Regression

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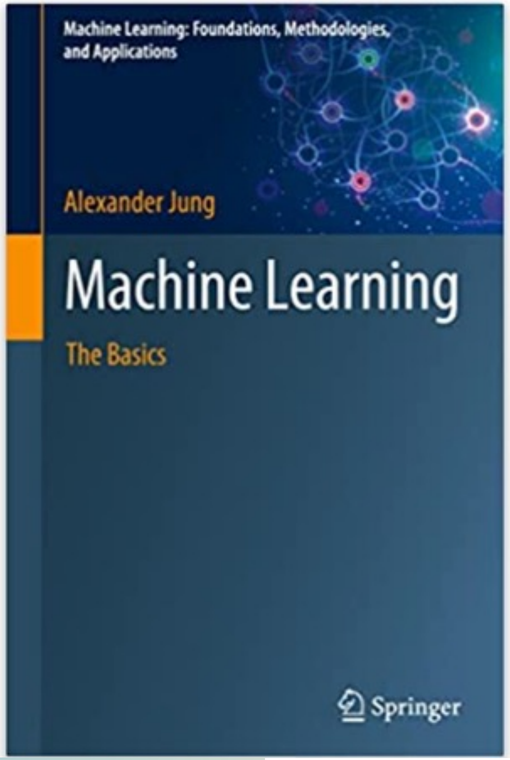
Reading.

- Chapter 3.1-3.2 of AJ, “Machine Learning: The Basics”, Springer, 2022.https://mlbook.cs.aalto.fi



https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html

Learning Goals:

- know about notion of expected loss or risk
- know that average loss approximates risk
- know about empirical risk minimization
- know some regression methods
- know comp./stat. trade offs for diff. loss func.

What is ML About ?

fit models to data to make

predictions or forecasts !

Data. Model. Loss.

data: set of data points (x,y)

model: set of hypothesis maps h(.)

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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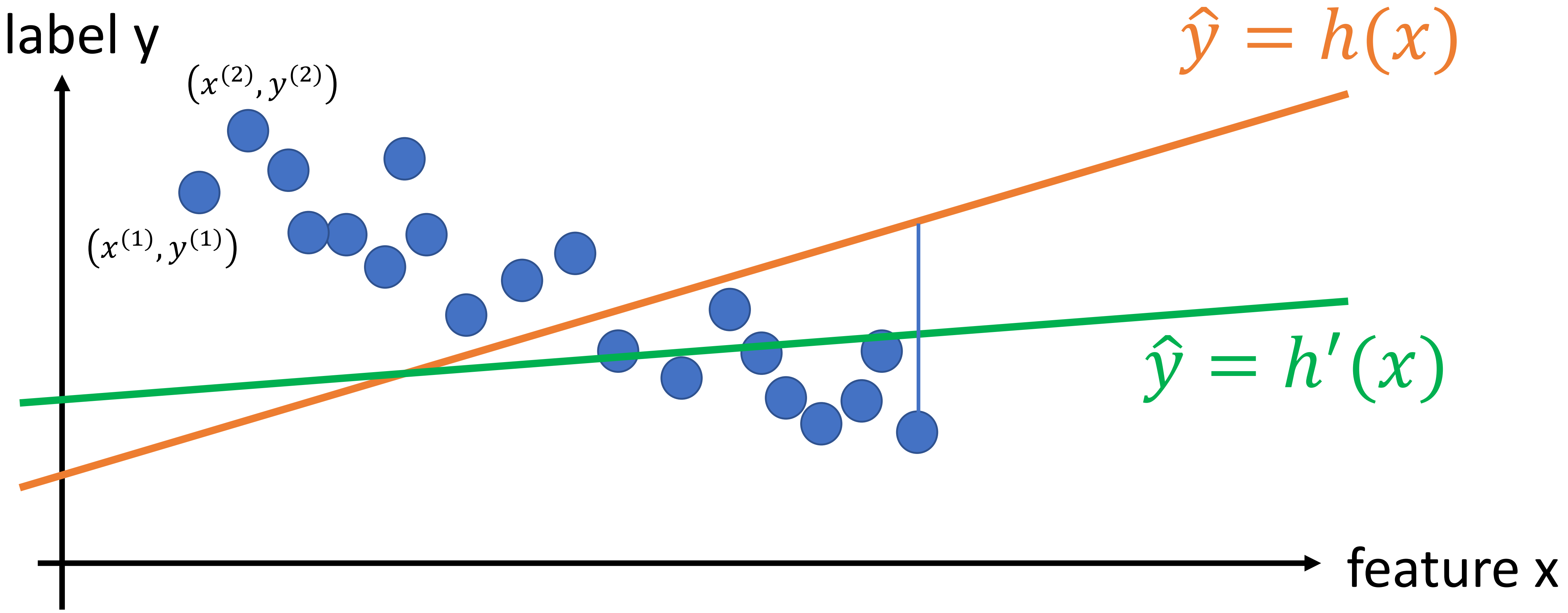
stack feature vecs into matrix

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

stack labels into vector

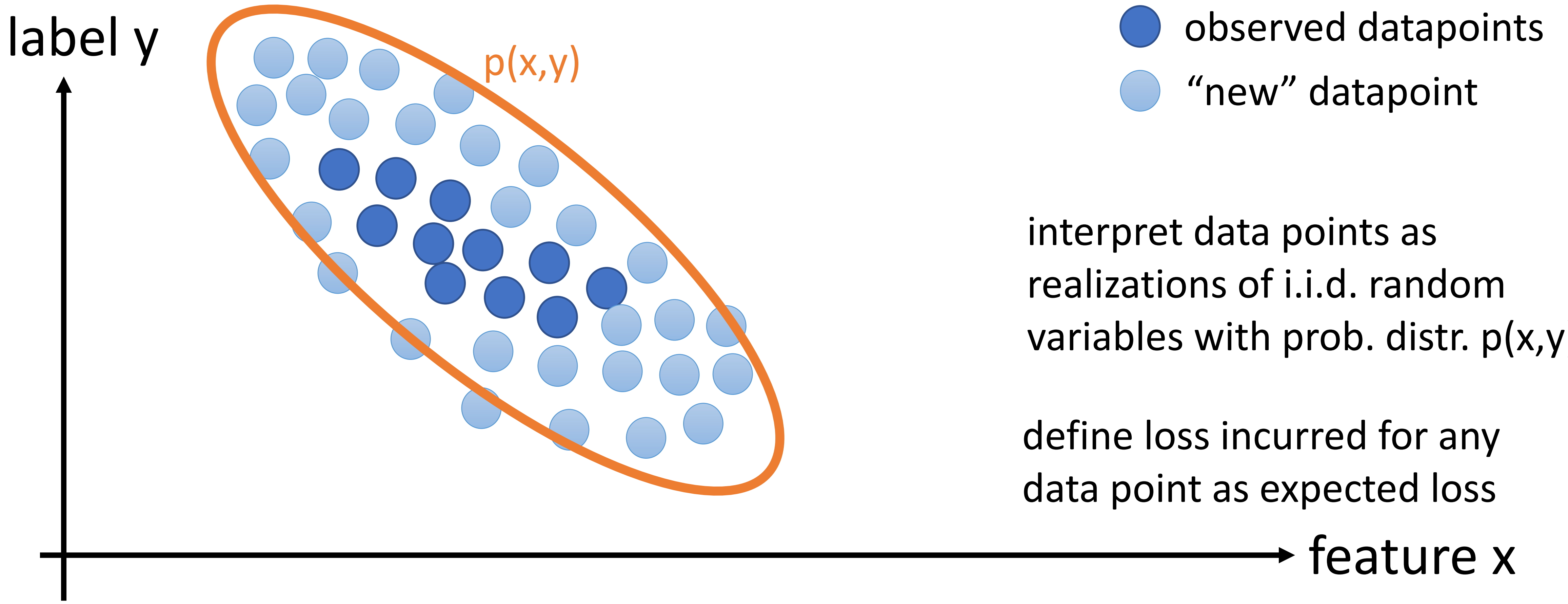
$$\mathbf{y} = (y^{(1)}, \ldots, y^{(m)})^T \in \mathbb{R}^m$$


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

Machine Learning.

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

What is Any Datapoint?



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

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

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)

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

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

with the average loss or empirical risk

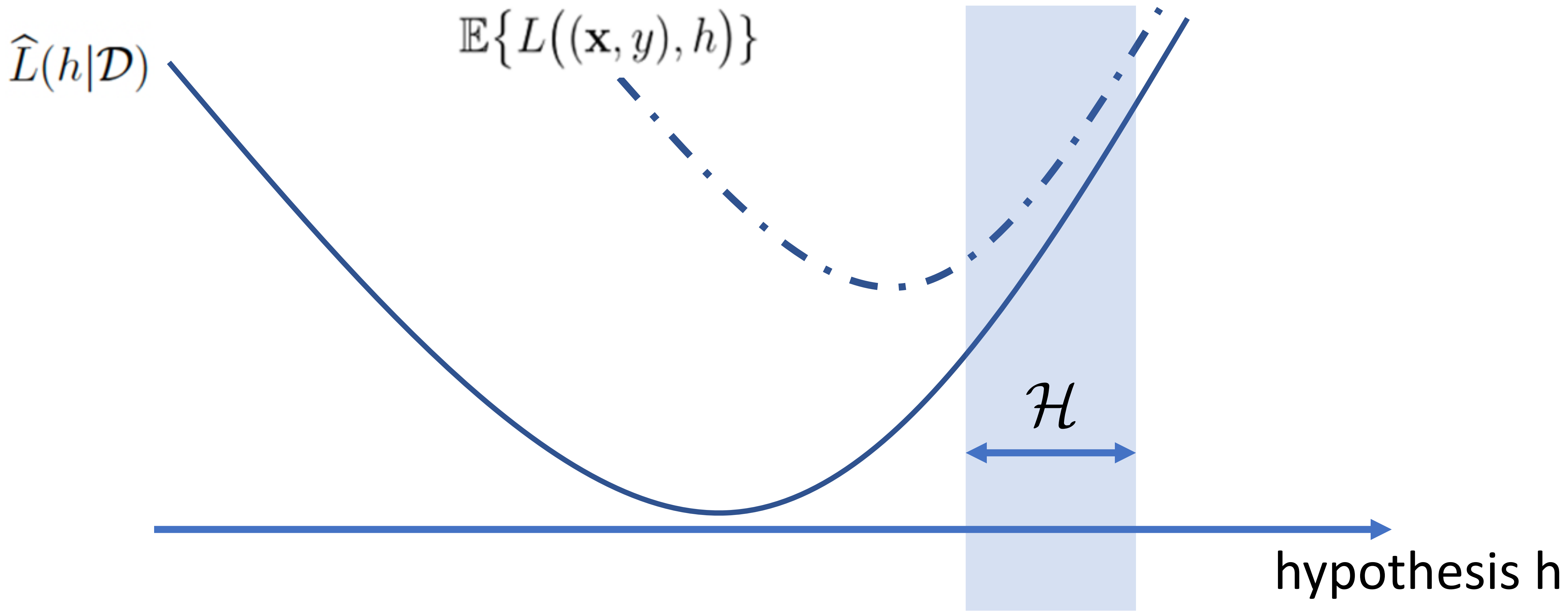
$$\widehat{L}(h|\mathcal{D}) = (1/m) \sum_{i=1}^{m} L((\mathbf{x}^{(i)}, y^{(i)}), h). \quad (2.16)$$

