Linear Regression

Supervised

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Bristol, UK
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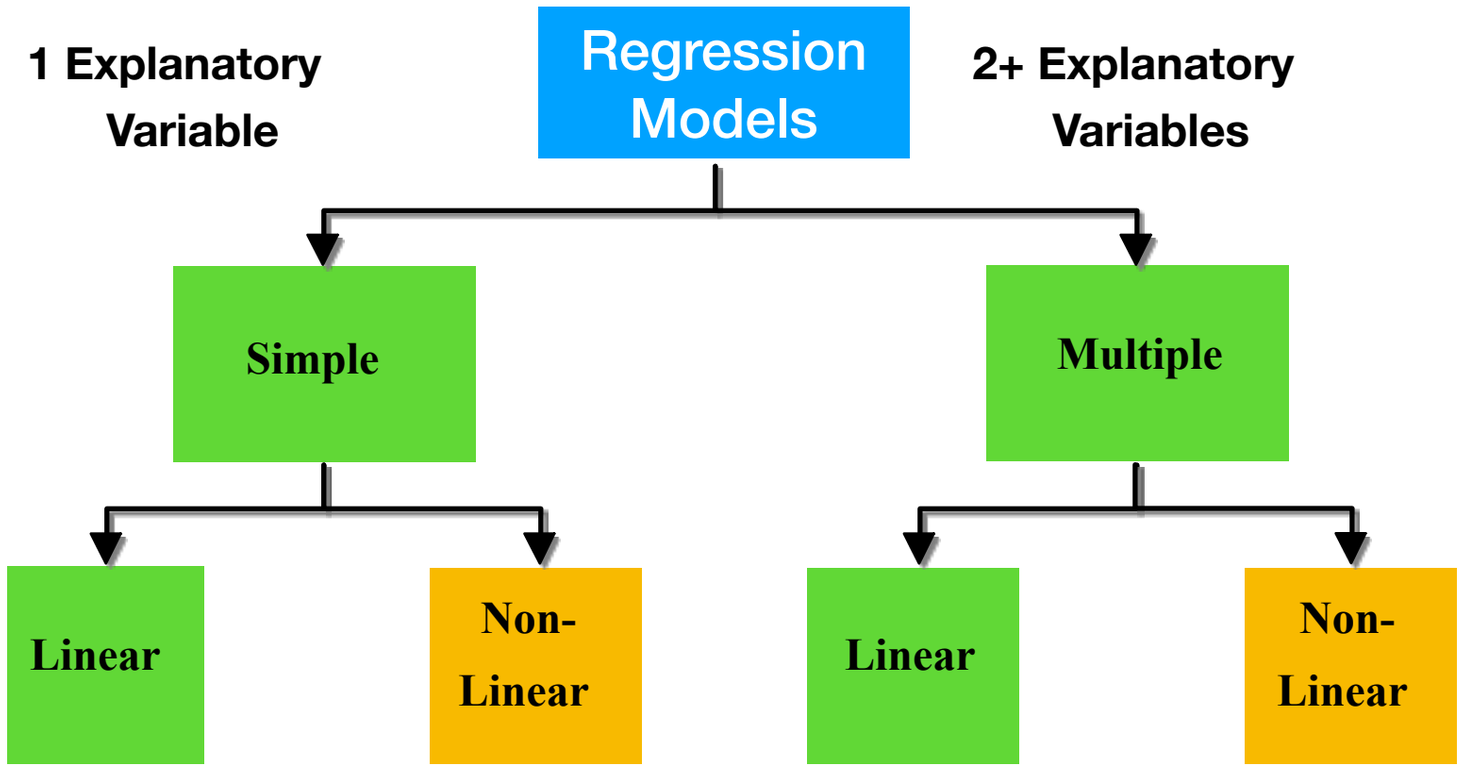
Agenda

- ➡ Motivation
- ➡ Linear Regression Models
  - ◉ Estimation
  - ◉ Evaluation
- ➡ Tutorial (1) — you will be provided with further exercise later on.

Note: if you see many equations and dislike them, you're absolutely OK (these are just an extra).

I'll show you what we need to minimally understand by the end of this lecture!

Regression Models



Motivation

- Analyse the *specific* relationships between the independent variables and the dependent one.
- Predict the value of a *dependent* variable (Y_i) from the value of *independent* variable ($X1_i$, $X2_i$, …, Xn_i)

