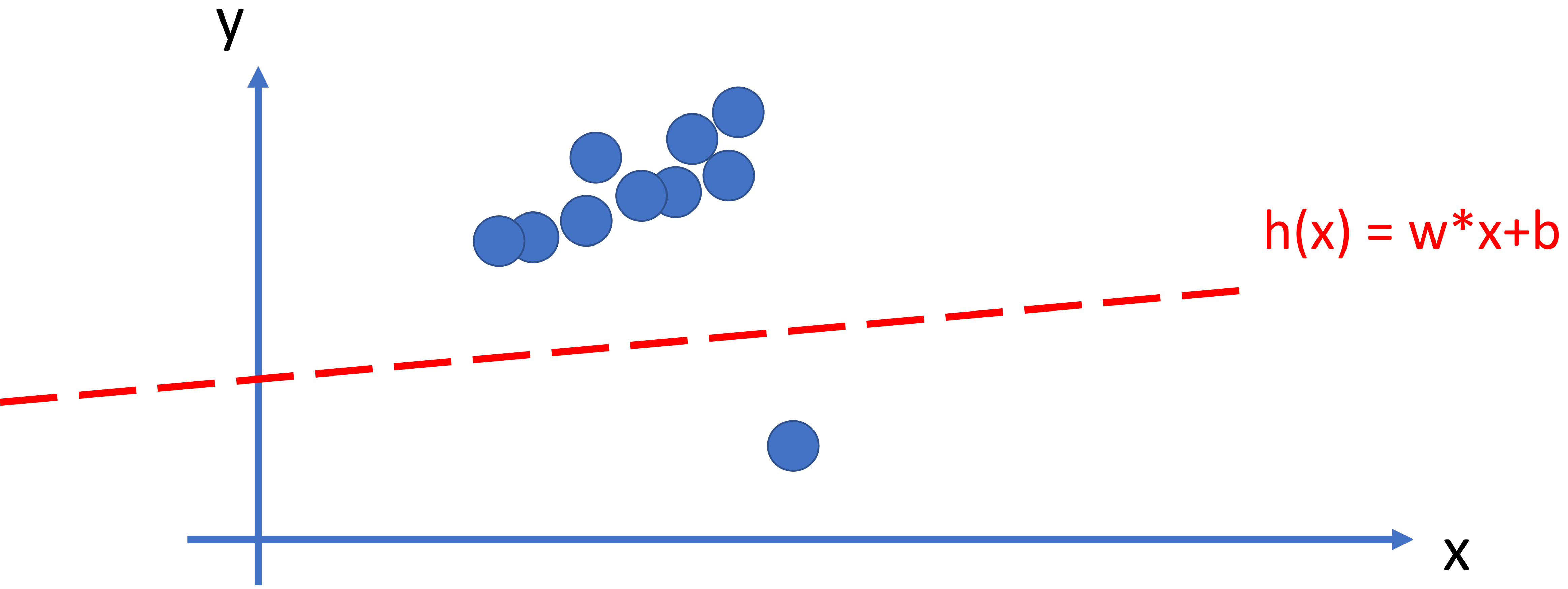


min. squared error loss forces predictor towards outlier

Train Linear Model on “Clean Data”

