Linear Regression

Fitting a **line** through data points

Faculty of Mathematics and Computer Science, University of Bucharest
and
Sparktech Software

Academic Year 2018/2019, 1st Semester

History of Linear Regression

- ***"Nouvelles méthodes pour la détermination des orbites des comètes"***

  Legendre, Adrien-Marie, 1805
  - The first clear and concise exposition of the "least squares method"

- ***"Regression Towards Mediocrity in Hereditary Stature"***

  Francis Galton, 1886
  - Children with tall parents tend to be shorter... They "regressed" towards the mean

- ***"The Law of Ancestral Heredity"***

  Karl Pearson, G. U. Yule, Norman Blanchard and Alice Lee, 1903

- ***"The goodness of fit of regression formulae, and the distribution of regression coefficients"***

  Sir R.A. Fisher, 1922

Linear Regression Objectives

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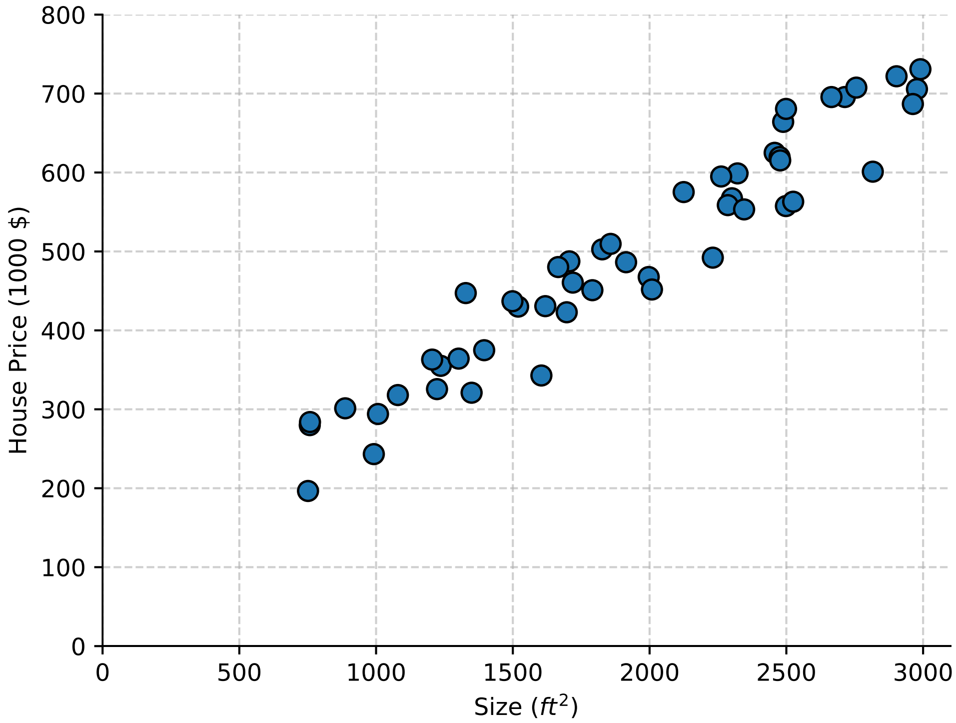
- **Forecast** new observations.
  - Use the established relationship to make *predictions* about new data.

Simple
Linear Regression

Simple Linear Regression



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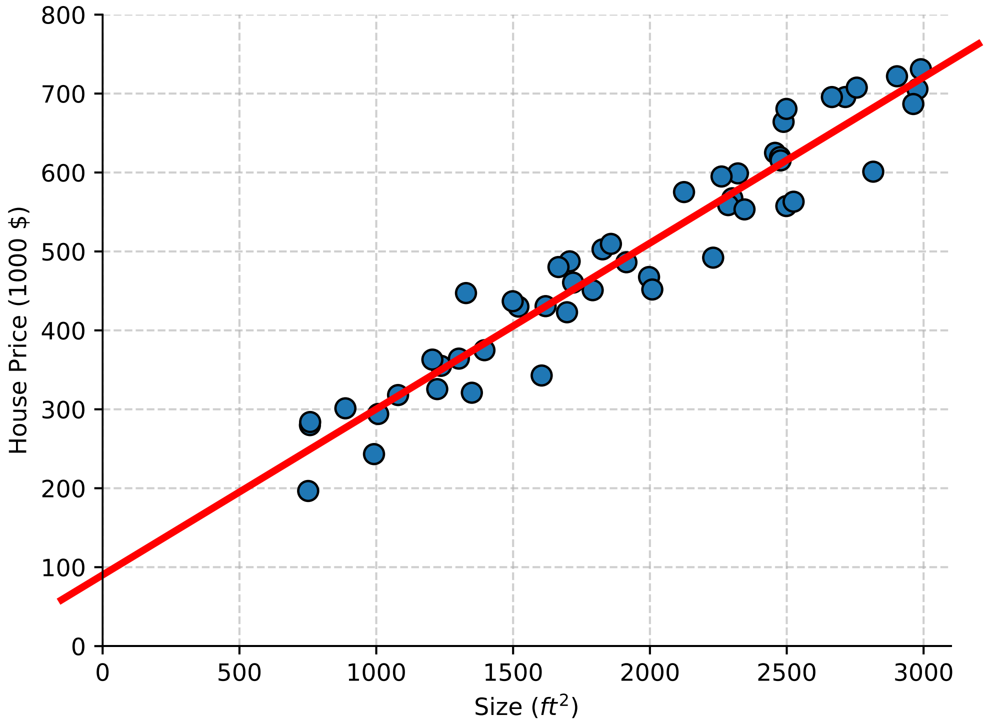
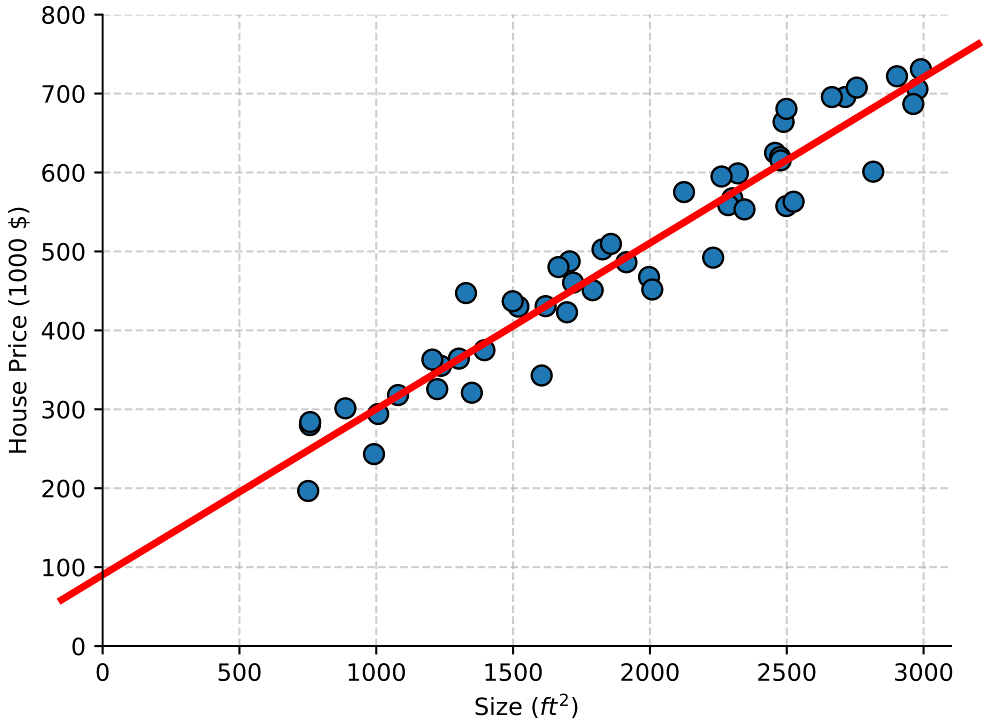


We find a straight *line* which *best fits* the data.

Simple Linear Regression

Slope is positive → *Positive correlation* between price and size (i.e. price tends to grow with size).



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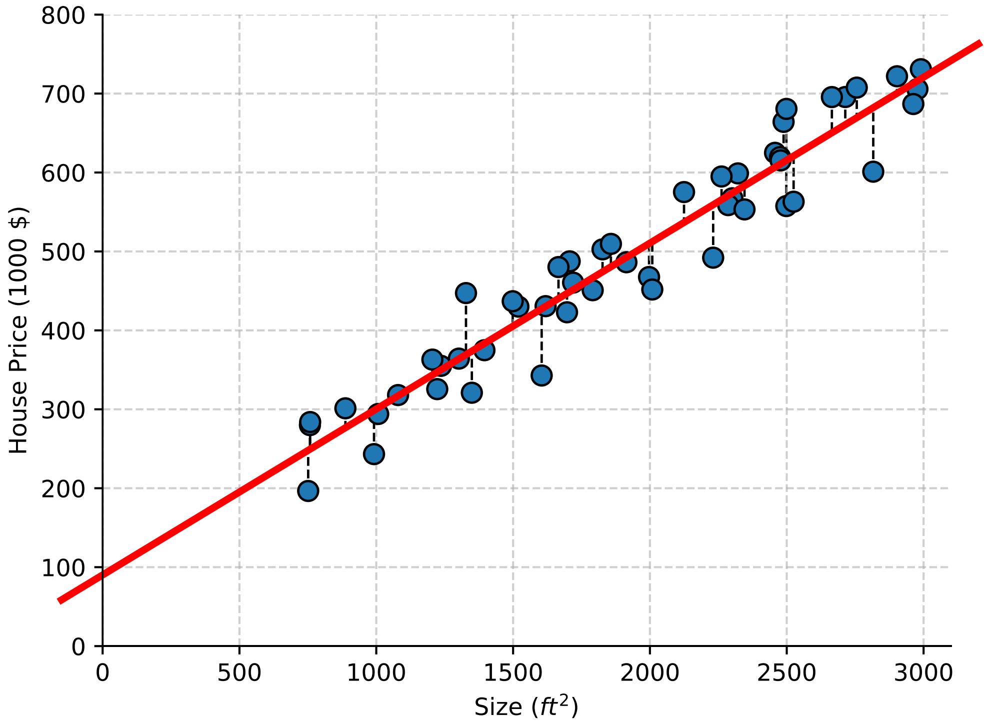