Motivation

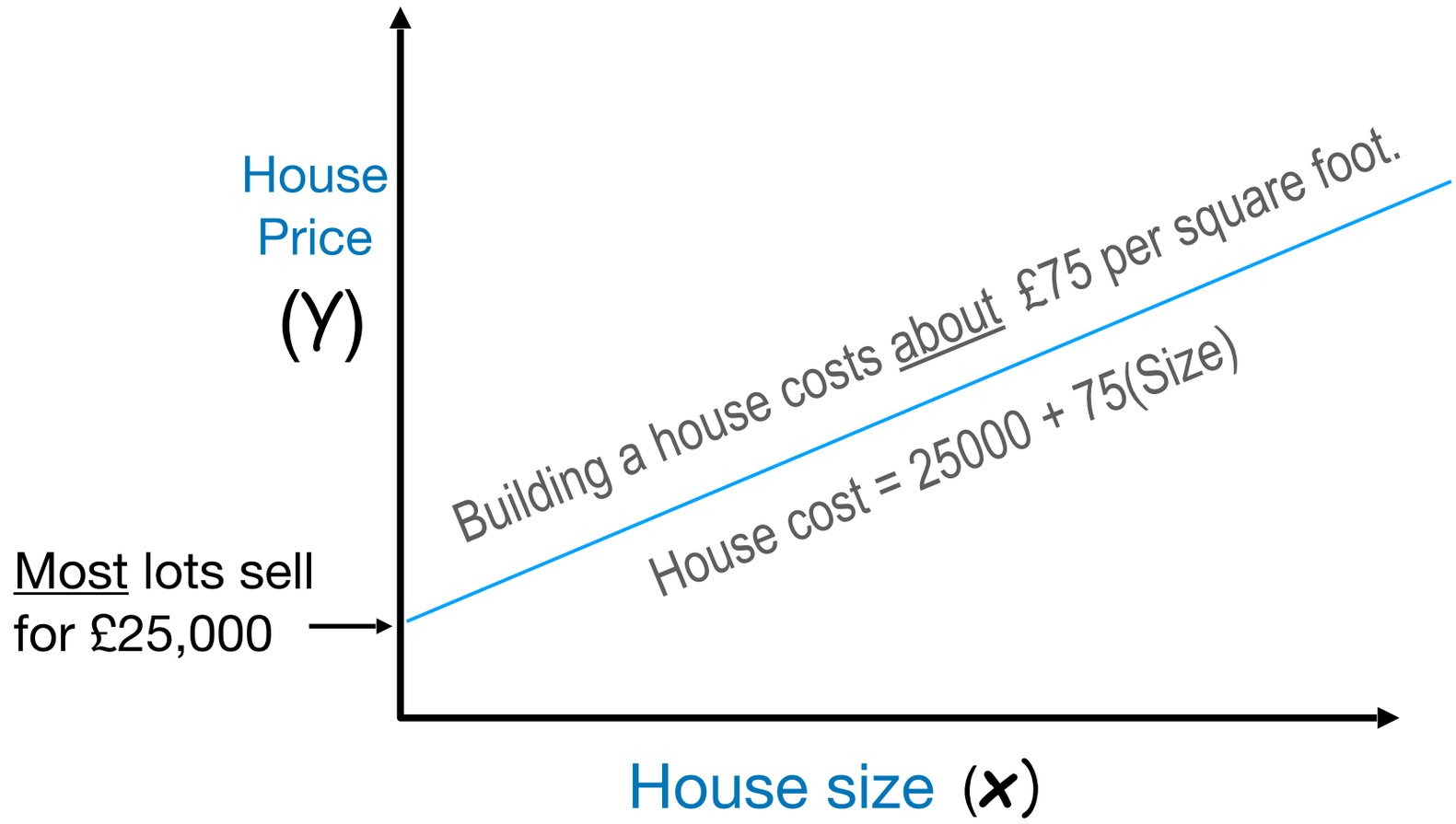
simple LR

- Predict the value of a *dependent* variable (Y_i) from the value of *independent* variable ($X1_i$, $X2_i$, …, Xn_i)

- Analyse the specific relationships between the independent variables and the dependent one