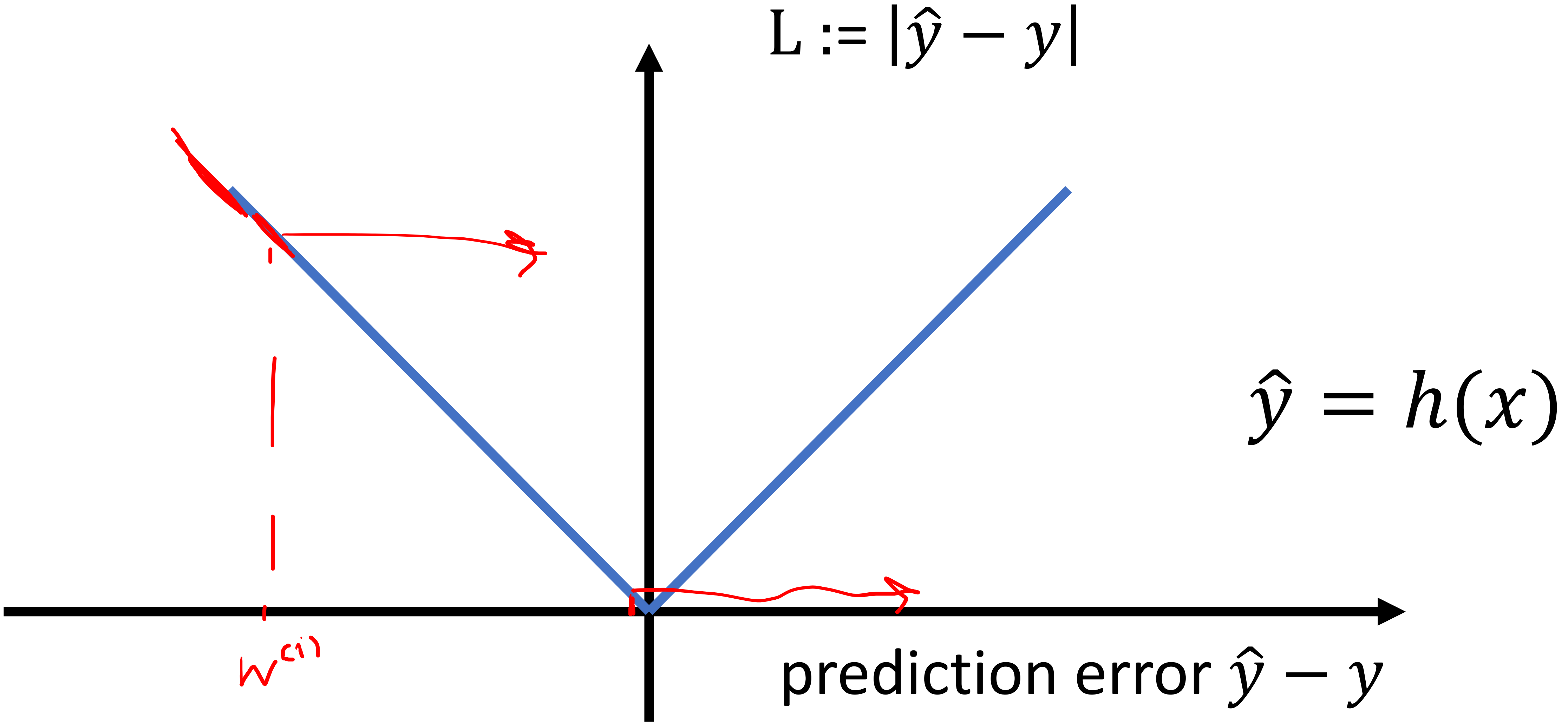


Training Set with a SINGLE OUTLIER !