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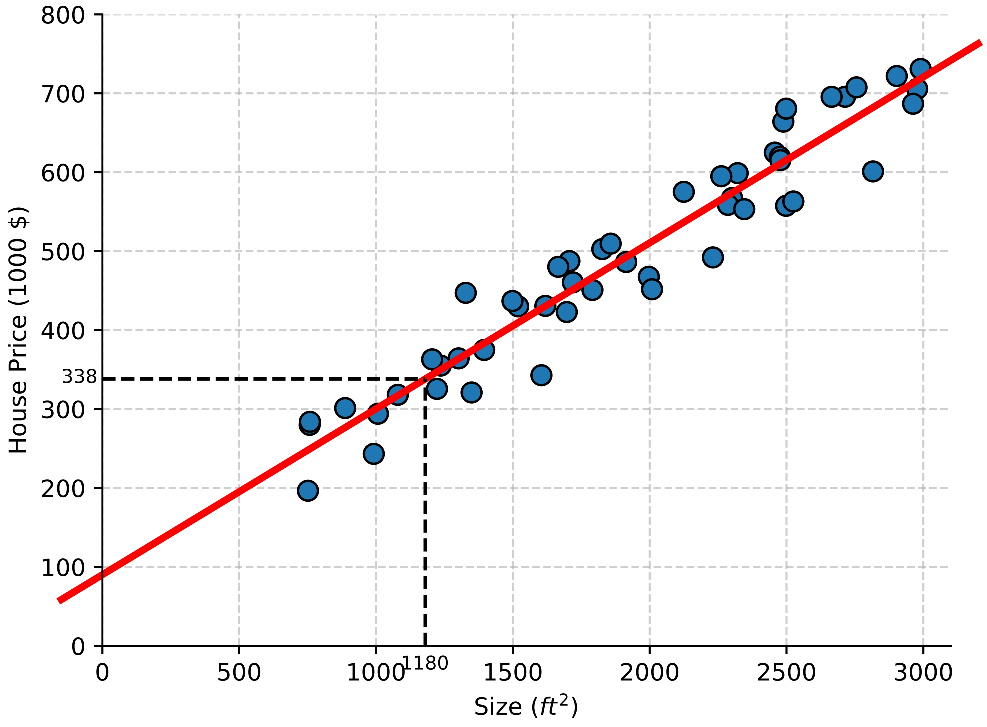

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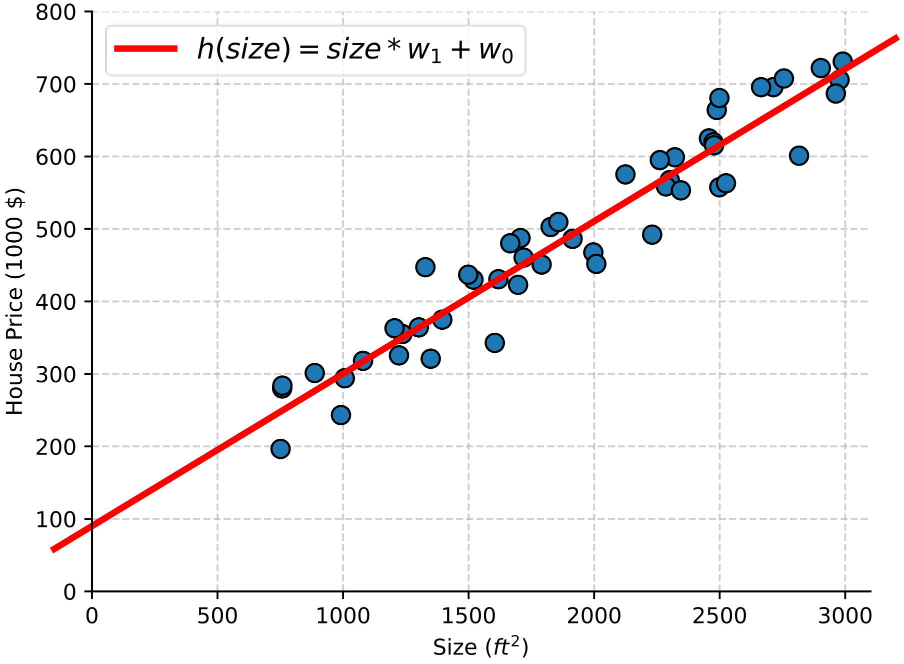
We can also determine how much of the variance in price is *explained* by size.

We can use the model for forecasting →
The model *predicts* that a 1220 ft^2 house will cost \$347K.

Linear Model

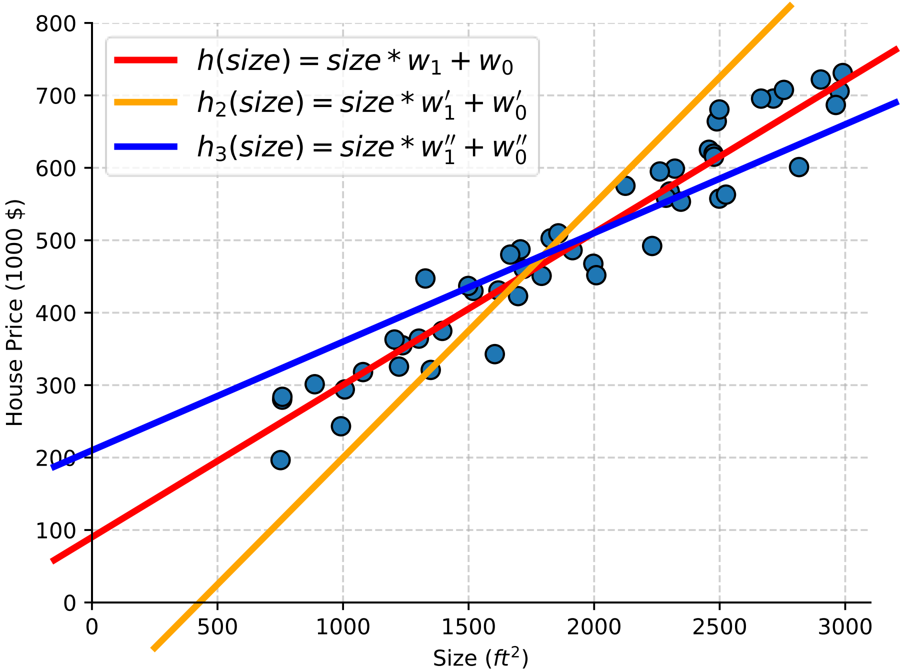
- The relationship is modeled with a *linear function*:



Linear Model

- The relationship is modeled with a *linear function*:

There are many linear functions to choose from.



We need a way of choosing the *best* w_0 and w_1.

Notation

- $x \in \mathbb{R}$ is the independent variable (i.e. size)
- $y \in \mathbb{R}$ is the dependent variable (i.e. price)
- $h : \mathbb{R} \to \mathbb{R}$ is the hypothesis, which has parameters w_0 and w_1
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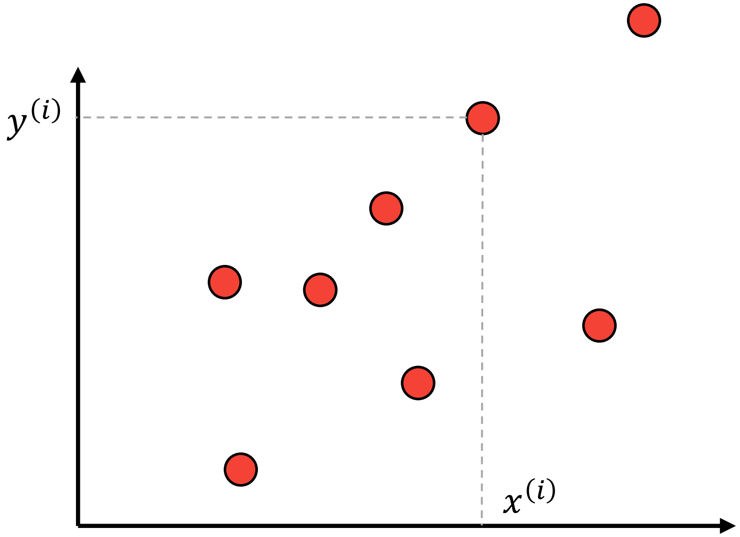
- $\hat{y} = h(x)$ is the predicted value.
- Simple Linear Regression:

$$\hat{y} = h(x) = \mathrm{w}_0 + w_1 x$$

- We need to find w_0 and w_1 such that $\hat{y}$ is as close to y as possible.