Multiple LR

Relationship between 2 variables

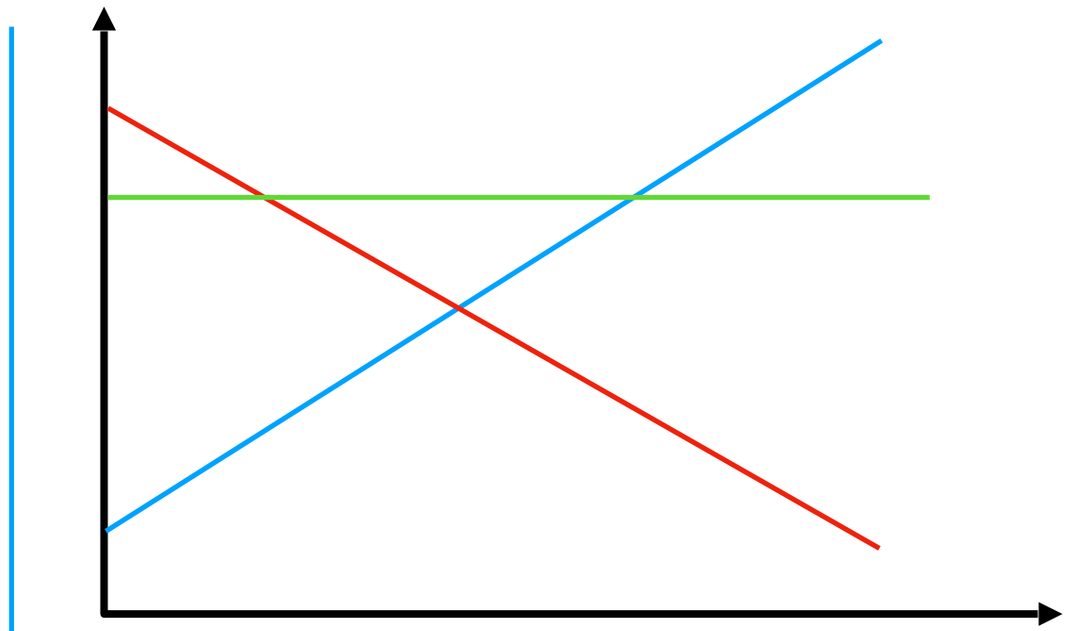


! **Extrapolation vs Interpolation**

General Model

- $\beta_1 > 0 \Rightarrow$ Positive Association
- $\beta_1 < 0 \Rightarrow$ Negative Association
- $\beta_1 = 0 \Rightarrow$ No Association

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$



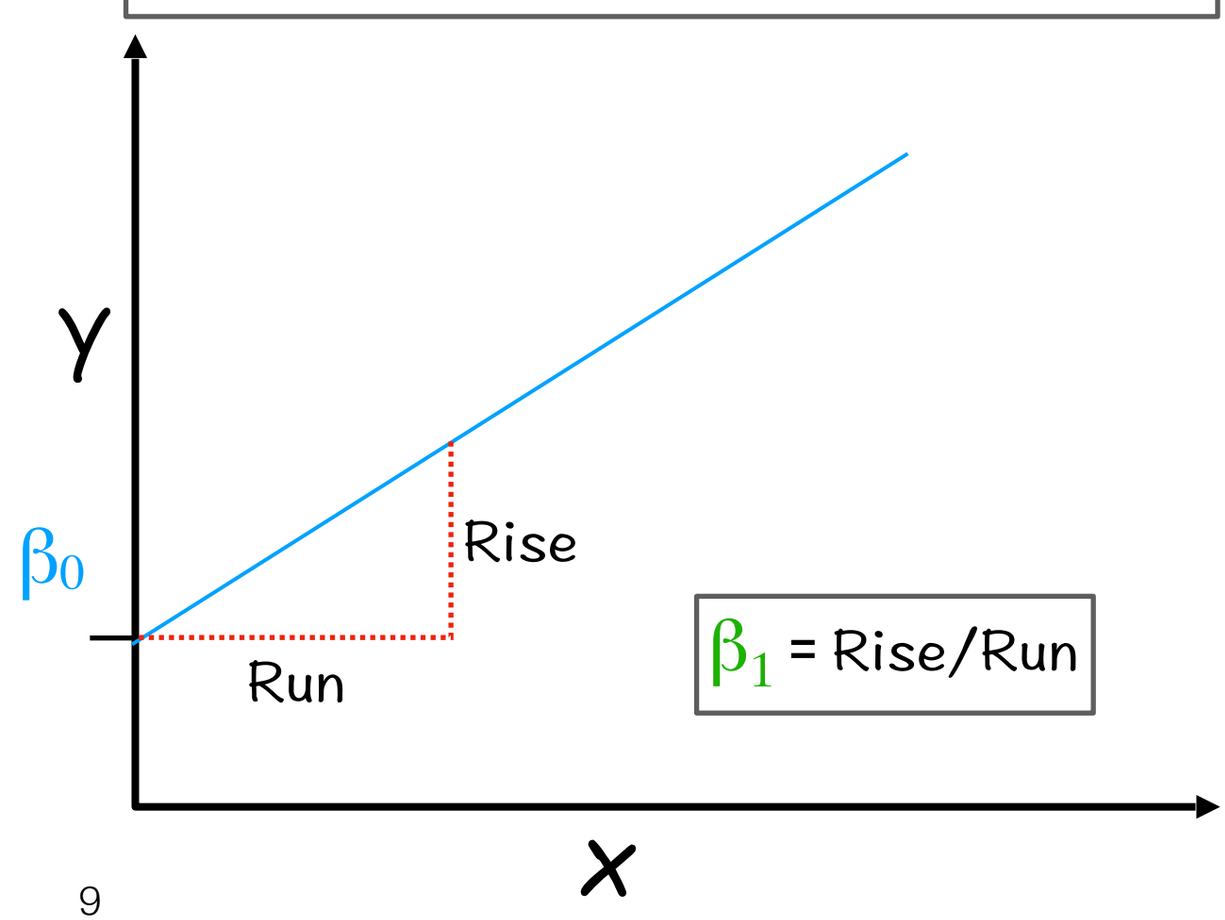
- $\beta_0 \equiv$ Mean response when x=0 (y-intercept)
- $\beta_1 \equiv$ Change in mean response when x increases by 1 unit (slope)
- β_0, β_1 are unknown parameters (like μ)
- $\beta_0+\beta_1 x \equiv$ Mean response when independent variable takes on the value x