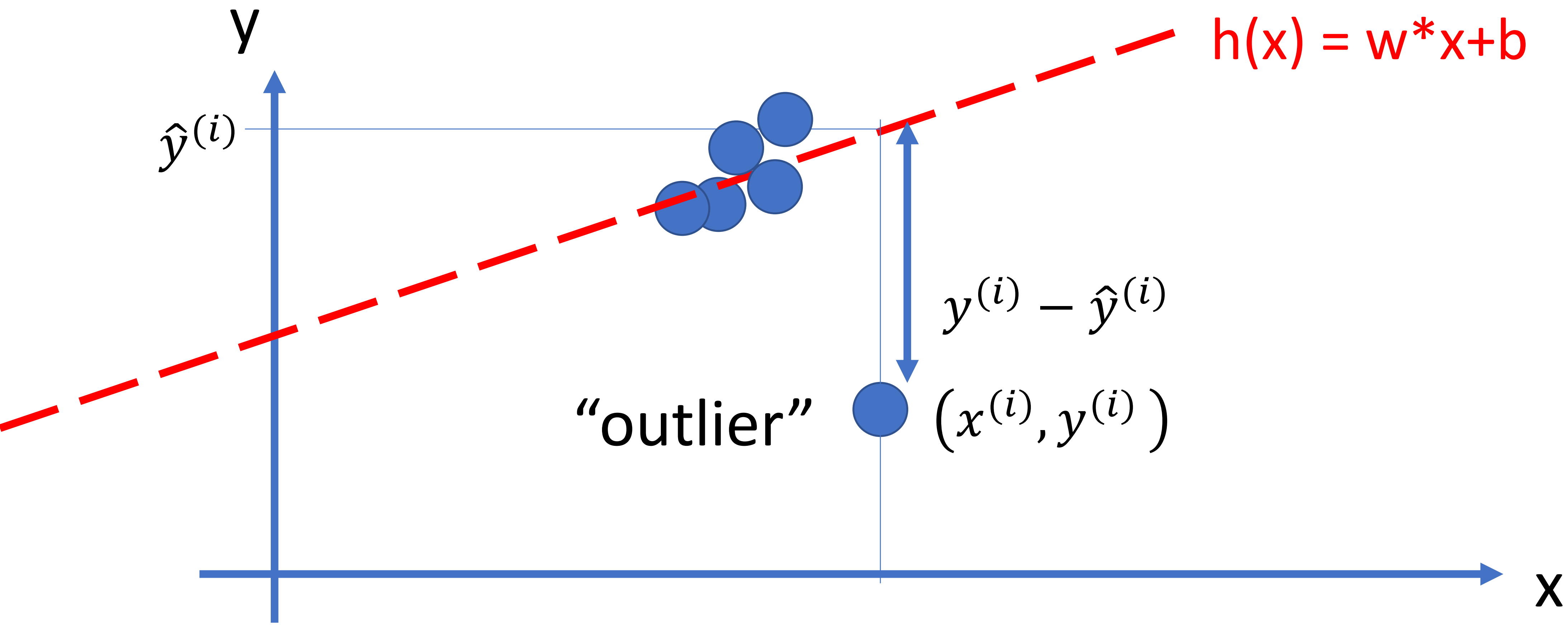


How to make learning robust against presence of few outliers in training set ?