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

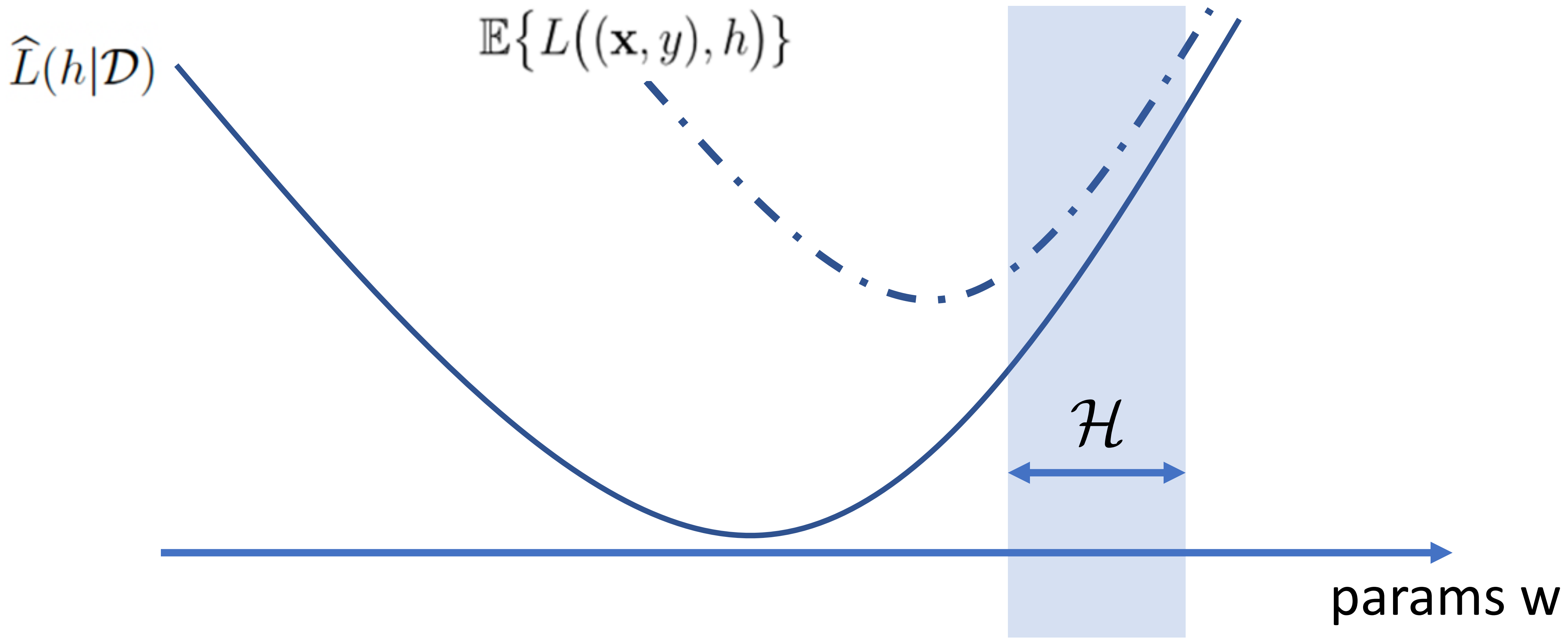
loss incurred by h(.) for i-th data point

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

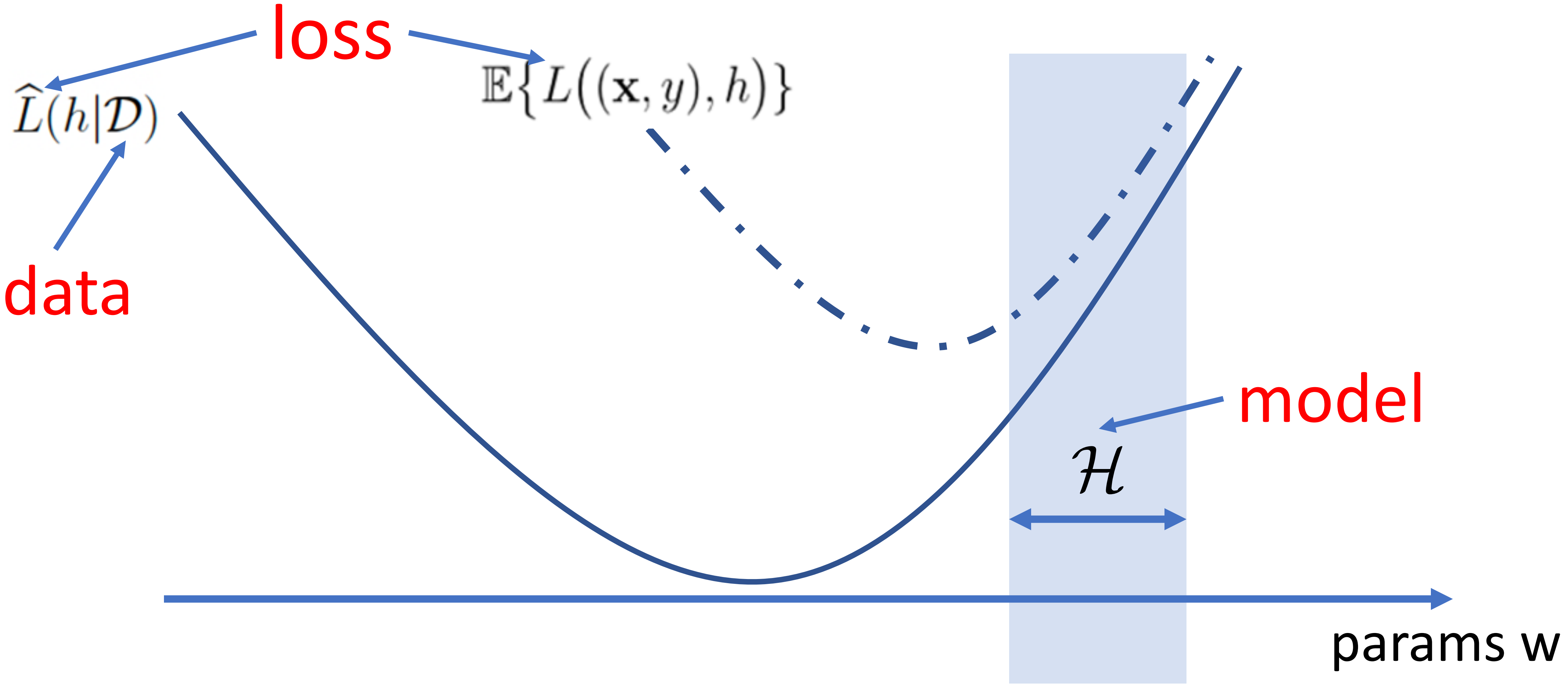
$$\text{with } f(\mathbf{w}) := \underbrace{(1/m) \sum_{i=1}^{m} L\big((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})}\big)}_{\widehat{L}\left(h^{(\mathbf{w})} | \mathcal{D}\right)} .$$

average loss or empirical risk

ERM for Param. Models



Design Choices in ERM



Design Choice:
Model and Data

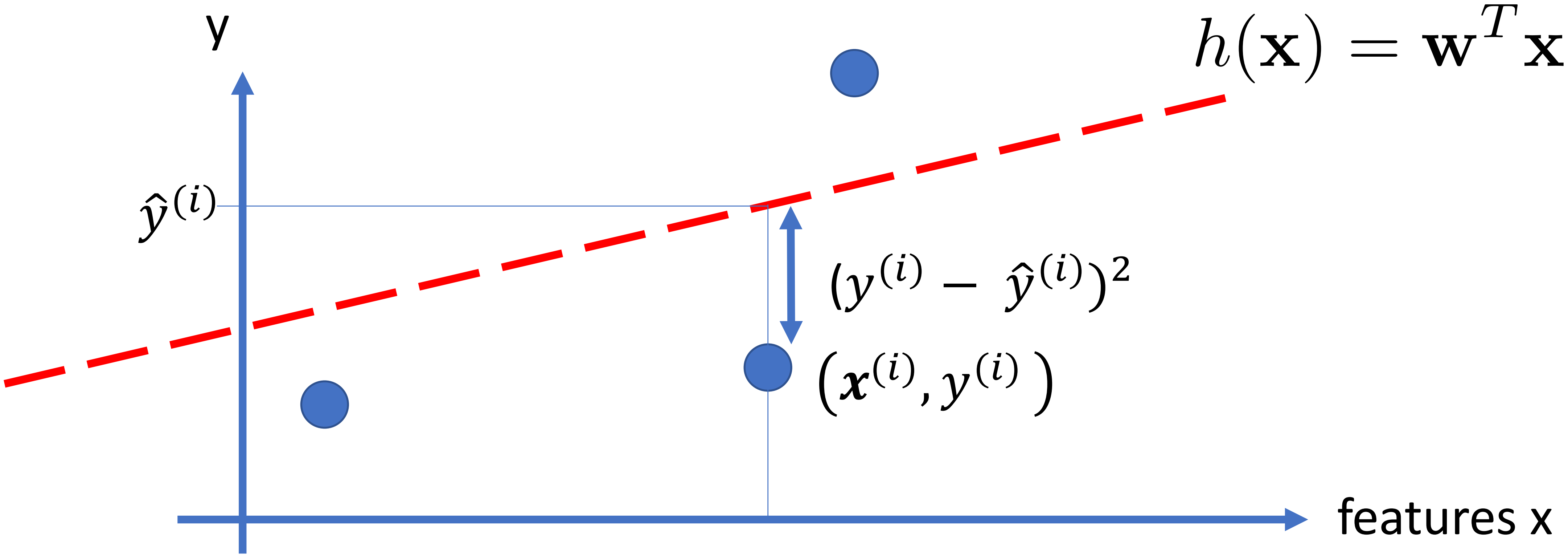
Linear Regression

- datapoints with numeric features and label
- model consists of linear maps
- squared error loss

sklearn.linear_model.LinearRegression

class `sklearn.linear_model.`**`LinearRegression`**(**, fit_intercept=True, normalize='deprecated', copy_X=True, n_jobs=None, positive=False*) [source]