Simplified (simple LR)

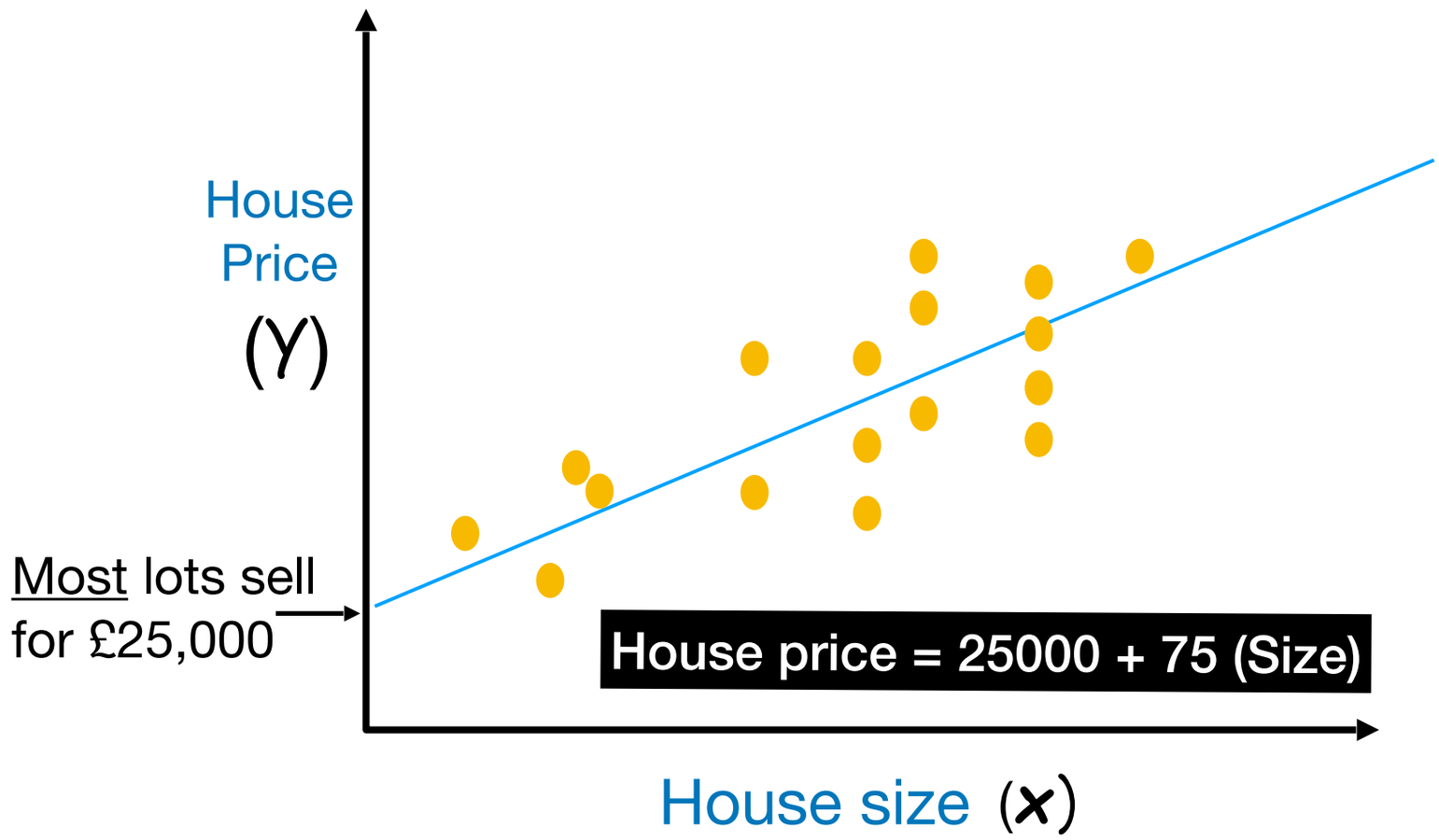
$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

- y = dependent variable
- x = independent variable
- β_0 = y-intercept
- β_1 = slope
- ε = error variable