Least Squares Method

- Given $E = \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$, with $x^{(i)}, y^{(i)} \in \mathbb{R}$



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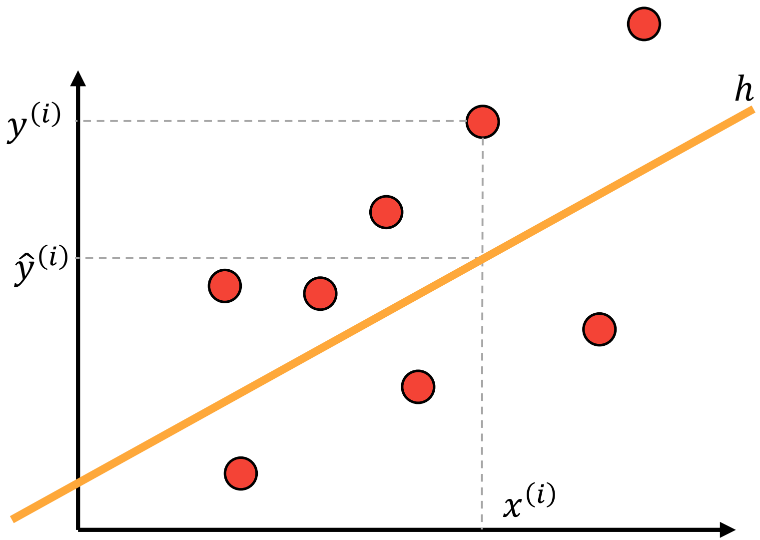

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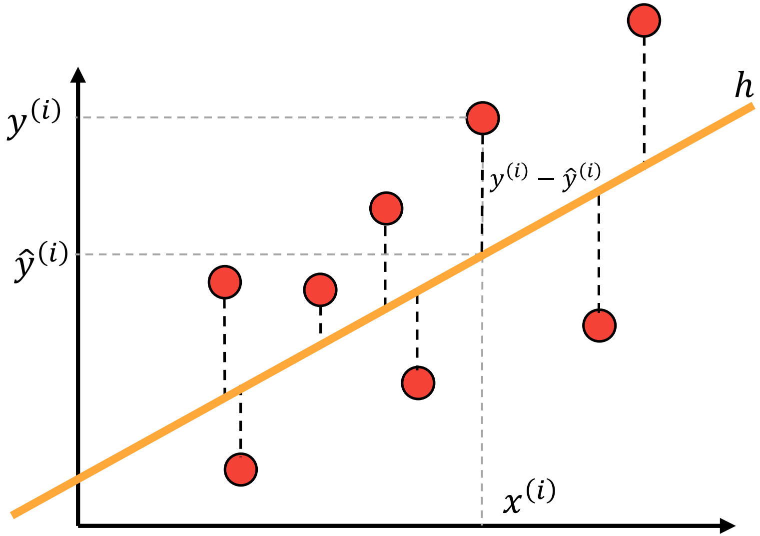

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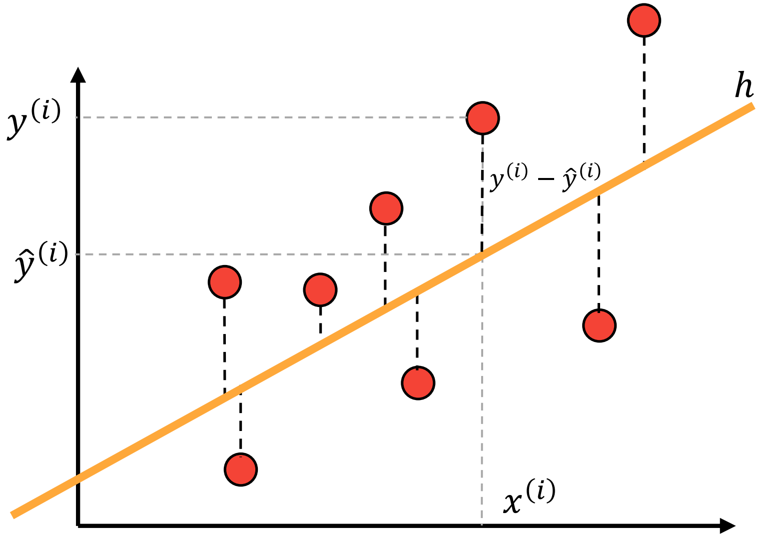
$$\frac{\partial \mathcal{L}_E}{\partial w_0} = 0, \qquad \frac{\partial \mathcal{L}_E}{\partial w_1} = 0$$



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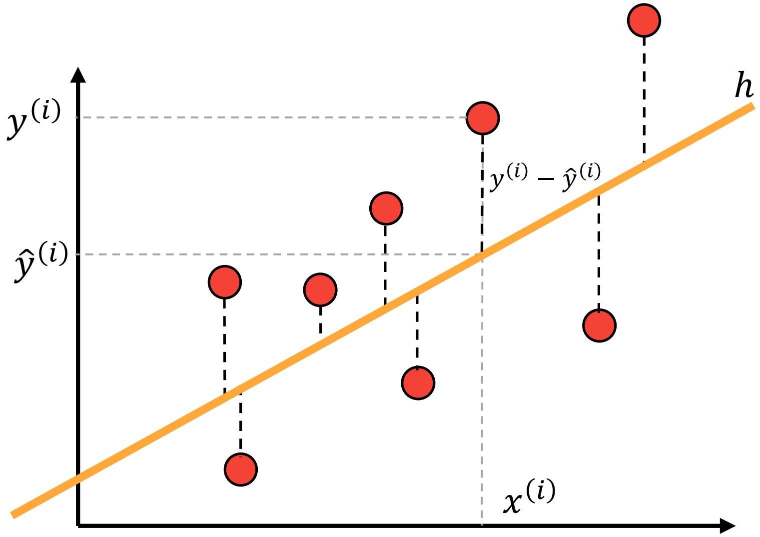
$$\Longrightarrow \quad w_1 = \qquad w_0 =$$

Let's do some math…



Least Squares Derivation

$$\mathcal{L}_E = \sum_{i=1}^{\mathrm{m}} (\mathrm{y} - w_1 \mathrm{x} - w_0)^2$$

To simplify notation let's assume:

$$y \overset{\text{not}}{=} y^{(i)}$$

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$$\mathcal{L}_E = \sum_{i=1}^{\mathrm{m}} (\mathrm{y} - w_1\mathrm{x} - w_0)^2 = \sum (\mathrm{y}^2 + w_1^2\mathrm{x}^2 + w_0^2 \; - 2\mathrm{w}_1\mathrm{xy} - 2\mathrm{w}_0\mathrm{y} + 2w_0w_1\mathrm{x})$$

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$$w_1 \sum x^2 - w_1 \frac{1}{m} \left(\sum x \right)^2 - \sum xy + \frac{1}{m} \sum x \sum y = 0$$

$$\Rightarrow w_1 = \frac{\sum xy - \frac{1}{m} \sum x \sum y}{\sum x^2 - \frac{1}{m} (\sum x)^2}$$

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$\bar{x} = \frac{1}{m}\sum x^{(i)}$

(the mean)

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Least Squares Method

$$\mathcal{L}_E \overset{\text{not}}{=} \sum_{(x,y)\in E} \mathcal{L}(y, h(x))$$

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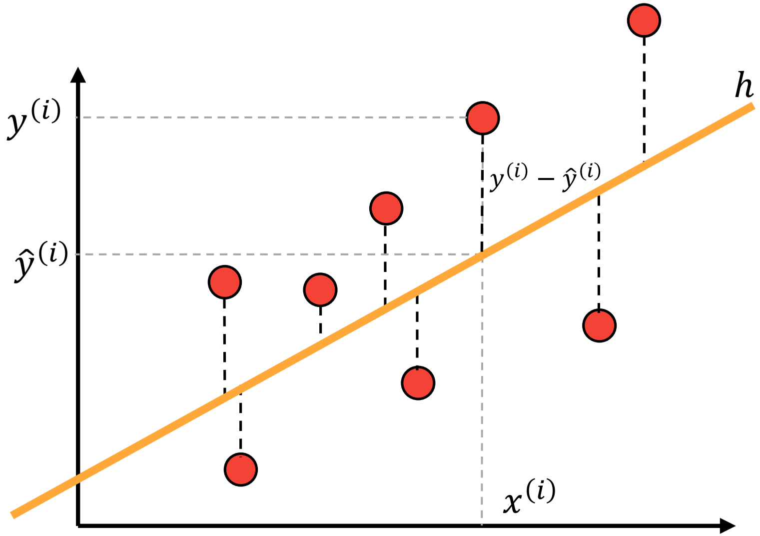


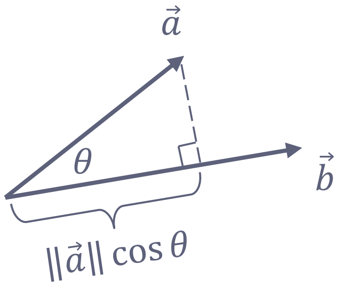
Multivariate Linear Regression

Refresher – Dot Product

- An operation which takes two vectors and returns a **scalar** value.
- Also called the *scalar product* or *inner product*.

$$\vec{a} \cdot \vec{b} = \langle \vec{a}, \vec{b} \rangle = \|a\| \|b\| \cos\theta = \sum_i a_i b_i$$

- It can be interpreted as a *similarity measure* between vectors.
- If we write it as $(\|\vec{a}\| \cos\theta)\|\vec{b}\|$, it can be viewed as the *length of the projection of $\vec{a}$ on $\vec{b}$*, measured in units of length $\|\vec{b}\|$.