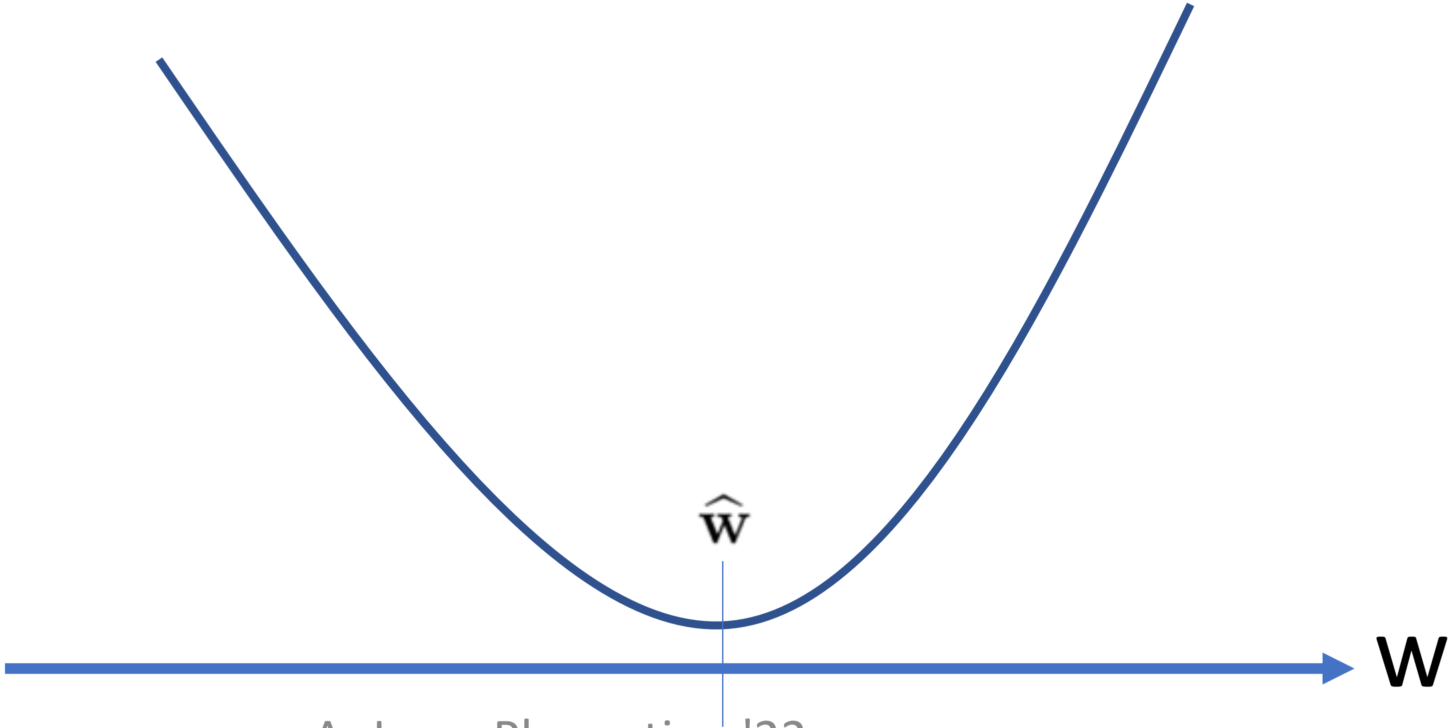
Linear Regression



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

ERM for Linear Regression

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



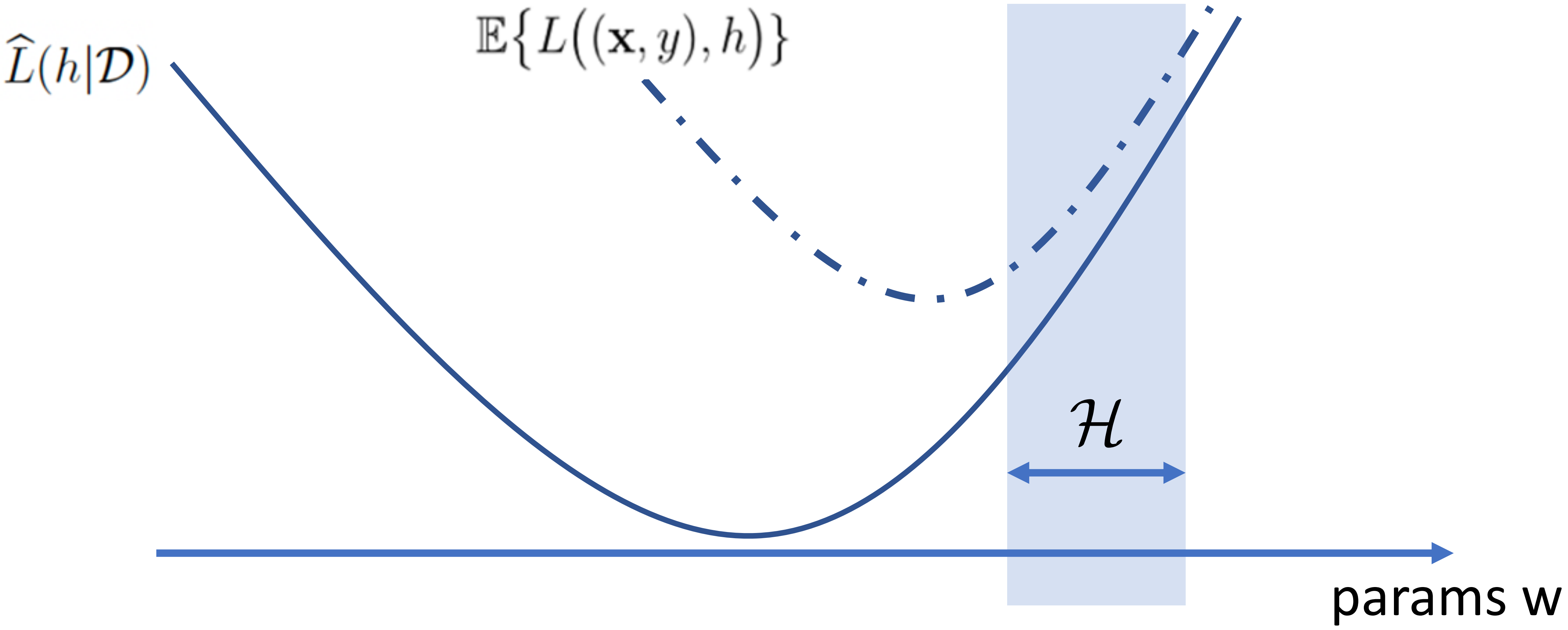
Linear Regression in Python

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

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

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

```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)
```