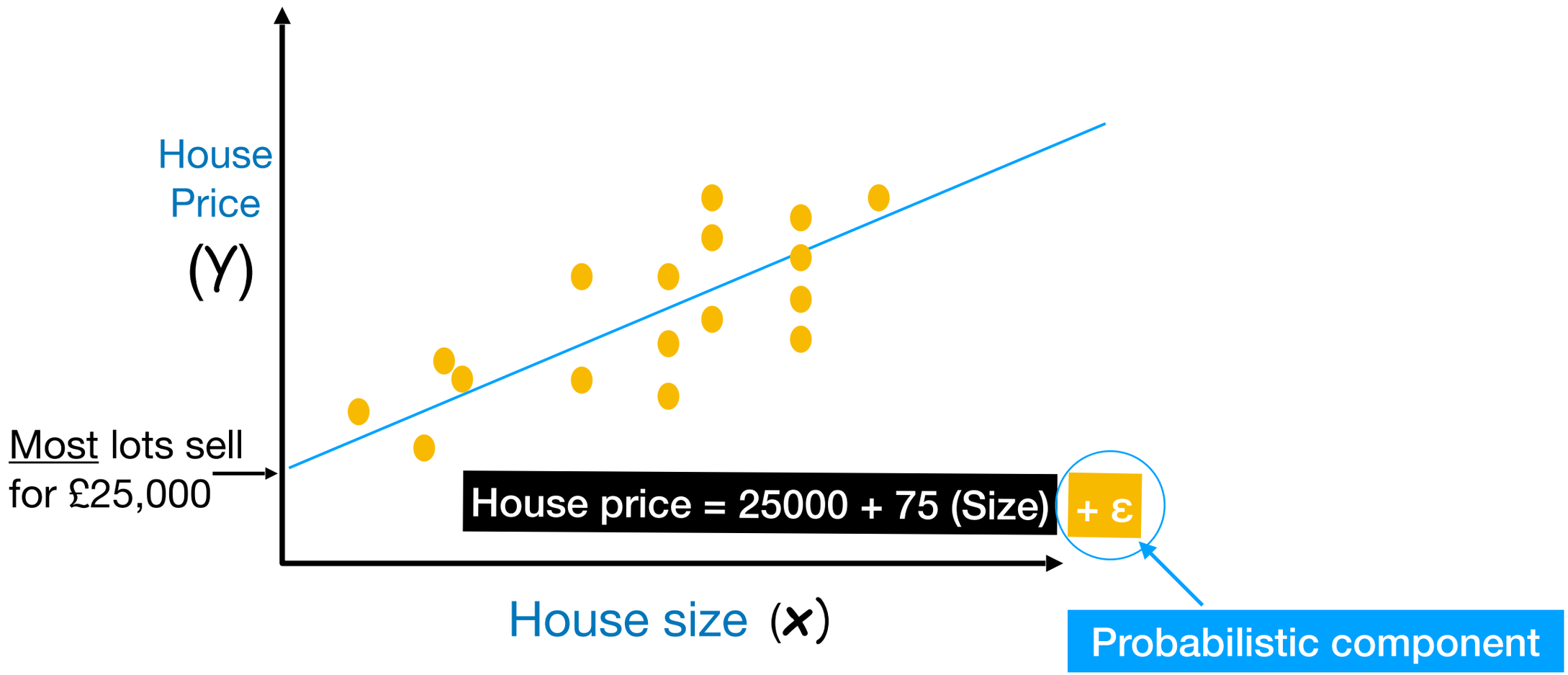
β_0 and β_1 are unknown *population* parameters, therefore are estimated from the data.



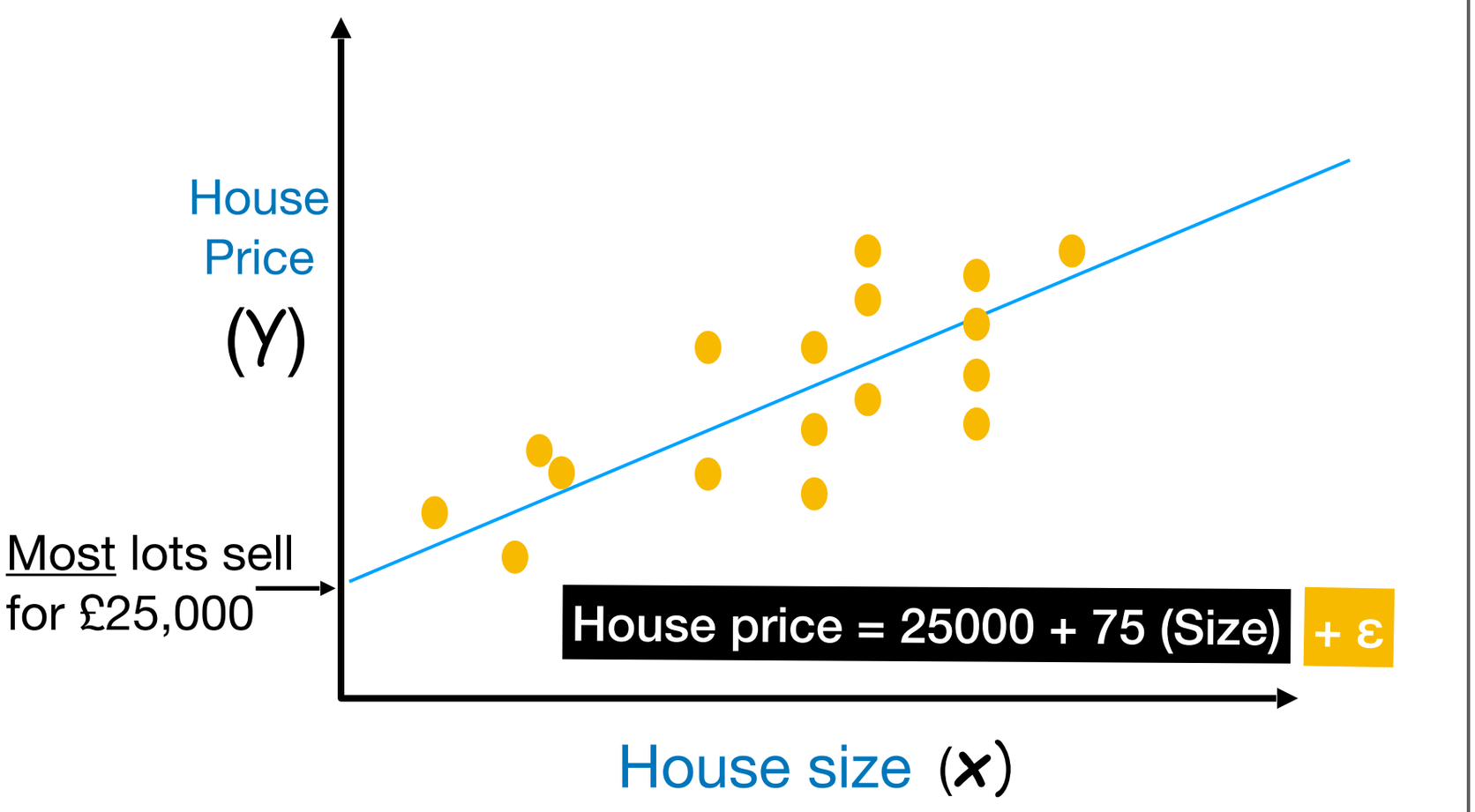
Deterministic and Probabilistic relationship