The Absolute Error Loss

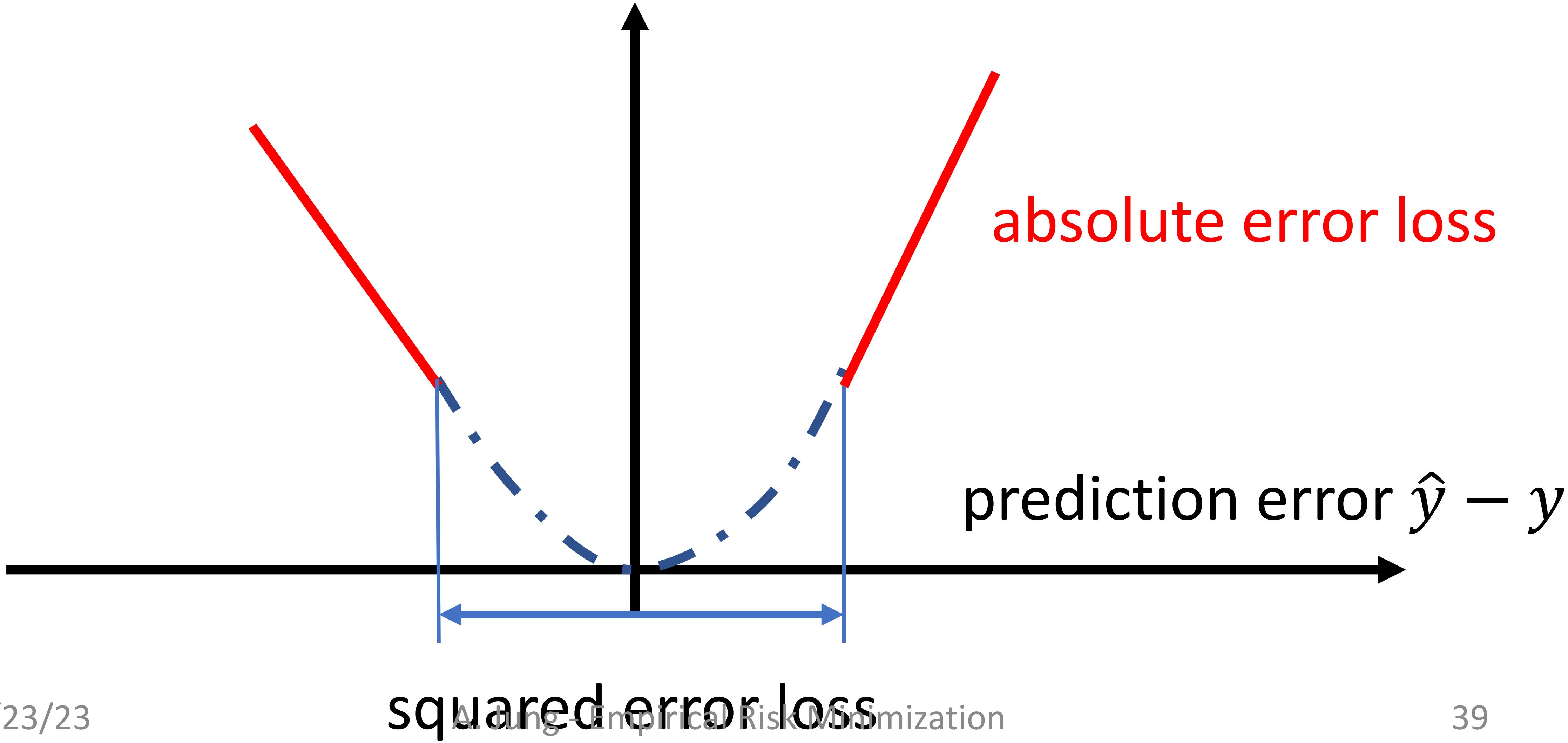


Absolute Error Loss Robust to Outliers



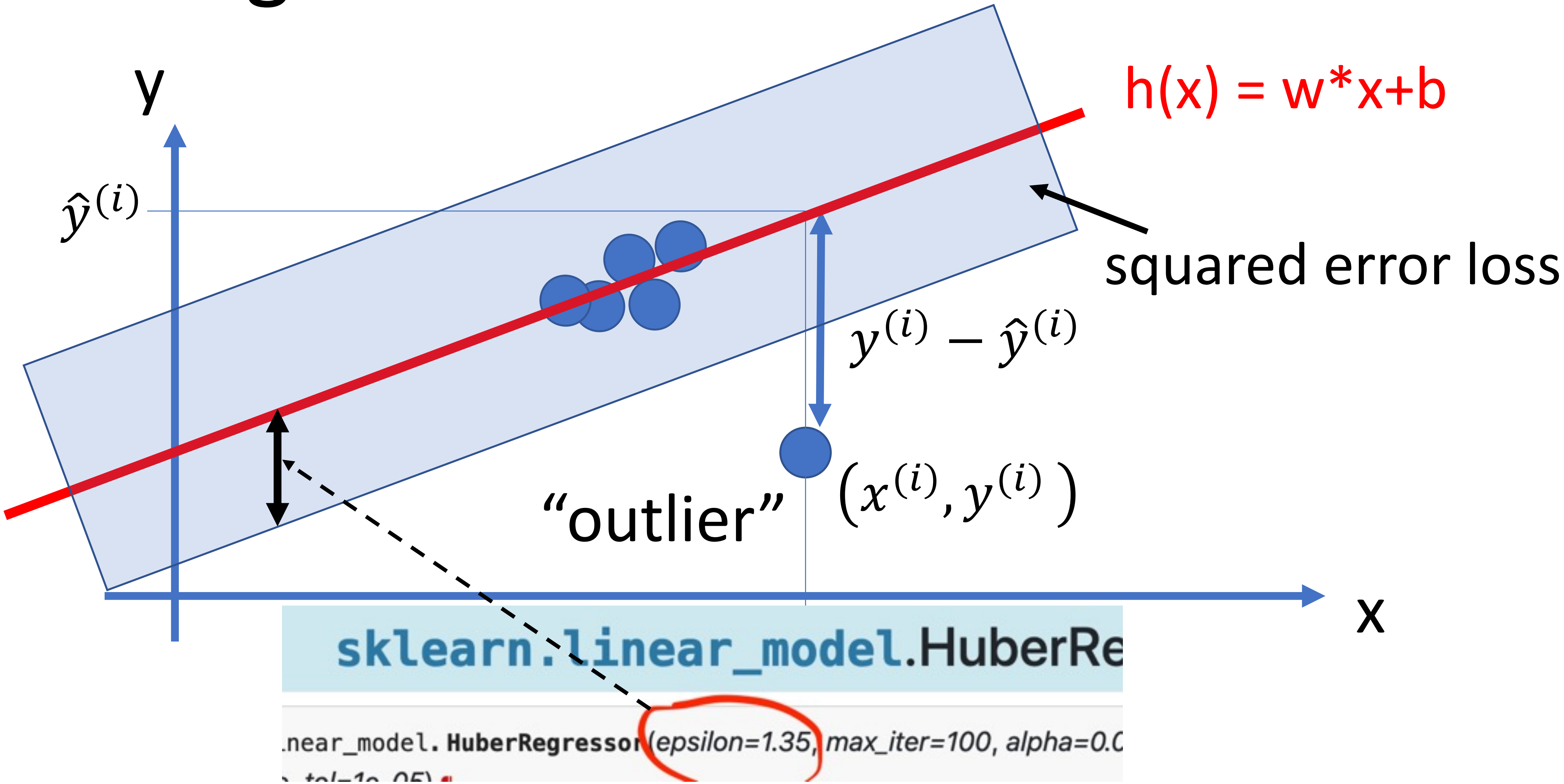
absolute error "tolerates" few outliers

Huber Loss