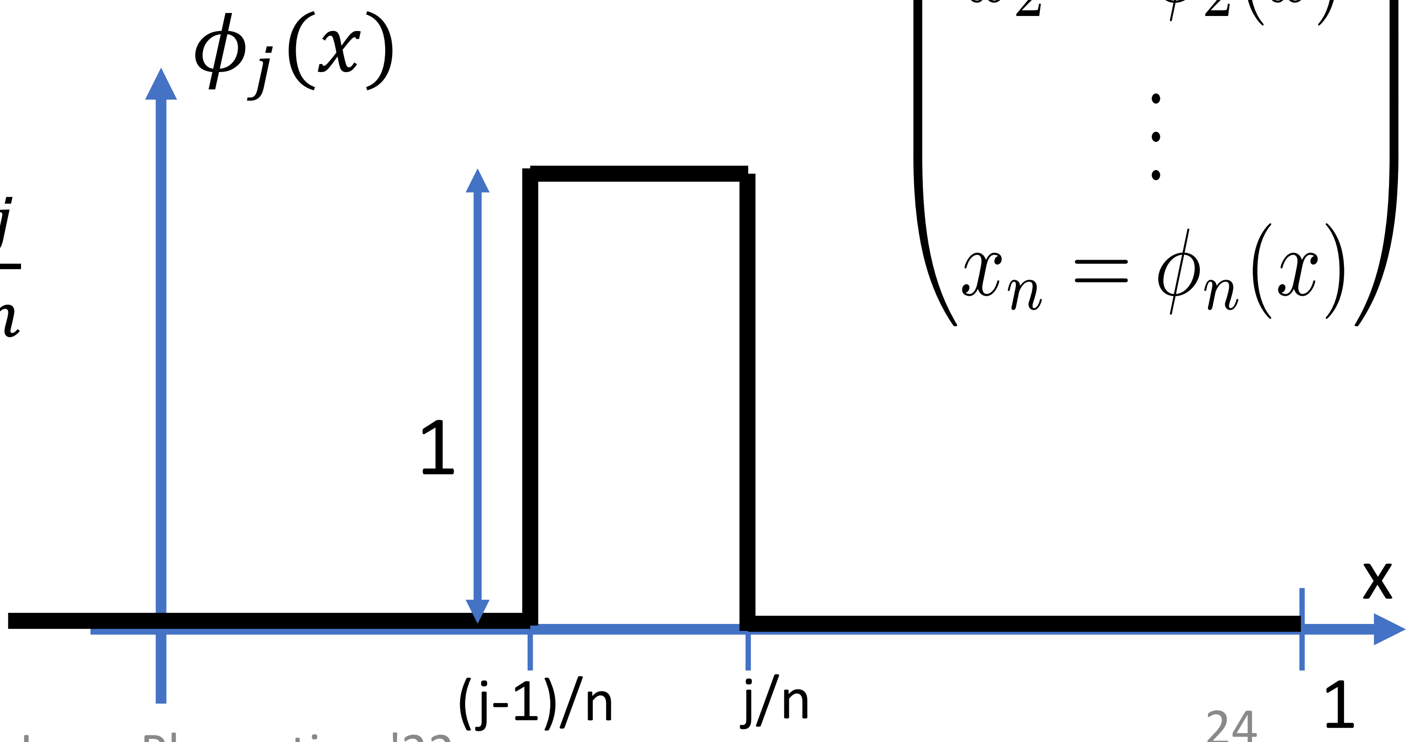


Upgrade Linear Model with new Features !

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

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

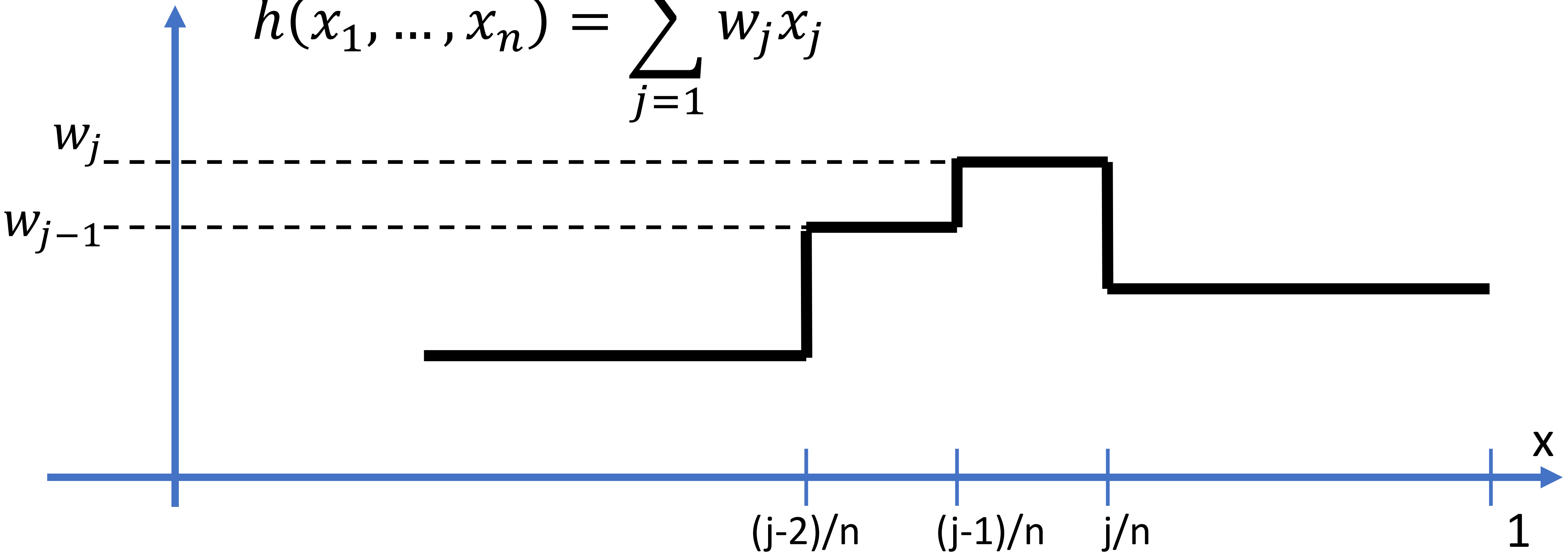
- $x_j = \begin{cases} 1 \; for \; \frac{j-1}{n} \leq x \leq \frac{j}{n} \\ 0 \; for \; all \; other \; x. \end{cases}$



You Can Do Anything with Linear Predictors!

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

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

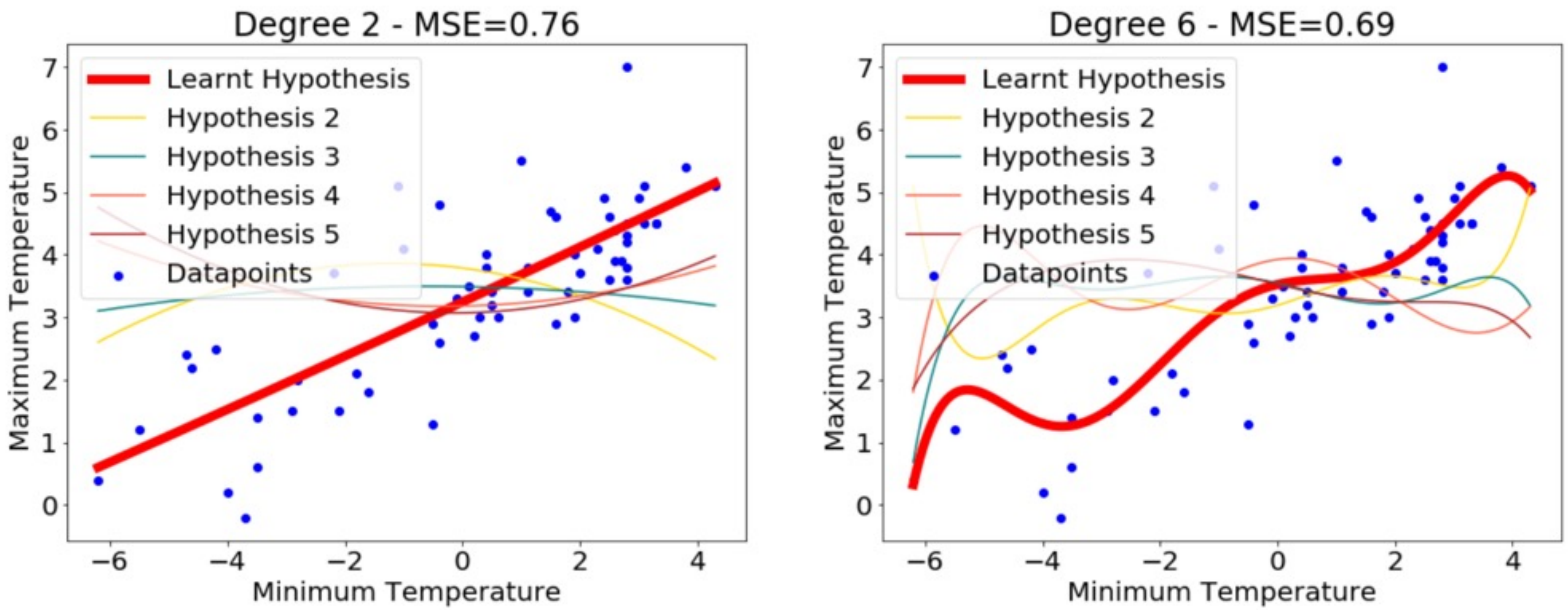


Polynomial Regression

$$\mathcal{H}_{\text{poly}}^{(n)} = \{h^{(\mathbf{w})} : \mathbb{R} \rightarrow \mathbb{R} : h^{(\mathbf{w})}(x) = \sum_{j=1}^{n} w_j x^{j-1},$$

$$\text{with some } \mathbf{w} = (w_1, \ldots, w_n)^T \in \mathbb{R}^n\}. \quad (3.4)$$