Deterministic and Probabilistic relationship



Deterministic and Probabilistic relationship

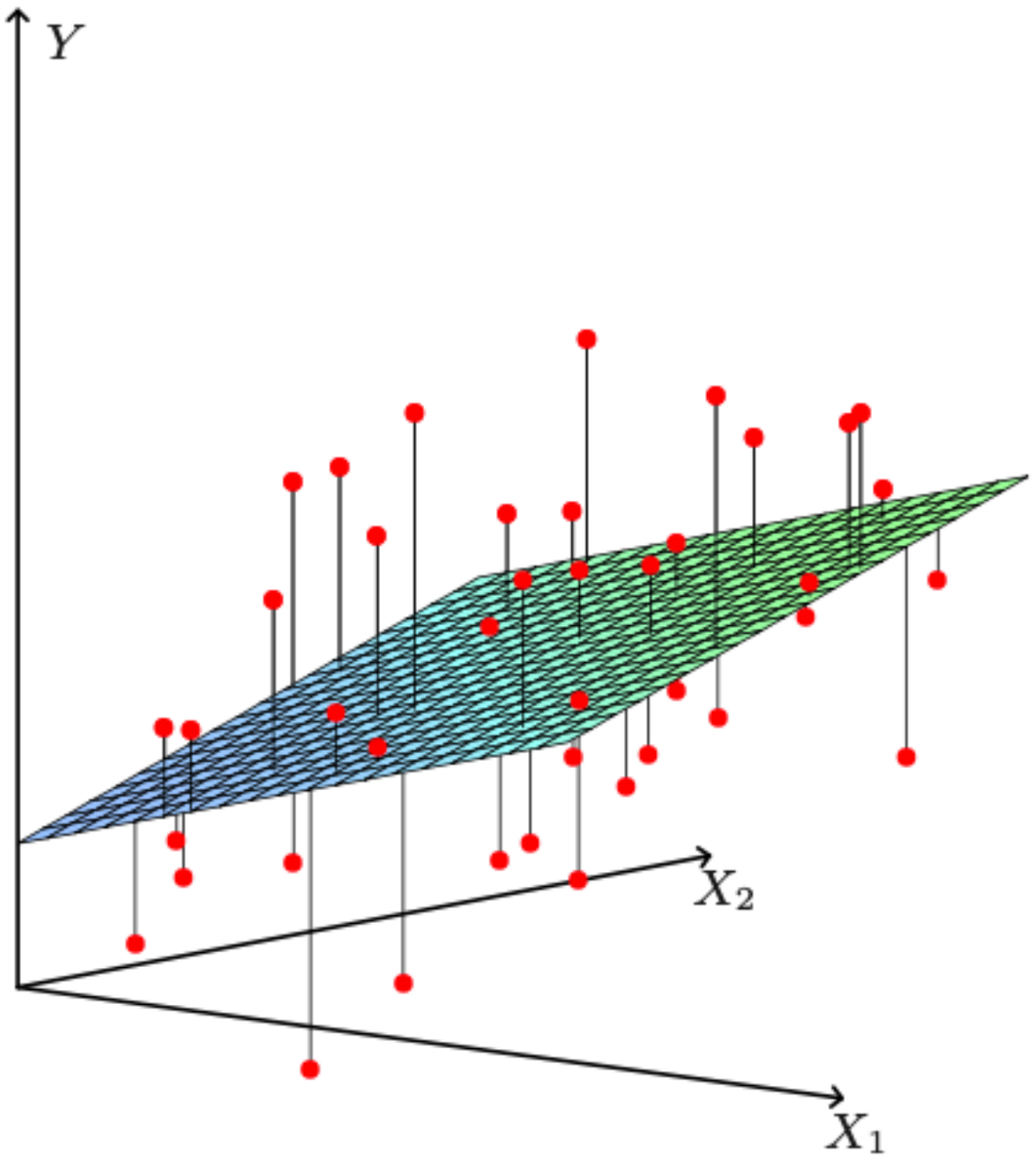


$$y_i = \beta_0 + \beta_1 x_i + \epsilon$$

$$\epsilon \sim N(0, \sigma^2)$$

Note that the intercept β_0, the slope β_1, and the noise variance σ^2 are all treated as fixed (i.e., deterministic) but unknown quantities.

Motivation



$$h(x) = \beta_0 + \sum_{i=1}^{P} X_i \beta_i$$

Linear least squares fitting with $X \in IR^{\wedge}p$. We seek the linear function of X that minimises the sum of squared residuals from Y .

Assumptions

(1) The regression model is linear in parameters (Weak exogeneity)

- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$
- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon$

(2) Mean of residuals is zero & Homoscedasticity of constant variance

- $\epsilon \sim N(0, \sigma^2)$

(3) Feature vectors and residuals are uncorrelated.

(4) No perfect multicollinearity

- Variance Inflation Factor (VIF) $VIF_i = \frac{1}{(1 - {R_i}^2)}$

```
from statsmodels.stats.outliers_influence import variance_inflation_factor
```