Multivariate Regression

- $\vec{x} \in \mathbb{R}^n = [x_1 \quad x_2 \quad \cdots \quad x_n]$,
- $\vec{w} \in \mathbb{R}^n = [w_1 \quad w_2 \quad \cdots \quad w_n], w_0 \in \mathbb{R}$

Multivariate Regression

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$$\hat{y} = \mathrm{w}_0 + w_1 x_1 + w_2 \mathrm{x}_2 + \cdots + \mathrm{w}_\mathrm{n} \mathrm{x}_\mathrm{n} = w_0 + \langle \vec{w}, \vec{x} \rangle$$

Multivariate Regression

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- Common mathematical trick is to get rid of the intercept by considering:

$$\vec{x} \in \mathbb{R}^{n+1} = [1 \quad x_1 \quad x_2 \quad \dots \quad x_n]$$
$$\vec{w} \in \mathbb{R}^{n+1} = [w_0 \quad w_1 \quad w_2 \quad \dots \quad w_n]$$
$$\Longrightarrow$$
$$\hat{y} = \langle \vec{w}, \vec{x} \rangle$$

Multivariate Regression

- Given $E = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), \ldots, (\vec{x}^{(m)}, y^{(m)})\}, \vec{x}^{(i)} \in \mathbb{R}^n, \mathrm{y}^{(i)} \in \mathbb{R}$

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- We can use matrix multiplication to compute the predictions for all samples:

$$\begin{pmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{pmatrix} = \begin{pmatrix} 1 & x_1^{(1)} & \dots & x_n^{(1)} \\ 1 & x_1^{(2)} & \dots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{pmatrix} \quad \Rightarrow \quad \widehat{\boldsymbol{Y}} = \mathbf{Xw}$$

Multivariate Regression

- Given $E = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), \dots, (\vec{x}^{(m)}, y^{(m)})\}, \vec{x}^{(i)} \in \mathbb{R}^n, y^{(i)} \in \mathbb{R}$

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$$\mathcal{L}_E = \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

Multivariate Regression

- Given $E = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), \dots, (\vec{x}^{(m)}, y^{(m)})\}, \vec{x}^{(i)} \in \mathbb{R}^n, y^{(i)} \in \mathbb{R}$

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$$\mathcal{L}_E = \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(Y - \hat{Y}\right)^T \left(Y - \hat{Y}\right)$$

Multivariate Regression

- Given $E = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), \dots, (\vec{x}^{(m)}, y^{(m)})\}, \vec{x}^{(i)} \in \mathbb{R}^n, \mathrm{y}^{(i)} \in \mathbb{R}$

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Multivariate Regression

$$\mathcal{L}_E = \left(Y - \hat{Y}\right)^2$$

Multivariate Regression

$$\mathcal{L}_E = \left(Y - \hat{Y}\right)^2 = (Y - Xw)^2 = (Y - Xw)^T(Y - Xw)$$

Multivariate Regression

$$\mathcal{L}_E = \left(Y - \hat{Y}\right)^2 = (Y - Xw)^2 = (Y - Xw)^T(Y - Xw)$$
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Multivariate Regression

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$$= Y^T Y - Y^T Xw - w^T X^T Y + w^T X^T Xw$$

Multivariate Regression

$$\mathcal{L}_E = \left(Y - \hat{Y}\right)^2 = (Y - Xw)^2 = (Y - Xw)^T(Y - Xw)$$
$$= (Y^T - w^T X^T)(Y - Xw)$$
$$= Y^T Y - Y^T Xw - w^T X^T Y + w^T X^T Xw = Y^T Y - 2w^T X^T Y + w^T X^T Xw$$

- $Y^T Xw = [\ddots]_{1\times m}\,[\ddots]_{m\times n}\,[\ddots]_{n\times 1} = [\ddots]_{1\times 1}$ (scalar)
- $Y^T Xw = (w^T X^T Y)^{\mathrm{T}}$
- Transpose of a scalar is the same scalar

Multivariate Regression

$$\mathcal{L}_E = Y^T Y - 2w^T X^T Y + w^T X^T X w$$

Multivariate Regression

$$\mathcal{L}_E = Y^T Y - 2w^T X^T Y + w^T X^T X w$$

- Minimize $\mathcal{L}_E$ with respect to w:

$$\frac{\partial \mathcal{L}_E}{\partial w} = 0$$

Derivative w.r.t. to a vector $\Longrightarrow$ derivative w.r.t. each component.

$$\begin{bmatrix} \frac{\partial \mathcal{L}_E}{\partial w_0} & \frac{\partial \mathcal{L}_E}{\partial w_1} & \cdots \end{bmatrix}$$

Multivariate Regression

$$\mathcal{L}_E = Y^T Y - 2w^T X^T Y + w^T X^T X w$$

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$$\frac{\partial \mathcal{L}_E}{\partial w} = 0 \Rightarrow -2X^T Y + 2X^T X w = 0$$

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$$\boldsymbol{w} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y}$$

Multivariate Regression

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Derivative w.r.t. to a vector $\Rightarrow$ derivative w.r.t. each component.
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- Observations:
    - $X^T X$ needs to be *invertible*.
    - If $X \in \mathbb{R}^{m \times n}$ with $n > m$ (more features than examples), there is a high chance of $X^T X$ being singular.
        - The problem is *"ill-posed"*.

Well-posed vs. Ill-posed problems

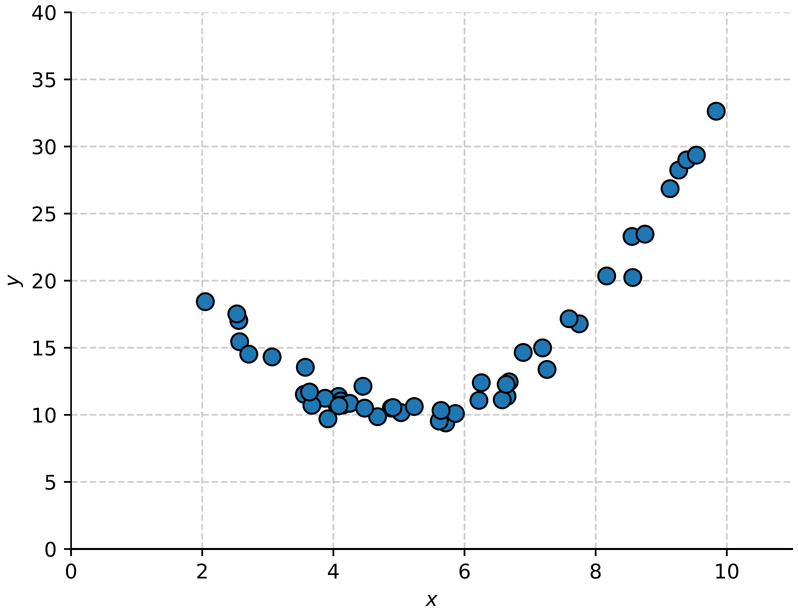
- A problem is **well-posed** if:
  - A solution exists.
  - The solution is unique.
  - The solution's behavior changes continuously with the initial conditions.

Jacques Hadamard, 1902

- If a problem is not well-posed, it is said to be **ill-posed**.
  - This usually implies that additional assumptions need to be taken into consideration for numerical treatment of the problem.
  - This process is called **regularization**
  - Inverse problems are often ill-posed (determining the cause by observing the effects)

Fitting a polynomial

- Linear regression is *linear in coefficients*, but we can have *non-linear features*.
  - If we use $[1 \quad x \quad x^2 \quad \dots \quad x^d]$ as features, we can fit a polynomial of degree d with linear regression



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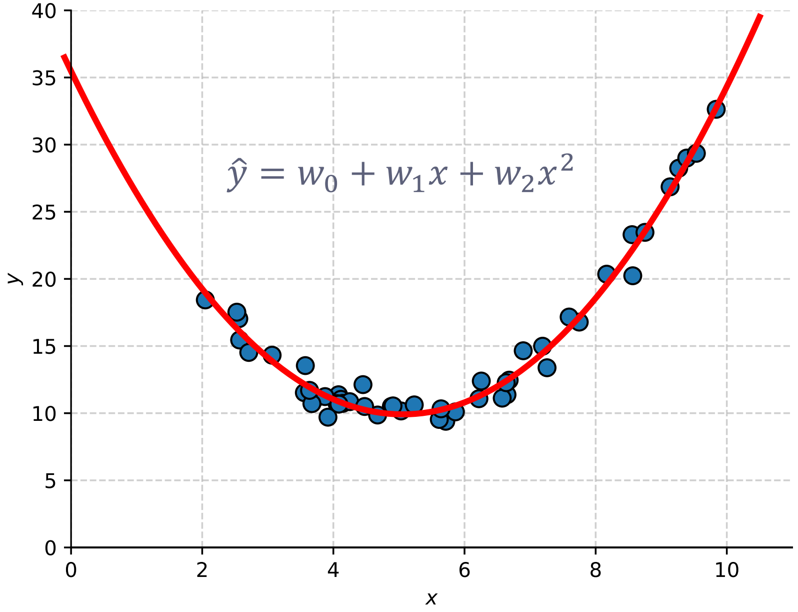


Ridge Regression

Linear regression with **regularization**

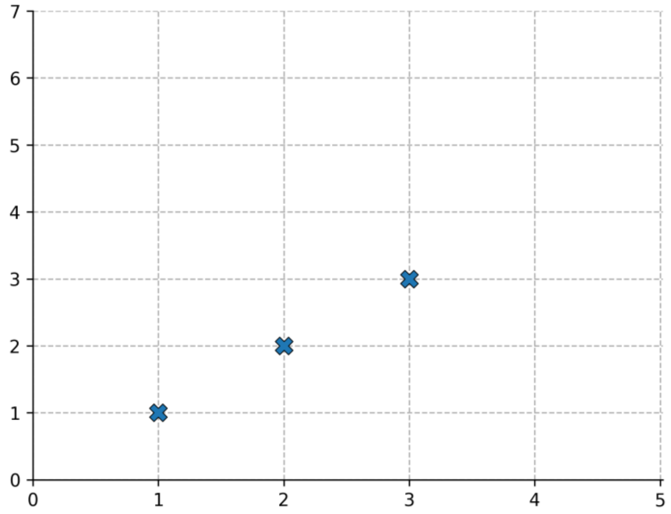
Faculty of Mathematics and Computer Science, University of Bucharest
and
Sparktech Software

Academic Year 2018/2019, 1st Semester

Ill-posed problems

- Let's say we have a function $f: \mathbb{R} \to \mathbb{R}$
- We are given:
    - $f(1) = 1$
    - $f(2) = 2$
    - $f(3) = 3$