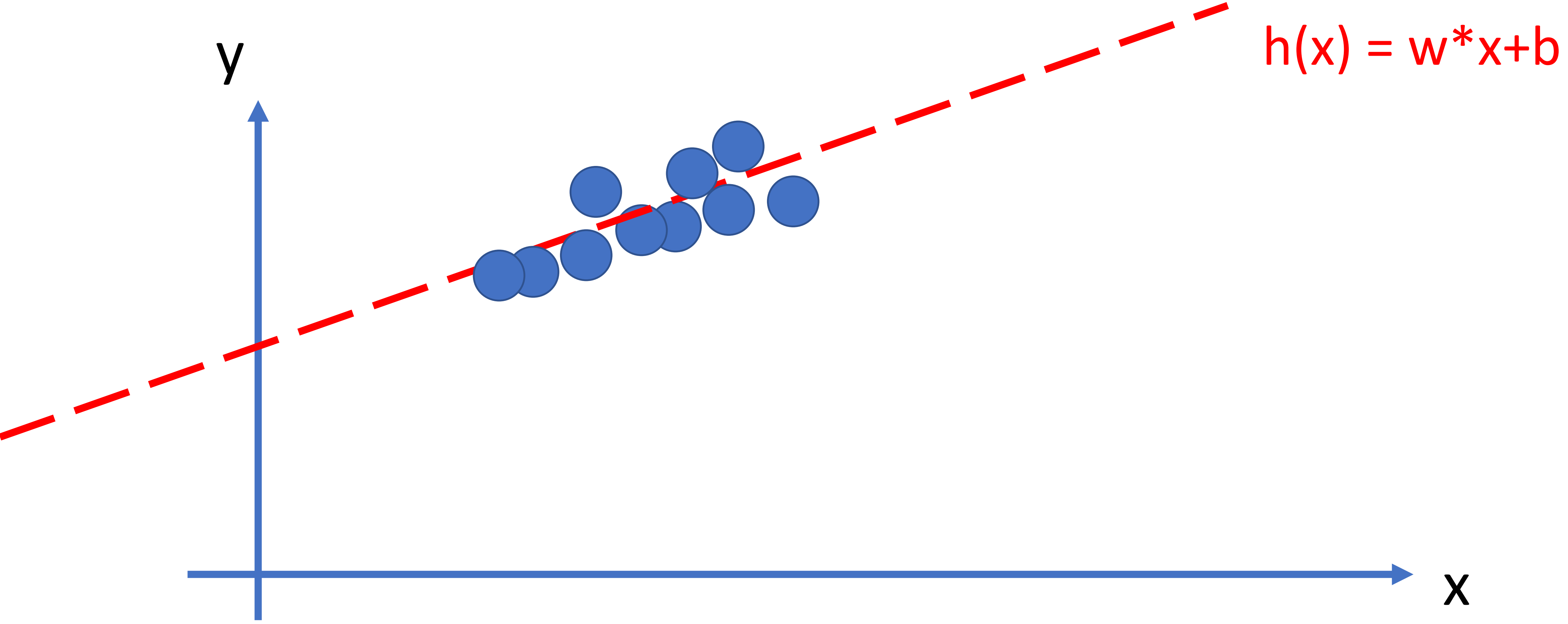


absolute error loss
prediction error $\hat{y} - y$
squared error loss

Fitting Linear Predictor with Huber Loss



Train Linear Model on “Clean Data”