Agenda

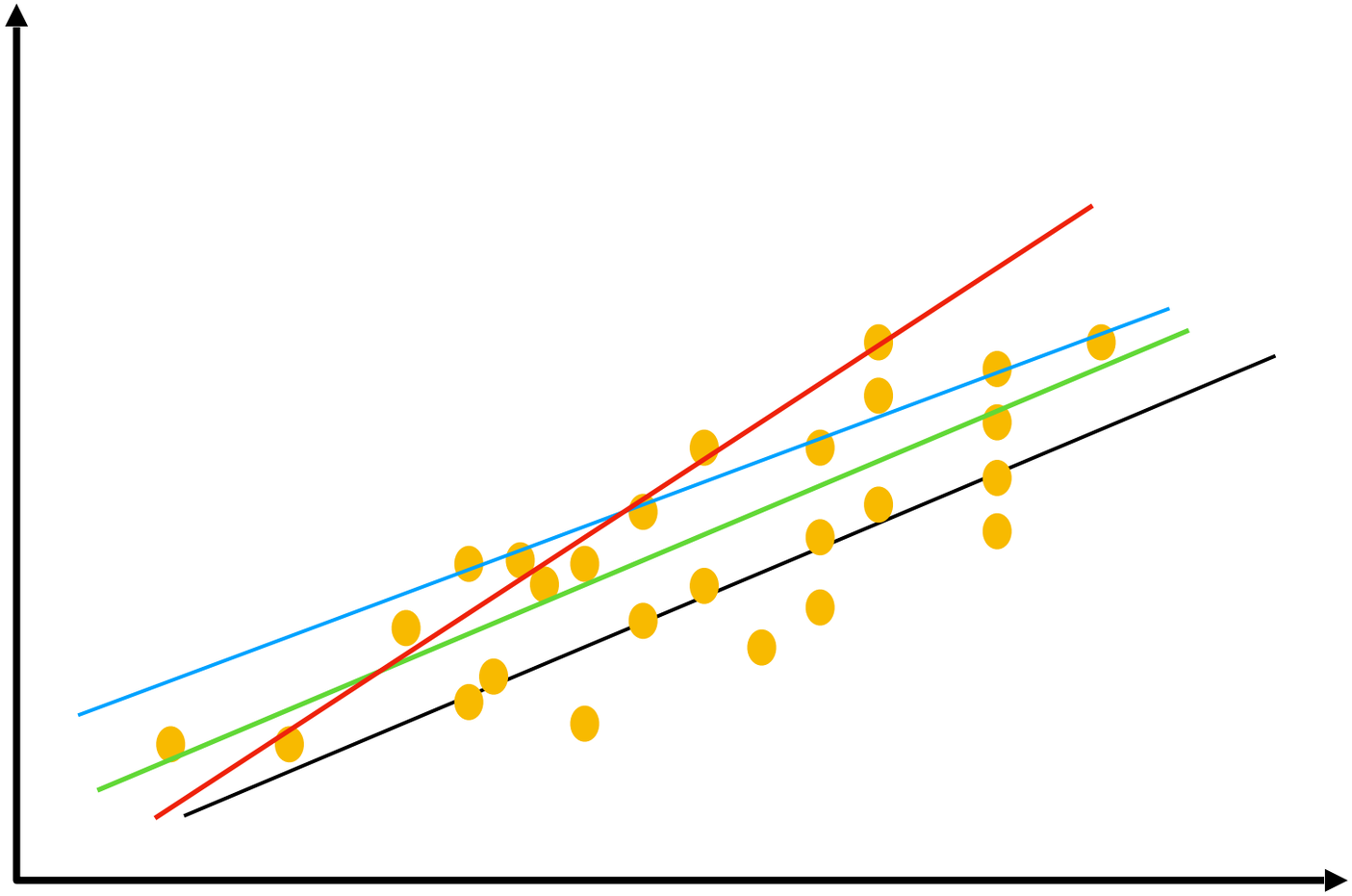
➡ Motivation

➡ Linear Regression Models

- ◉ Estimation
- ◉ Evaluation

➡ Tutorial (1) — you will be provided with further exercise later on.