- What is $f(4)$?
    - $f(4) = ?$



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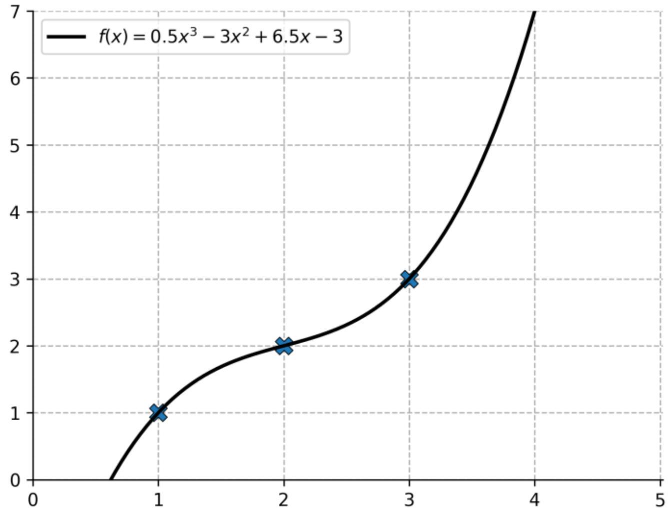
- What is $f(4)$?
  - $f(4) = 7$

$$f(\mathrm{x}) = 0.5x^3 - 3x^2 + 6.5x - 3$$



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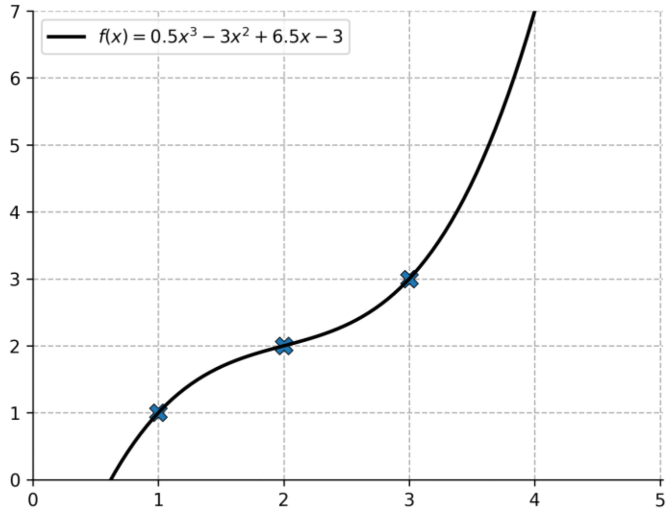
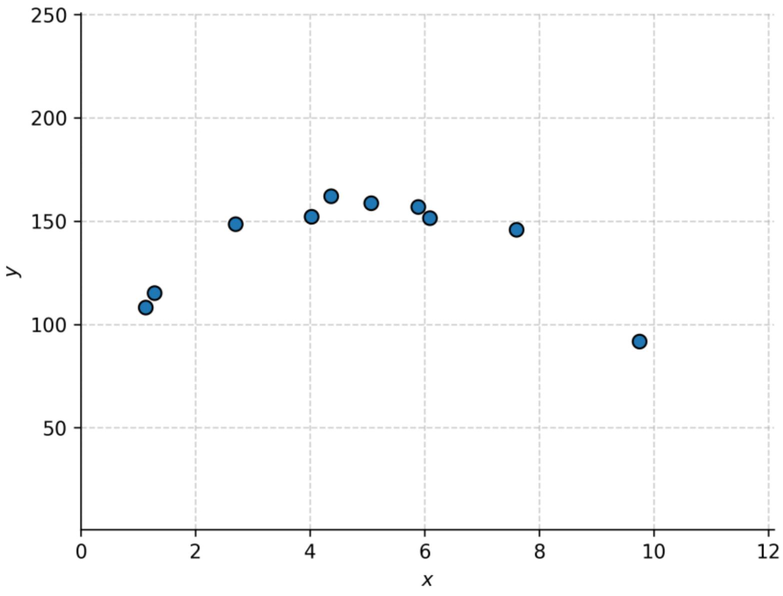


Ill-posed problems

- Lets consider a dataset $X \in \mathbb{R}^{10\times 10}$ (10 samples with 10 features each)
  - For ease of plotting let's consider the features to be $[1 \quad x \quad x^2 \quad \dots \quad x^{10}]$



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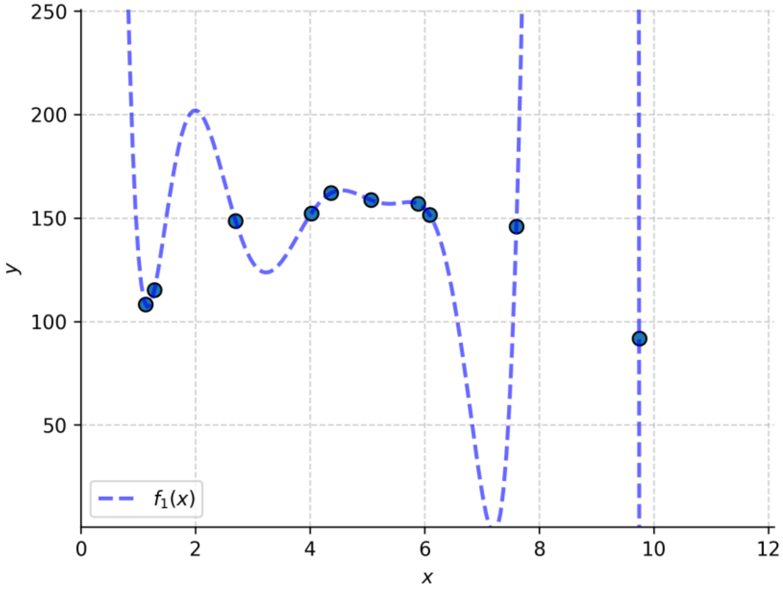
"Ill-posed" problem + unconstrained hypothesis space → data is overfitted.

$$\begin{aligned} f_1(x) &= 5.28 * 10^3 \\ &-1.50 * 10^4 x \\ &+1.72 * 10^4 x^2 \\ &-1.01 * 10^4 x^3 + \cdots \end{aligned}$$



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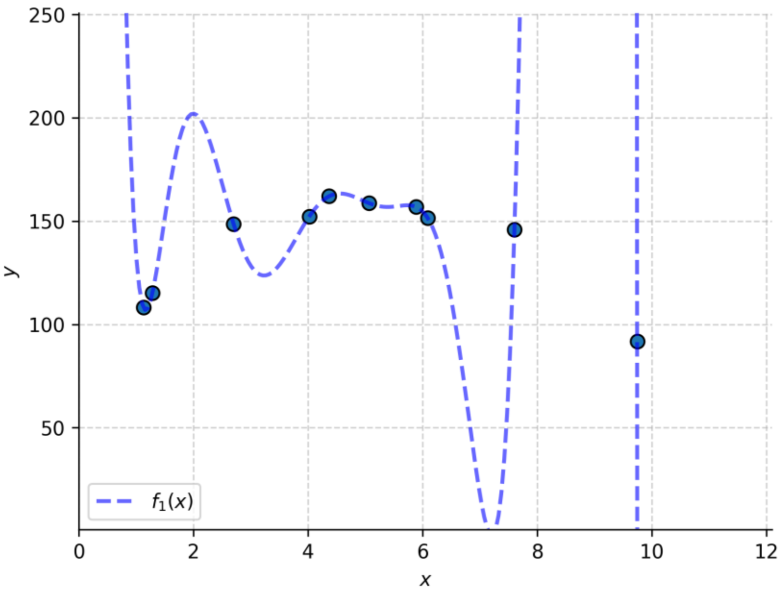
Large coefficients →

- Small changes in input cause large changes in output.



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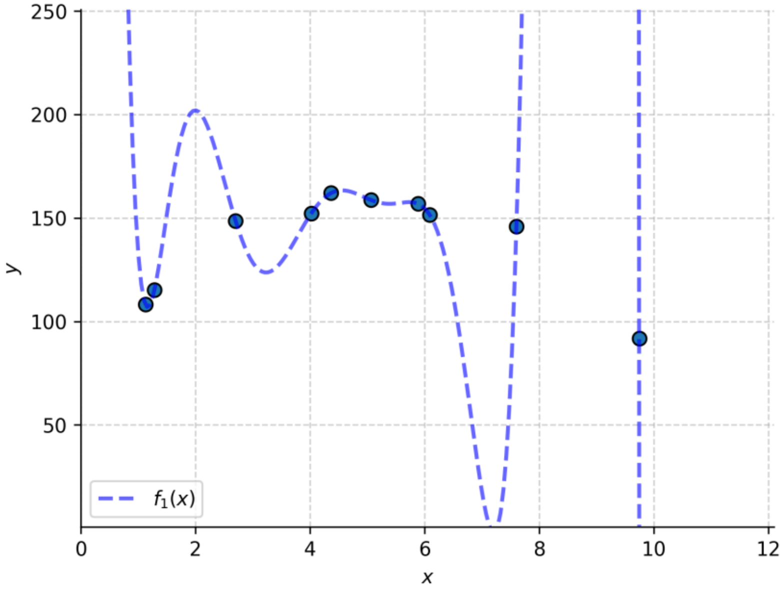

What if we *force coefficients to be small*?