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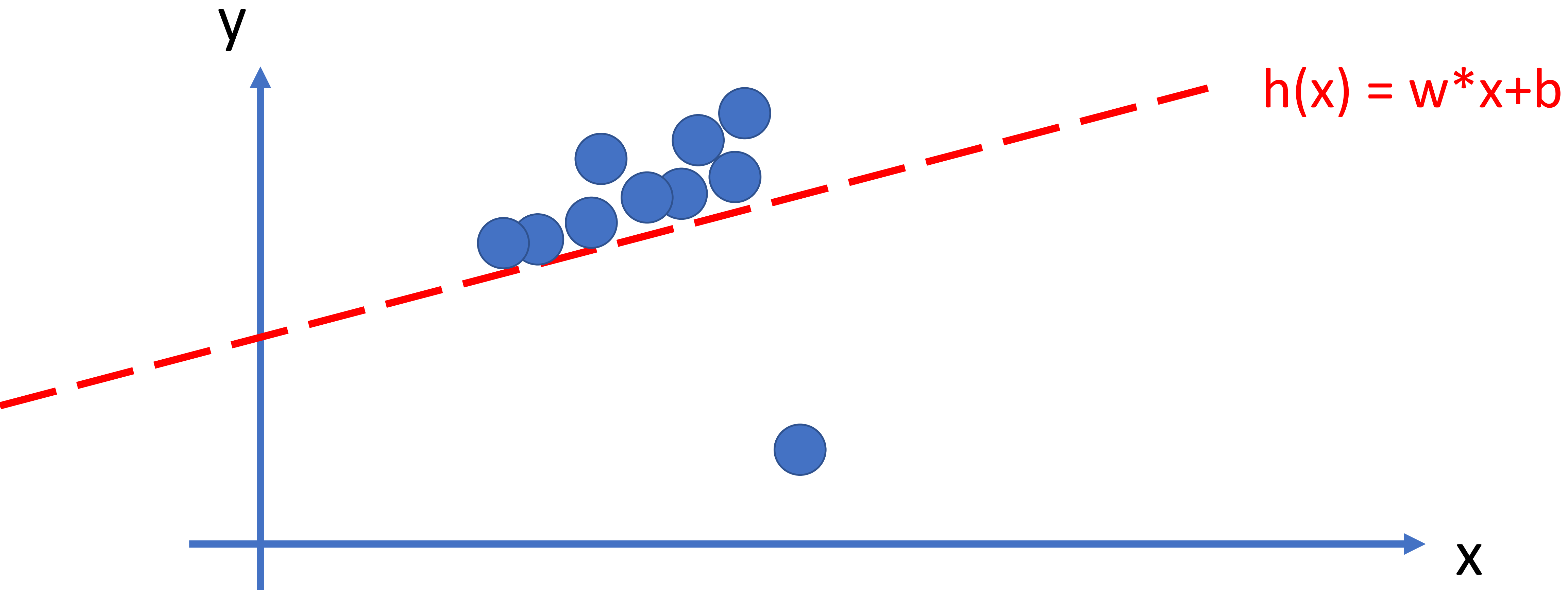

Huber vs. Squared Error Loss

Squared Error

- cvx and diff.able
- minimized via simple gradient descent
- sensitive to outliers

Huber

- cvx and non-diff.
- requires more advanced opt. methods
- robust against outliers

Summary

- ultimate quality measure: expected loss or risk
- approximate risk by average loss (empirical risk)
- many ML methods are instances of ERM
- three design choices of ERM: data, model and loss
- ERM can fail if empirical risk deviates from risk