Polynomial Regression



from notebook
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*

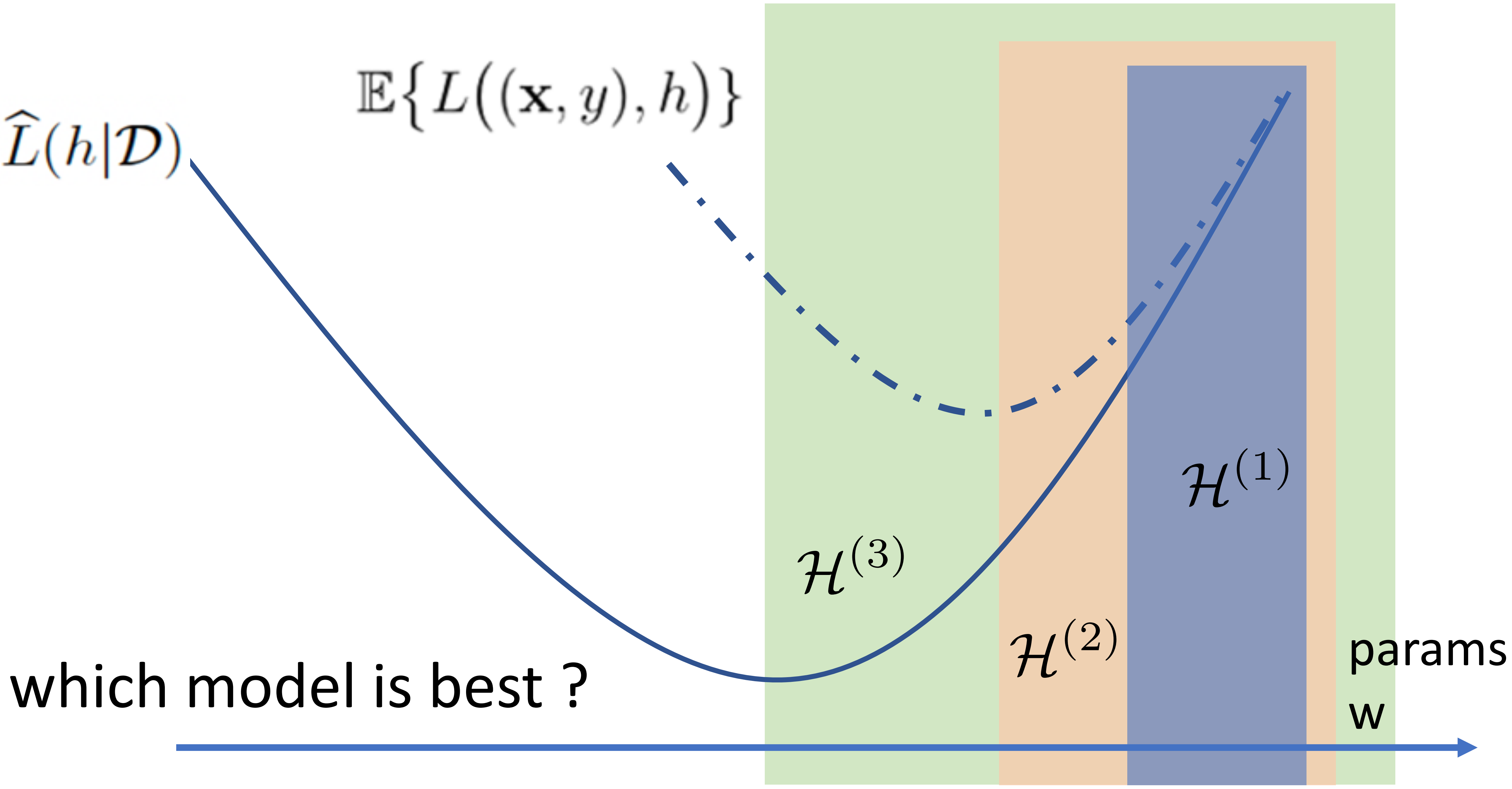
sklearn.linear_model.LinearRegression

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 !

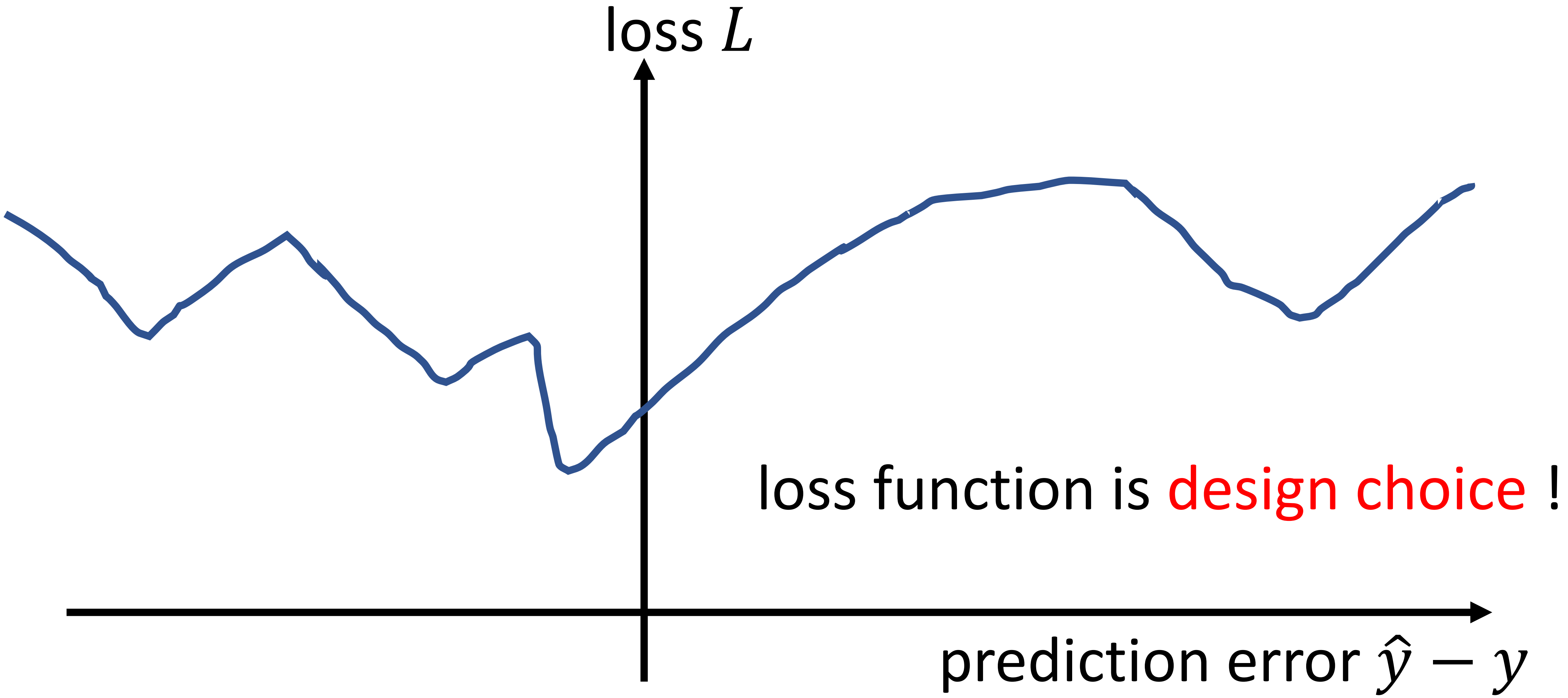
	Date	Max temp	Min temp	(Min temp)^2
0	2020-2-1	3.0	1.9	3.61
1	2020-2-2	4.9	2.4	5.76
2	2020-2-3	2.6	-0.4	0.16
3	2020-2-4	-0.2	-3.7	13.69
4	2020-2-5	2.5	-4.2	17.64



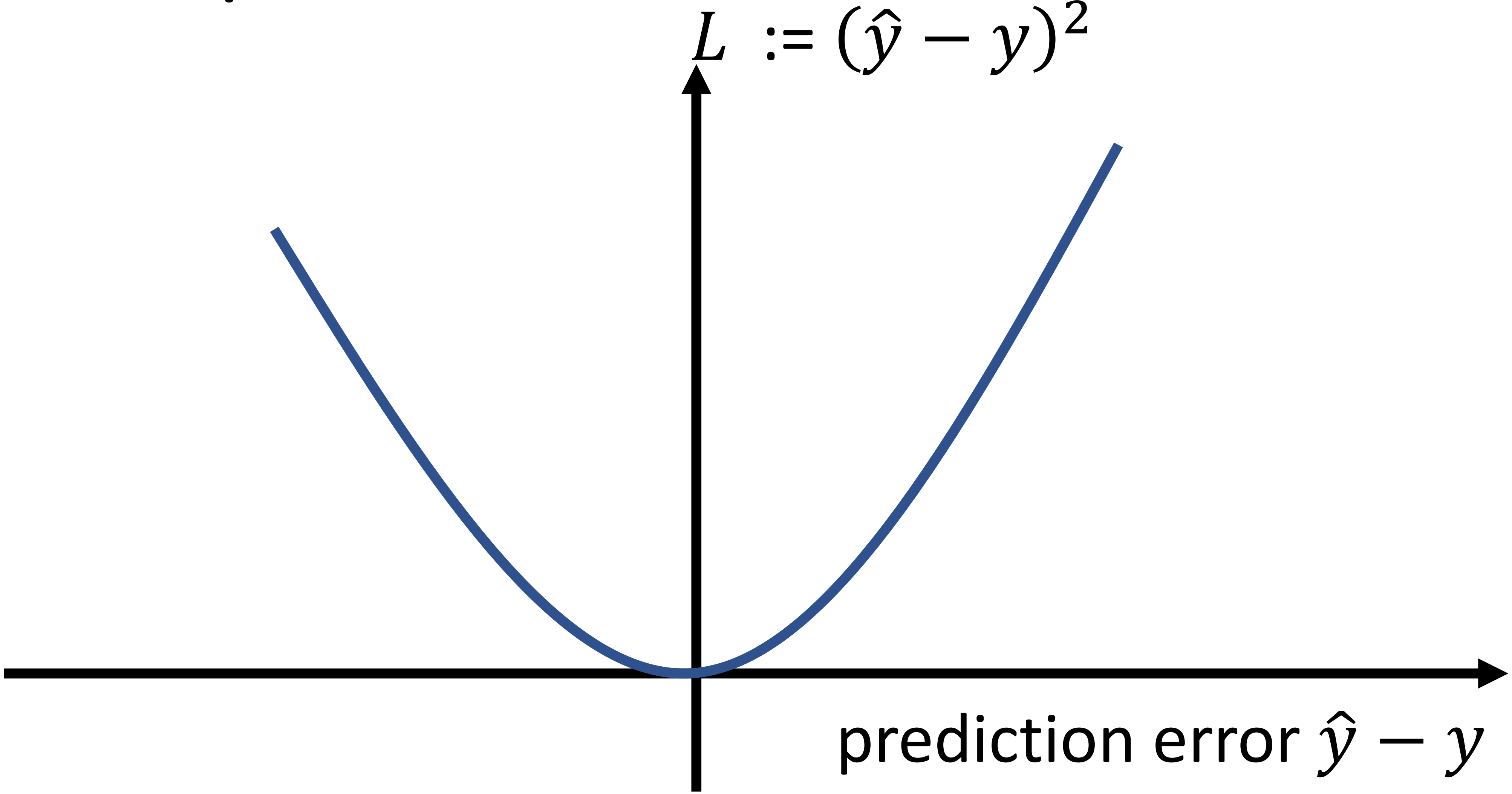
which model is best ?