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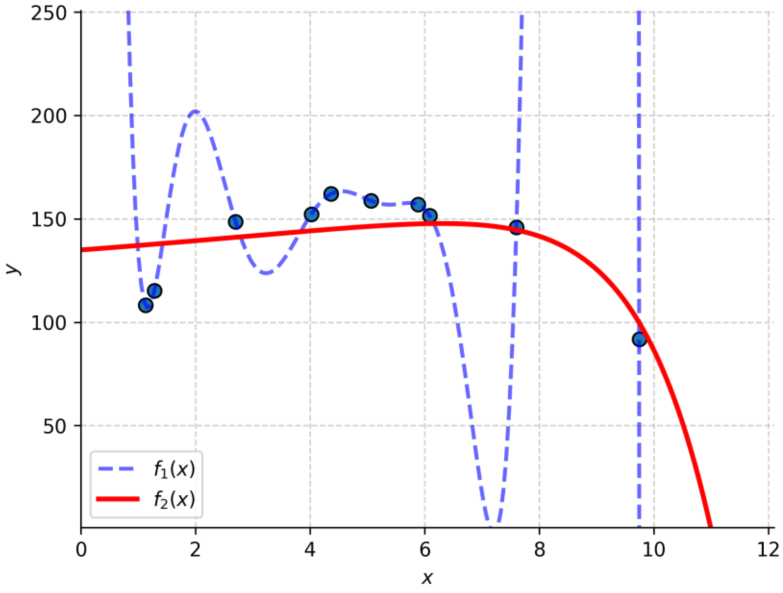

What if we *force coefficients to be small*?

$$f_2(x) = \boxed{\begin{aligned} &1.34 * 10^1 \\ +&2.09 * 10^1 x \\ +&7.11 * 10^{-2} x^2 \\ -&6.24 * 10^{-4} x^3 \end{aligned}} + \cdots$$

Small coefficients →
- Function is much smoother.

Ridge Regression

- We want small coefficients, so we add the norm of the weight vector to the loss:

$$\mathcal{L}_E = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda \|\vec{w}\|_2^2$$

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L_2 regularization

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L_2 regularization

- In matrix format:

$$\mathcal{L}_E = \left(Y - \hat{Y}\right)^2 + \lambda w^T w$$

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L_2 regularization

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$$\frac{\partial \mathcal{L}}{\partial w} = 0 \Rightarrow$$

$$\boldsymbol{w} = \left(\boldsymbol{X}^T \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y}$$

Ridge Regression

- We want small coefficients, so we add the norm of the weight vector to the loss:

$$\mathcal{L}_E = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda ||\vec{w}||_2^2$$

L_2 regularization

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Always invertible.

Other types of regularization

- **Lasso**
  - Same as Ridge Regression, but with L_1 regularization:

$$\mathcal{L}_E = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda \|\vec{w}\|_1$$

L_1 regularization

  - The L_1 penalty encourages some of the weights to be exactly 0, not just small.

Other types of regularization

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L_1 regularization

  - The L_1 penalty encourages some of the weights to be exactly 0, not just small.

- **Elastic Net**
  - Linear combination between Ridge Regression and Lasso Regression:

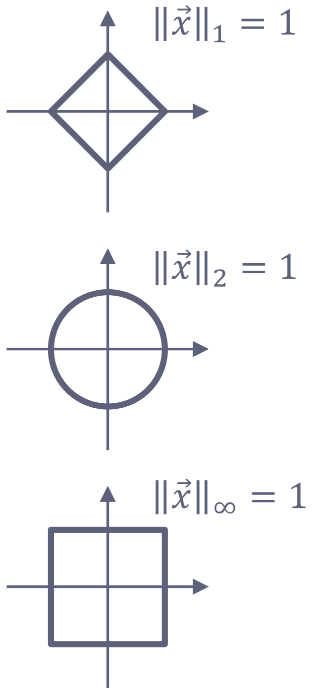
$$\mathcal{L}_E = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda_1 \|\vec{w}\|_2^2 + \lambda_2 \|\vec{w}\|_1$$

Other types of regularization

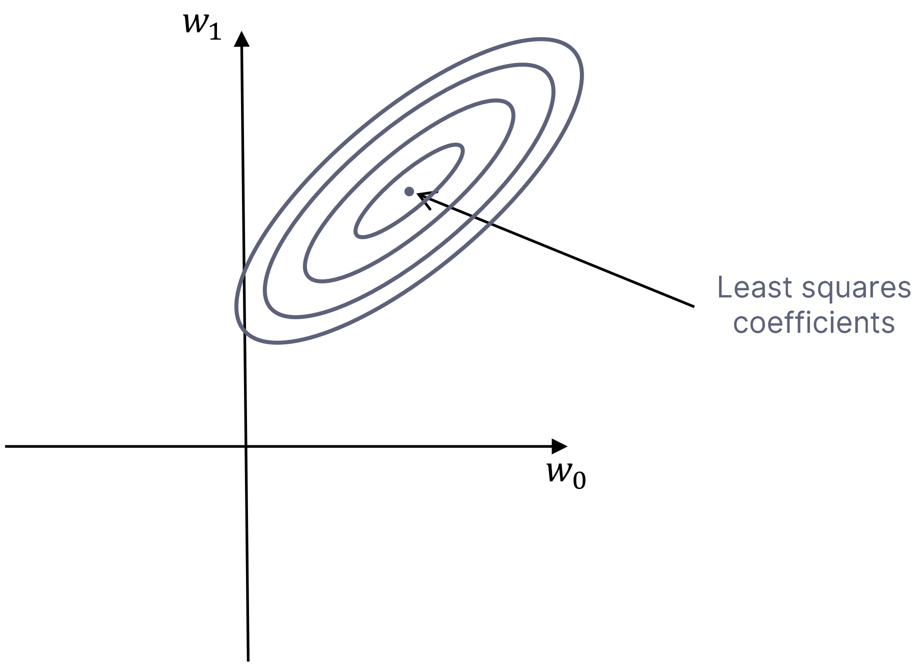
- L_p-norm of a vector $\vec{x} \in \mathbb{R}^n$:

$$\|\vec{x}\|_p = \sqrt[p]{\sum_{i=1}^{n} |x_i|^p}$$

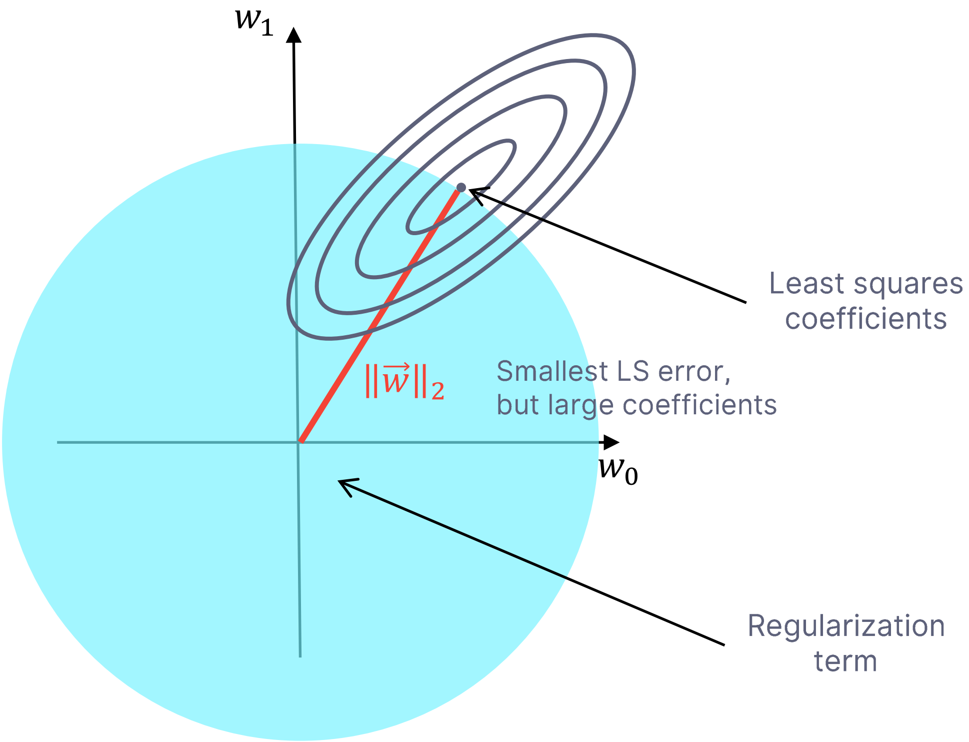
  - $p = 1 \Longrightarrow$ Manhattan Norm (sum of absolute element values)
  - $p = 2 \Longrightarrow$ Euclidean Norm
  - $p = \infty \Longrightarrow$ Maximum Norm (value of the absolute maximum element)



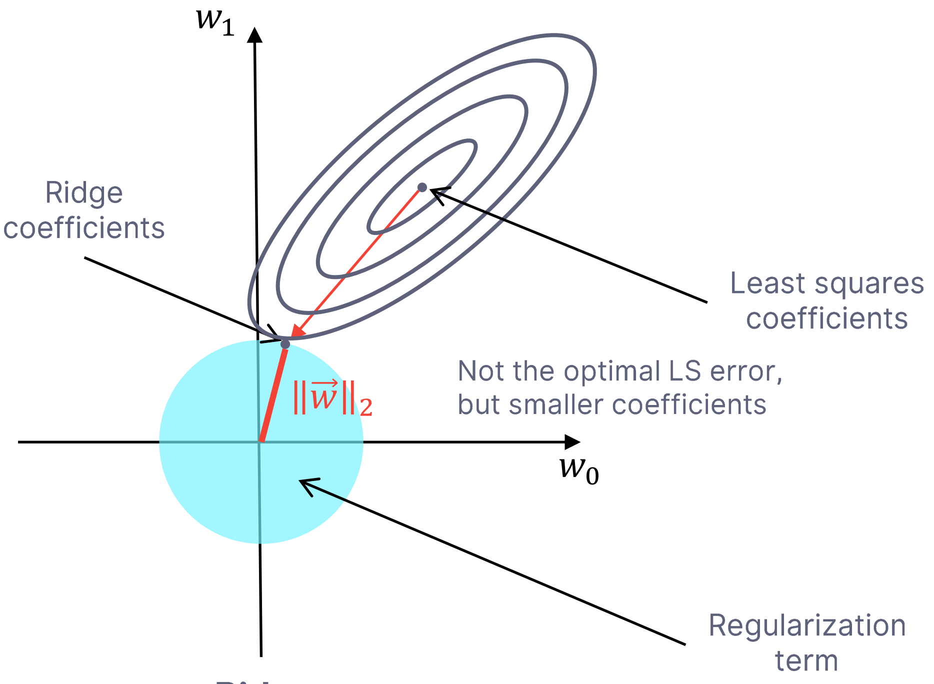
Other types of regularization



Other types of regularization

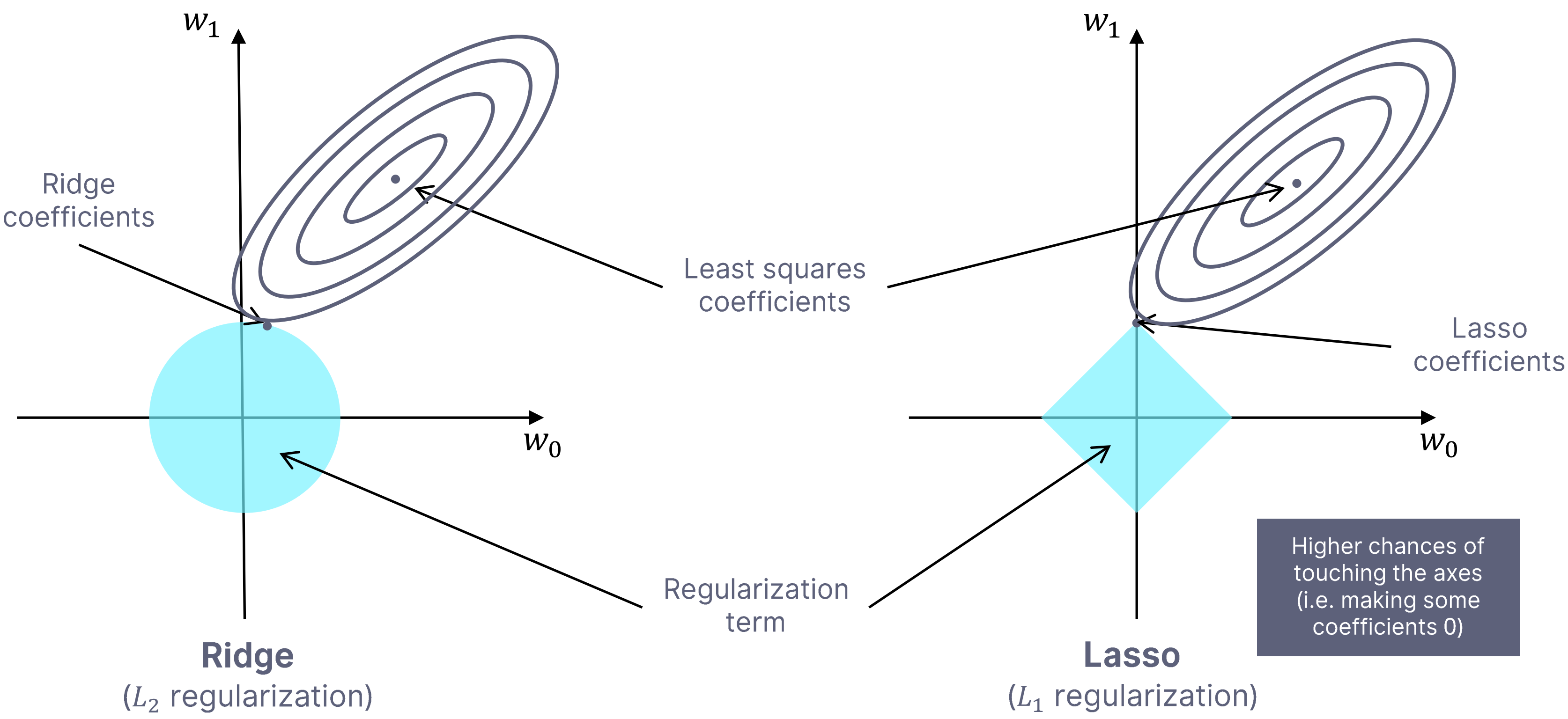


Other types of regularization



Ridge
(L_2 regularization)

Other types of regularization



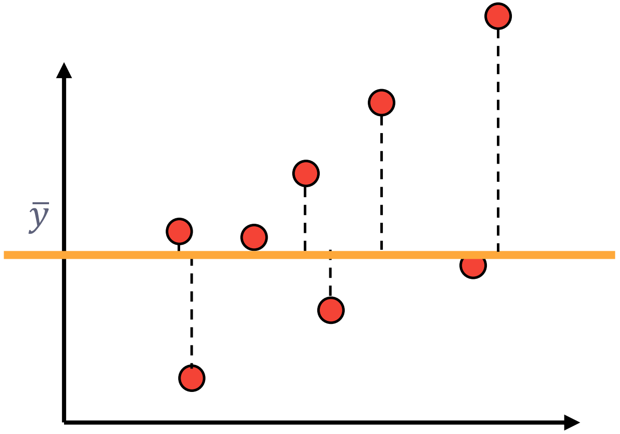
Recap

- **Linear regression**
  - Fits a *linear model* on the data:
    - $\hat{y} = \langle \vec{x}, \vec{w} \rangle = \mathrm{w}_0 + w_1 x_1 + w_2 \mathrm{x}_2 + \cdots + \mathrm{w}_\mathrm{n} \mathrm{x}_\mathrm{n}$
    - in matrix form: $\hat{Y} = Xw$
  - Minimizing the *squared-error loss* gives the following formula:
    - $\boldsymbol{w} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y}$
- **Ridge regression**
  - Forcing small coefficients makes the function smoother and less prone to overfitting.
  - Adding L_2 *regularization* (the Euclidean norm of the weight vector) to the loss gives:
    - $\boldsymbol{w} = \left(\boldsymbol{X}^T \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y}$

Coefficient of determination

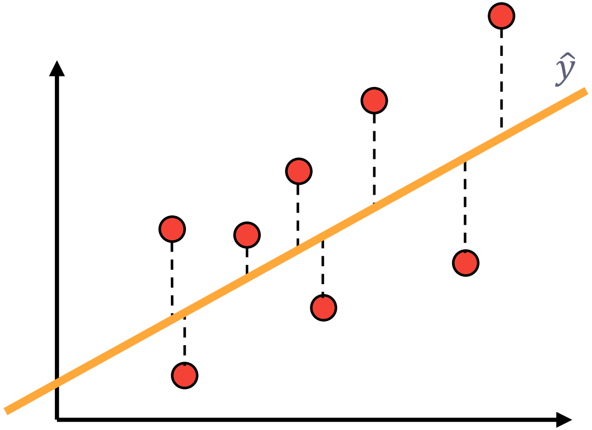
- The coefficient of determination (R^2, pronounced "R squared")
  - amount of variance in the dependent variable which is explained by the independent variables.

$$\overline{\mathcal{L}_E} = \sum_i \left(y^{(i)} - \bar{y}\right)^2$$



$$R^2 \stackrel{\text{def}}{=} \frac{\overline{\mathcal{L}_E} - \mathcal{L}_E(\vec{w})}{\overline{\mathcal{L}_E}}$$

$$\mathcal{L}_E(\vec{w}) = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

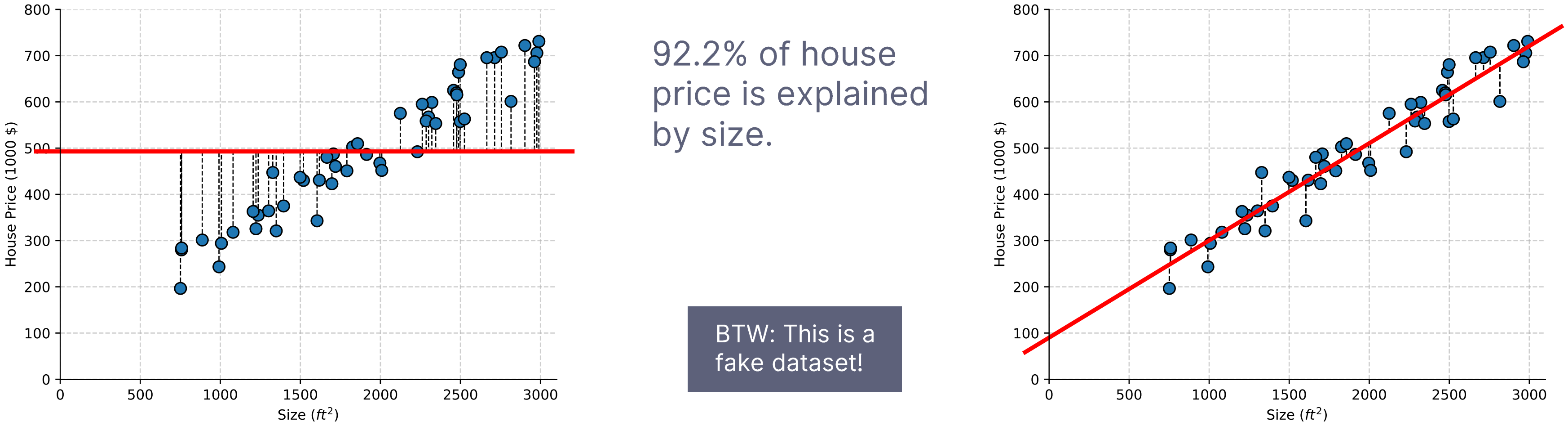


Coefficient of determination

$$R^2 = \frac{939{,}000.6 - 73{,}032.3}{939{,}000.6} = 0.922$$

$\overline{\mathcal{L}_E} = 939{,}000.6$

$\mathcal{L}_E(\vec{w}) = 73{,}032.3$



92.2% of house price is explained by size.

BTW: This is a fake dataset!