Design Choice: Loss Function

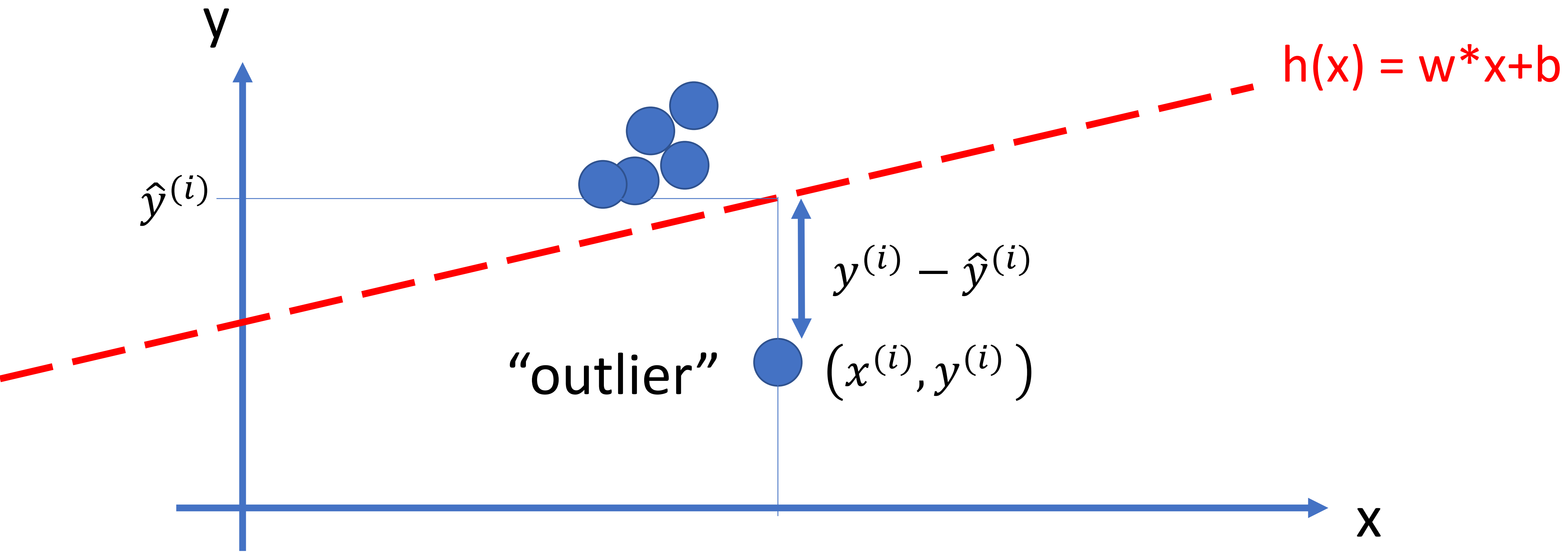
Measuring Error Size via Loss Functions



The Squared Error Loss

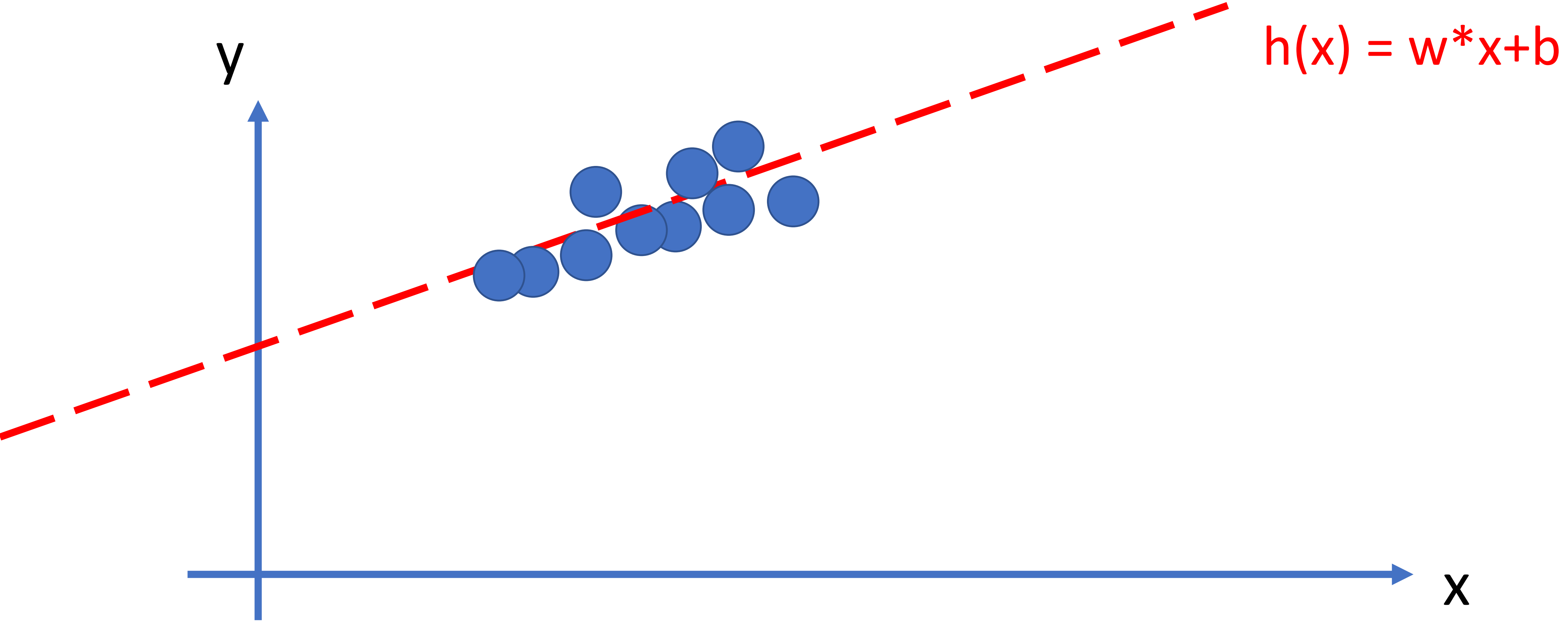


Squared Error Loss Sensitive to Outliers

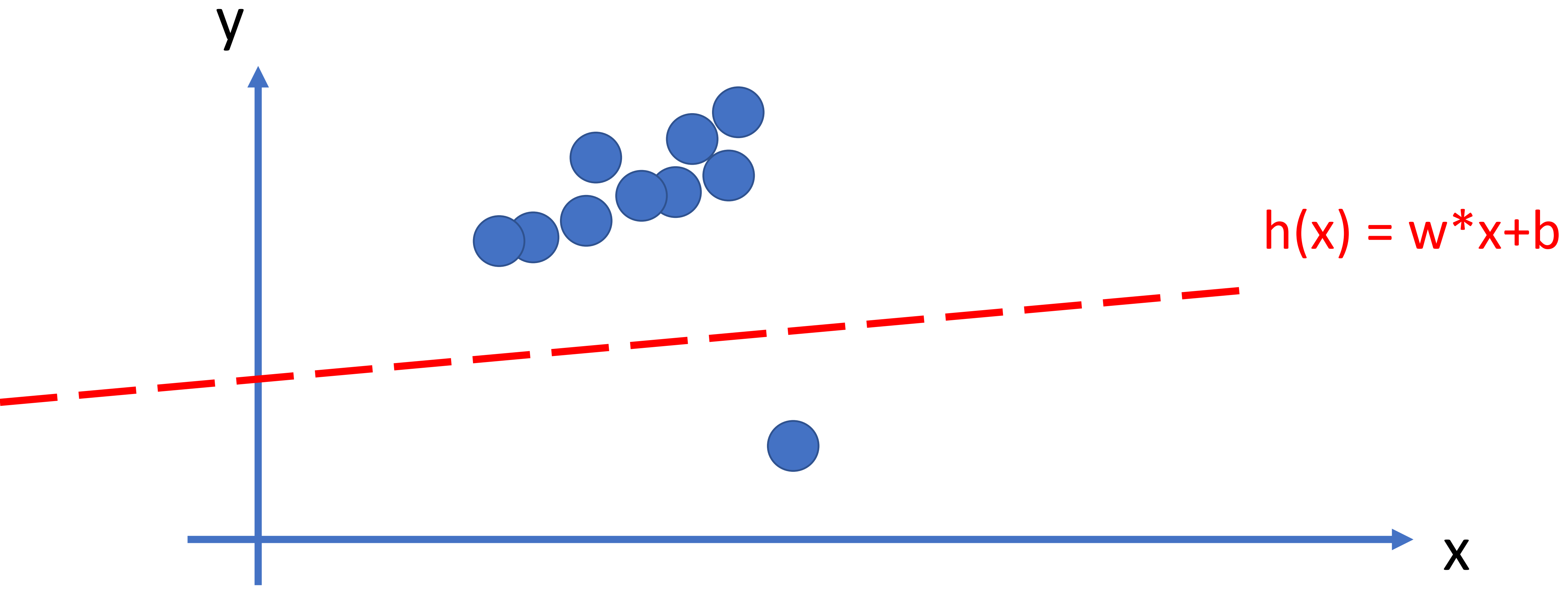


min. squared error loss forces predictor towards outlier

Train Linear Model on “Clean Data”