Linear Regression in Python

```python
from sklearn.linear_model import LinearRegression, Ridge, Lasso, ElasticNet

clf = LinearRegression()
clf.fit(X, y)

clf.predict([x]) # prediction for x

clf.score(X, y) # $R^2$ coefficient
clf._residues # Loss on the training samples $\mathcal{L}_{\hat{y}}$
clf.coef_ # $w_1, w_2 \dots w_n$
clf.intercept_ # $w_0$

clf = Ridge(alpha = 10) # alpha is the regularization strength $\lambda$
```

Conclusion

- **Linear Regression** uses a *linear function* to establish a relationship between a *dependent variable* and a number of *independent variables*.
- The parameters of the model are obtained by minimizing the **squared-error loss**.
- The fitted model can be used to determine the *correlation* between features and label.
- The fitted model can also be used to make *predictions* on future data.
- **Ridge Regression** adds *regularization* in order to deal with *ill-posed problems*.

Keywords

Linear Regression

Dependent / Independent Variable

Multivariate

Linear Function

Squared-error Loss

Ill-posed Problem

Regularization

Ridge Regression

Lasso

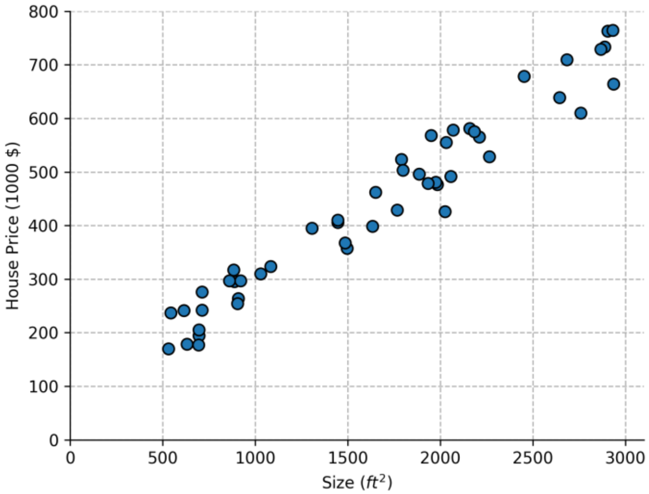
Elastic Net

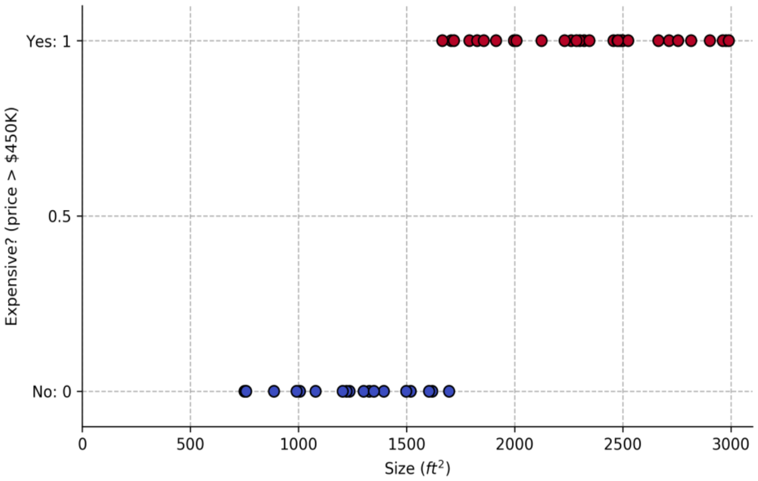
Correlation

R^2 (R squared)

Regression vs. Classification

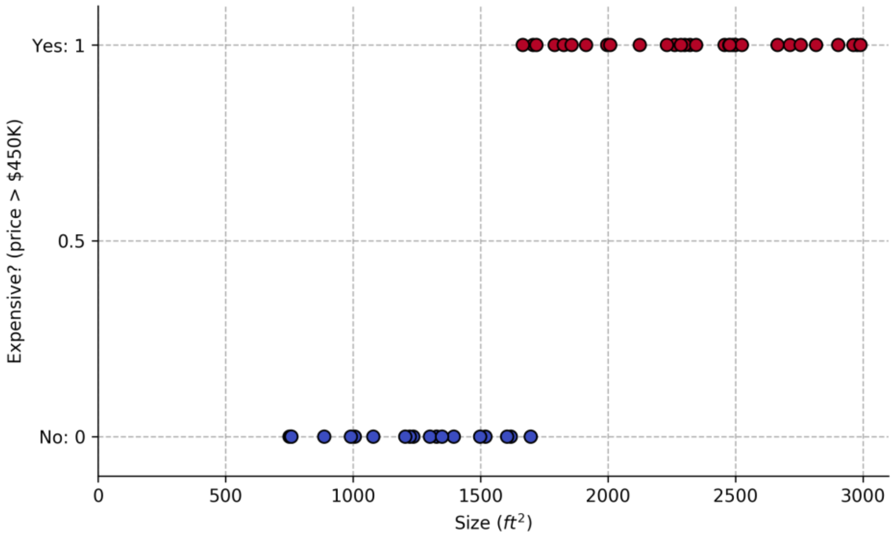
- What if we only knew and wanted to predict whether a house is expensive or not?
    - No information about the actual price → Binary classification problem.





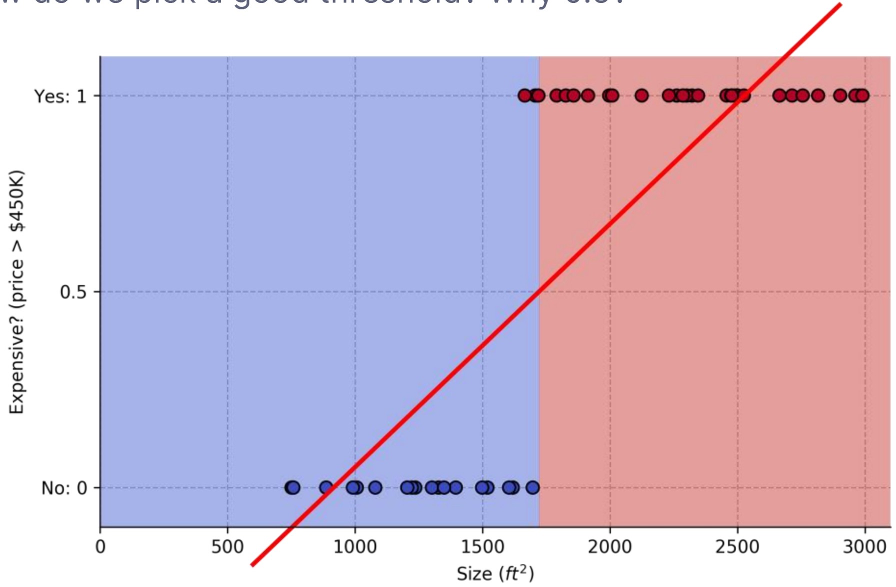
Regression vs. Classification

- Can we use Linear Regression to do Classification?



Regression vs. Classification

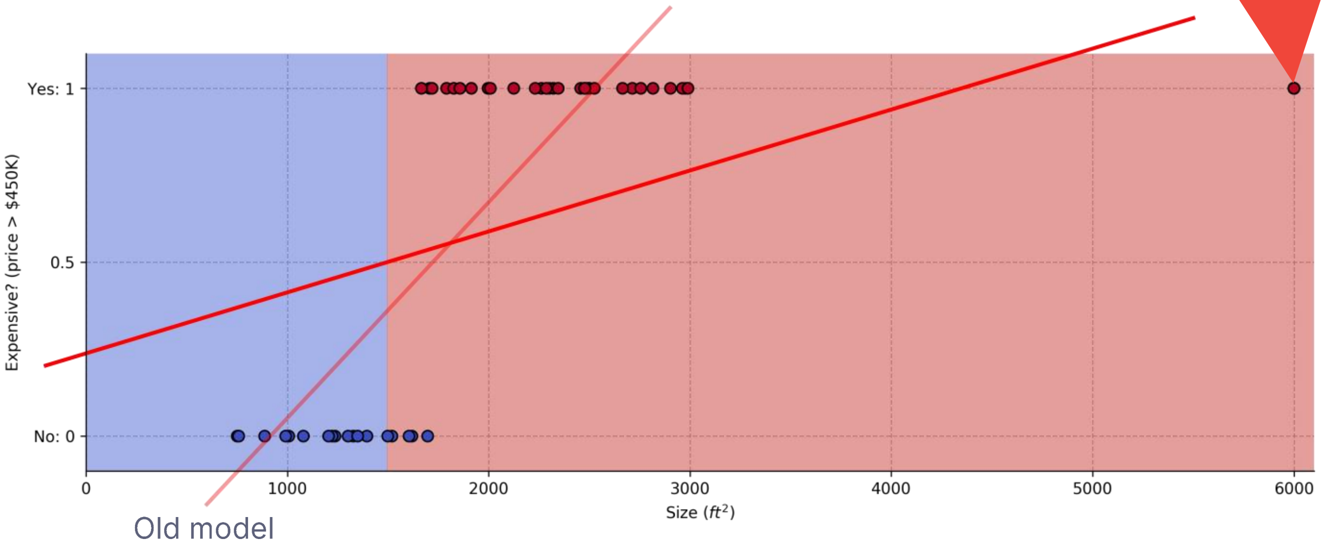
- Can we use Linear Regression to do Classification?
  - Not too bad, but a little hard to interpret the results.
  - Also, how do we pick a good threshold? Why 0.5?



Regression vs. Classification

- Same dataset as before, but with an added point.
  - Keeping the same 0.5 threshold makes some points get misclassified.
  - Can we find a better solution?

The old model "thinks" it is making a huge mistake for this point, even though it is getting the class right.



Regression vs. Classification

- Same dataset as before, but with an added point.
  - Keeping the same 0.5 threshold makes some points get misclassified.
  - Can we find a better solution? → ***Logistic Regression***

The old model "thinks" it is making a huge mistake for this point, even though it is getting the class right.