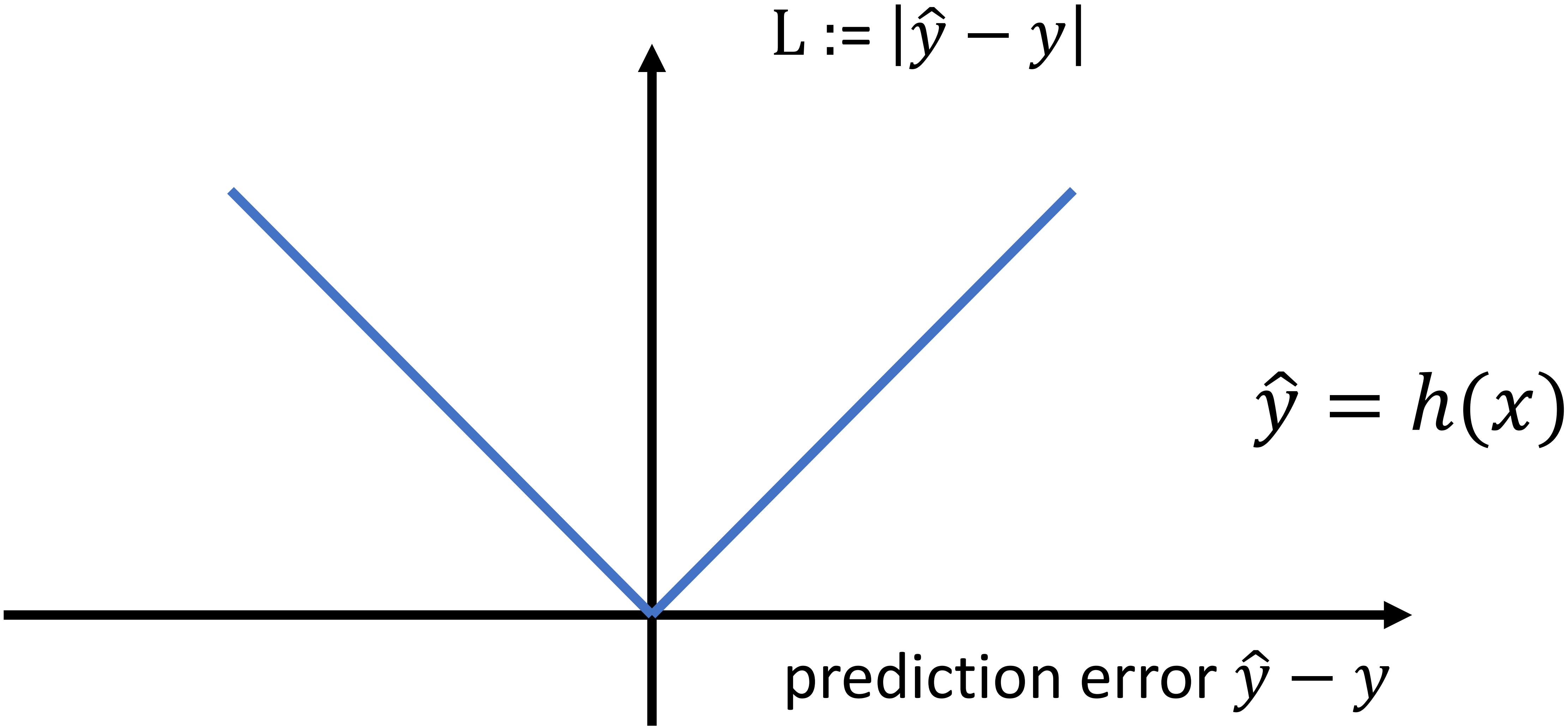


Training Set with a SINGLE OUTLIER !

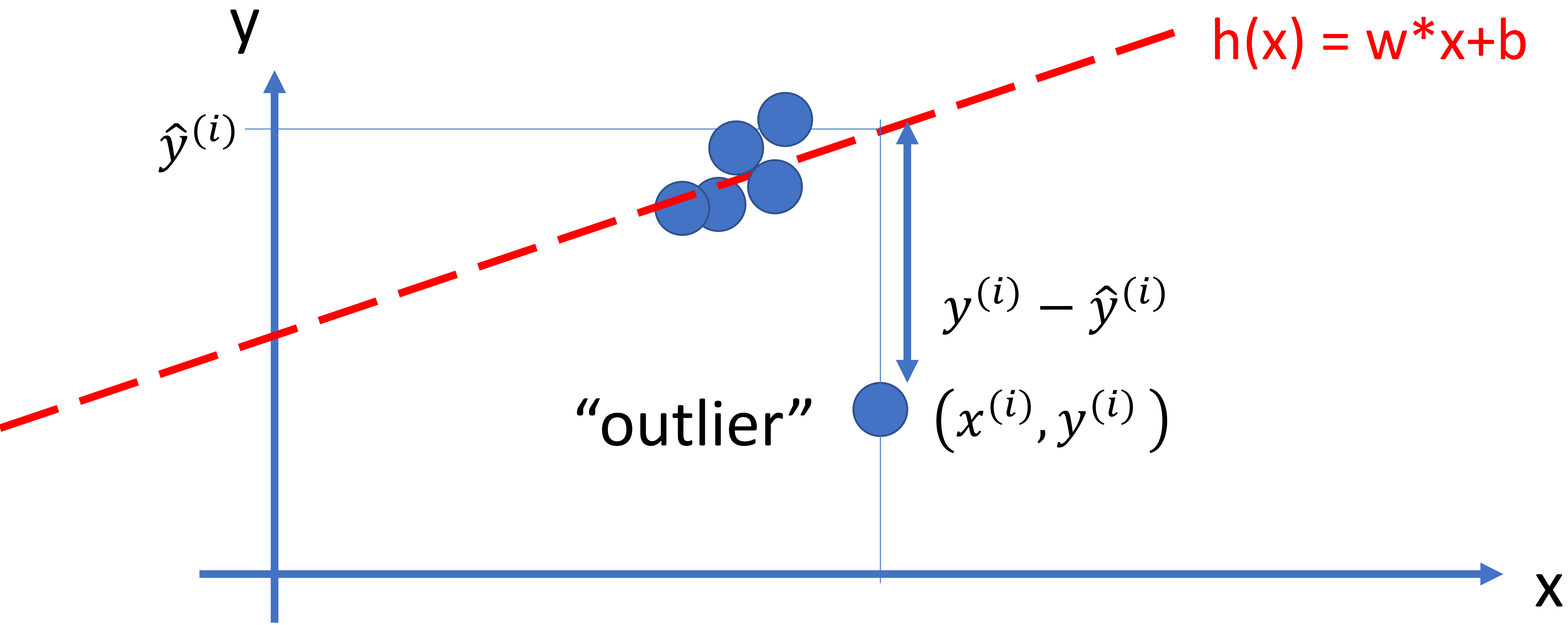


How to make learning robust against presence of few outliers in training set ?

The Absolute Error Loss

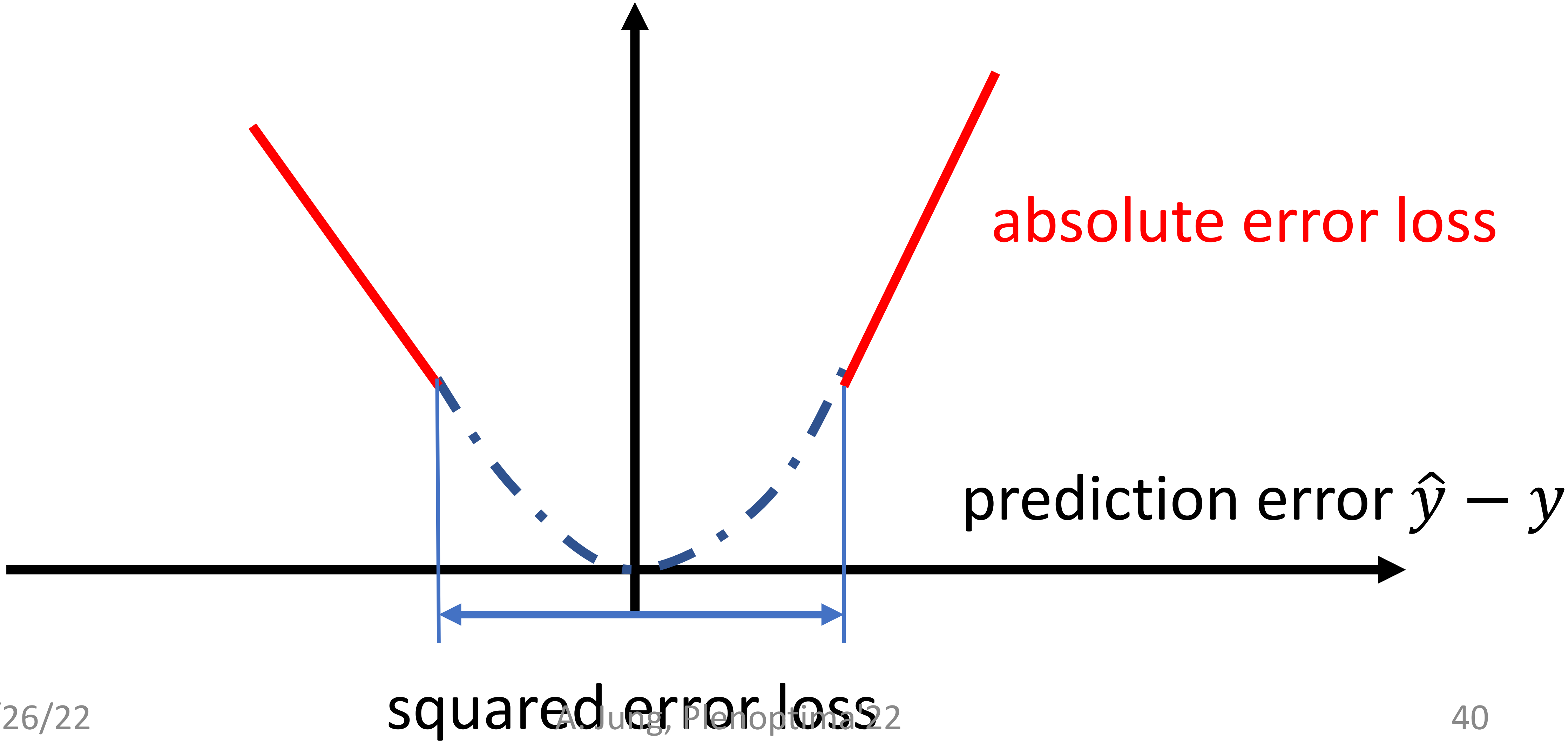


Absolute Error Loss Robust to Outliers

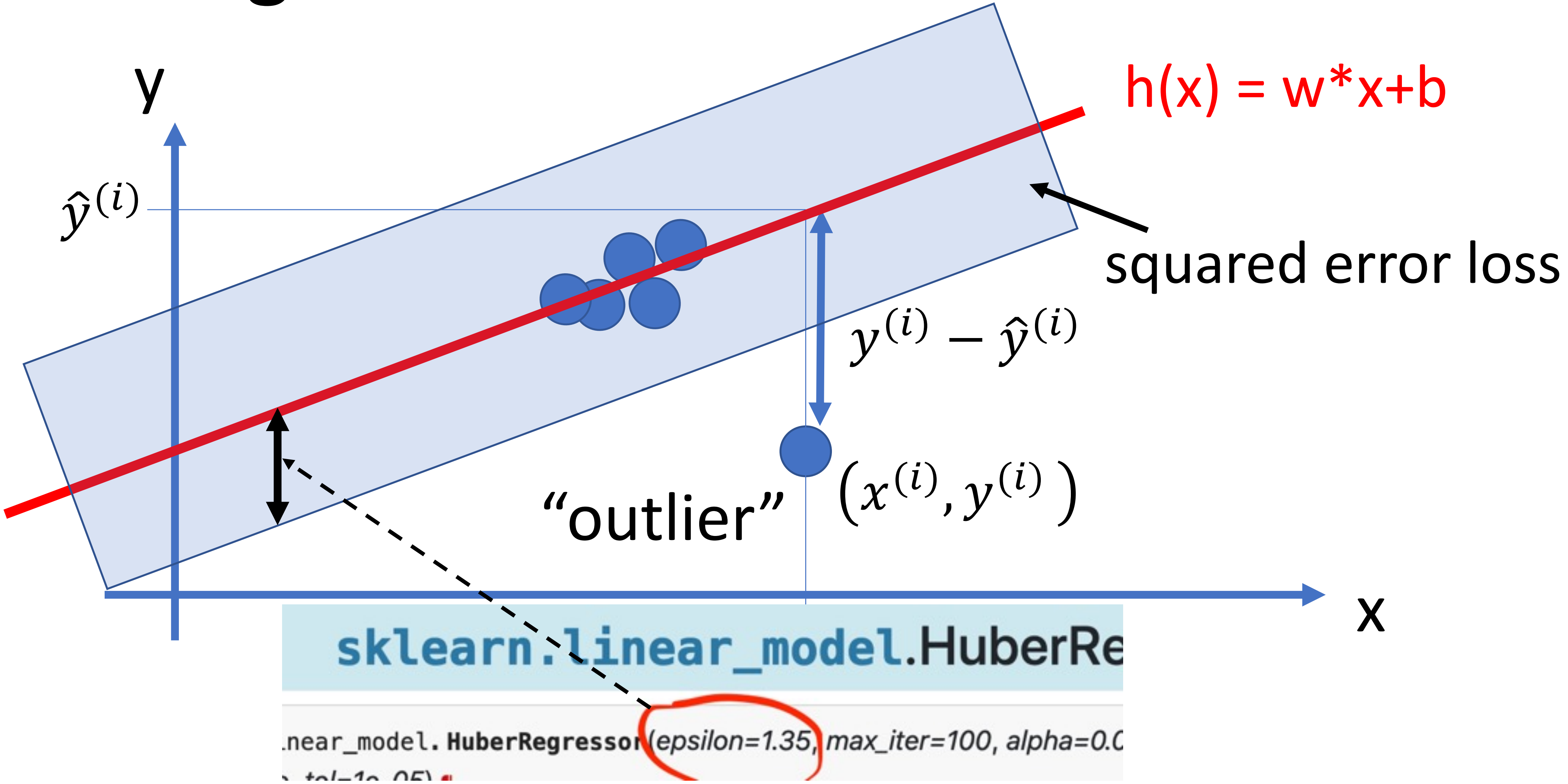


absolute error "tolerates" few outliers

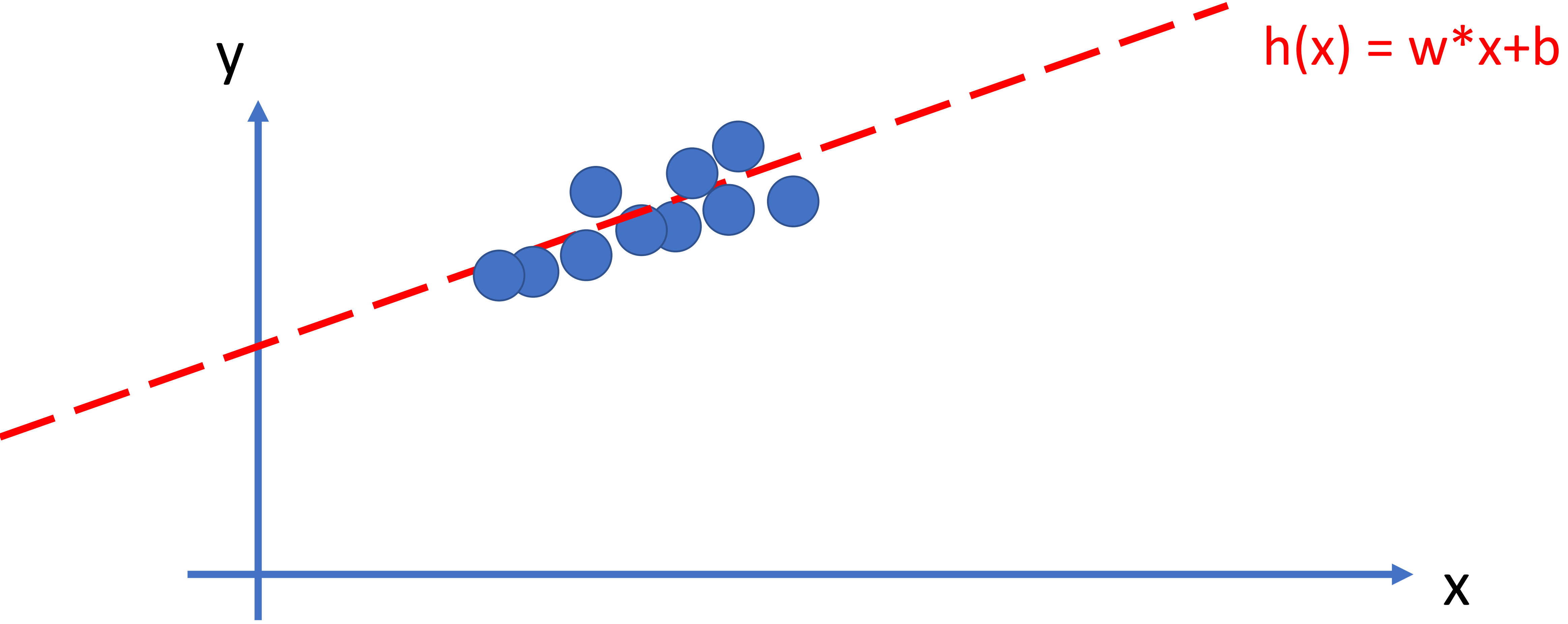
Huber Loss


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

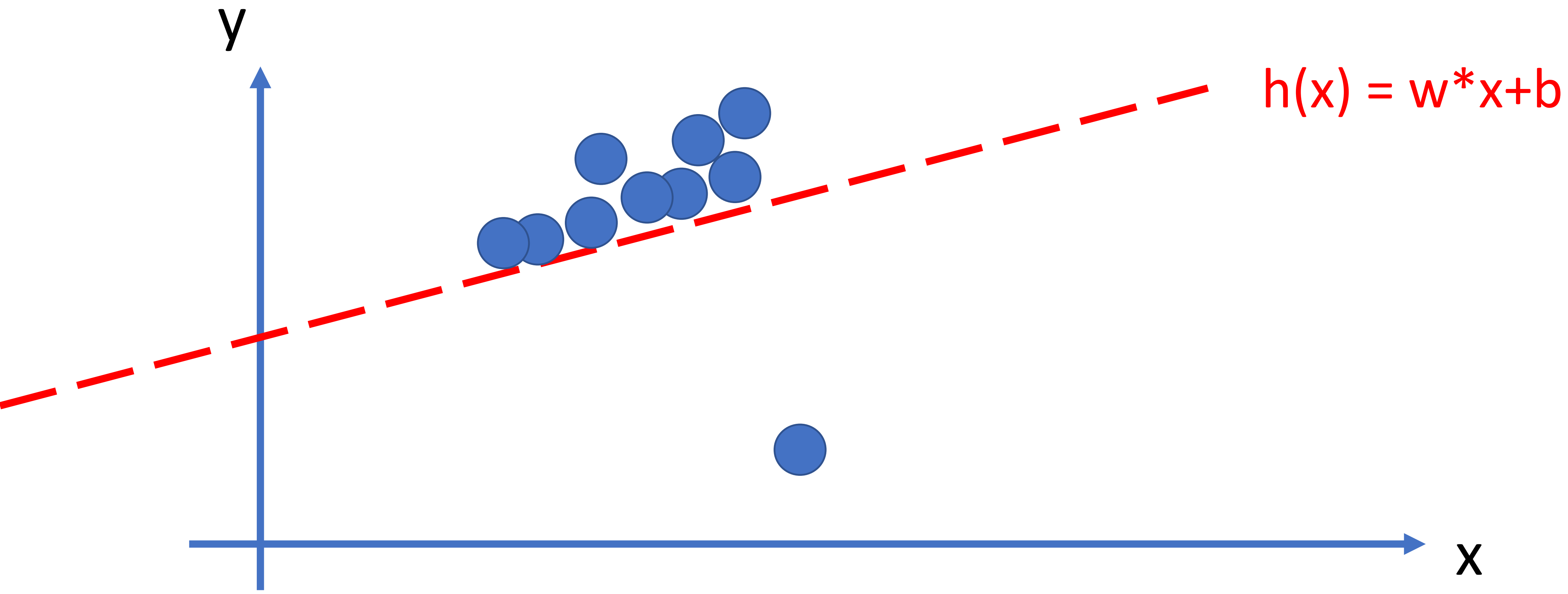
Fitting Linear Predictor with Huber Loss



Train Linear Model on “Clean Data”



Training Set with a SINGLE OUTLIER !



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 (“iid” asspt!)
- approximate risk by average loss (empirical risk)
- regression methods are instances of ERM
- three design choices of ERM: data, model and loss
- ERM can fail if empirical risk deviates from risk (e.g., due to outliers)

What’s Next ?

- tmrw, lecture “Classification”
- like regression, class. methods are instances of ERM
- class. use different label values and loss functions