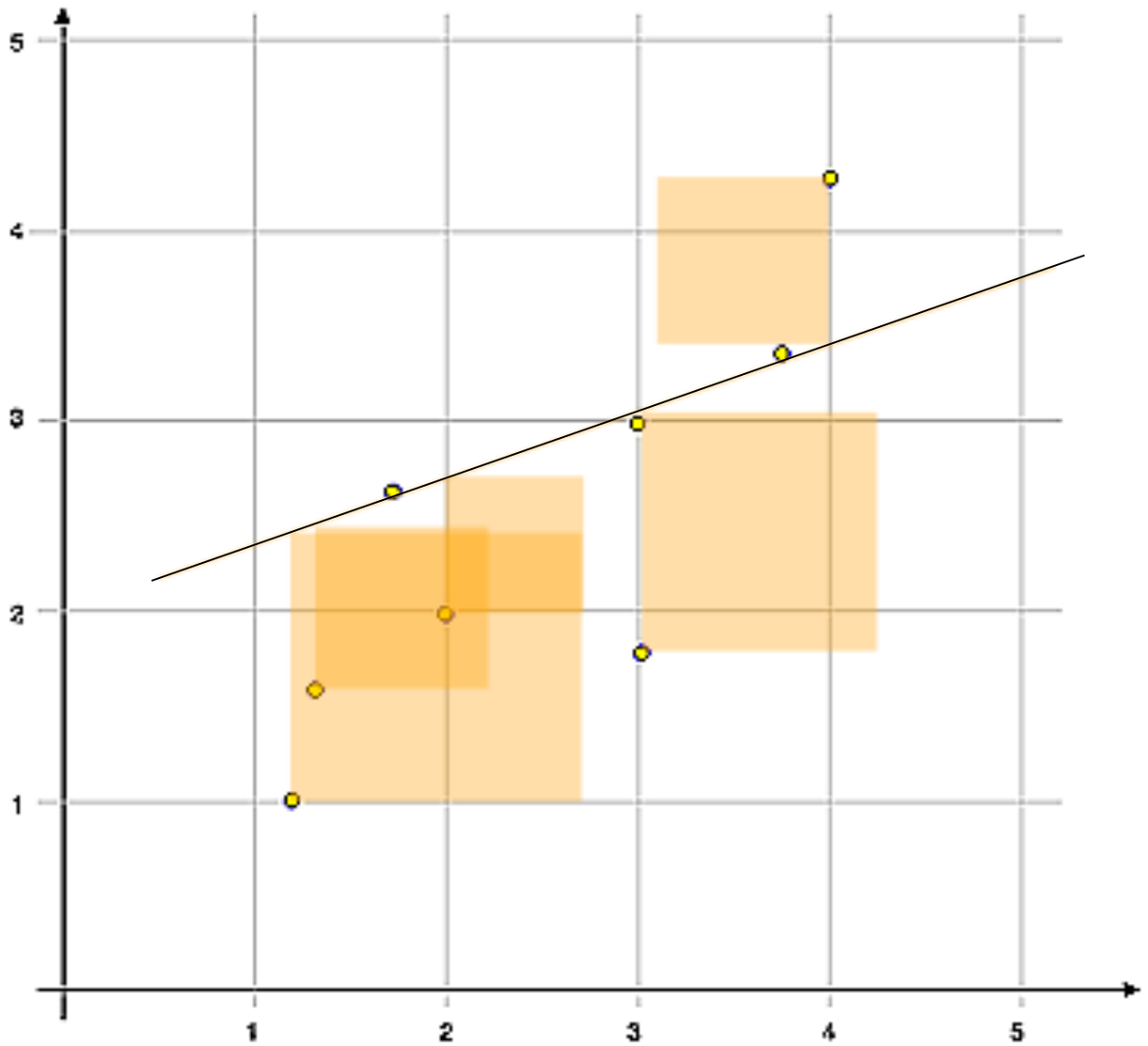
Which Line (model) then?



$\beta_0,\ \beta_1$

1) OLS {ordinary least squares} //

LSE Least Square Error

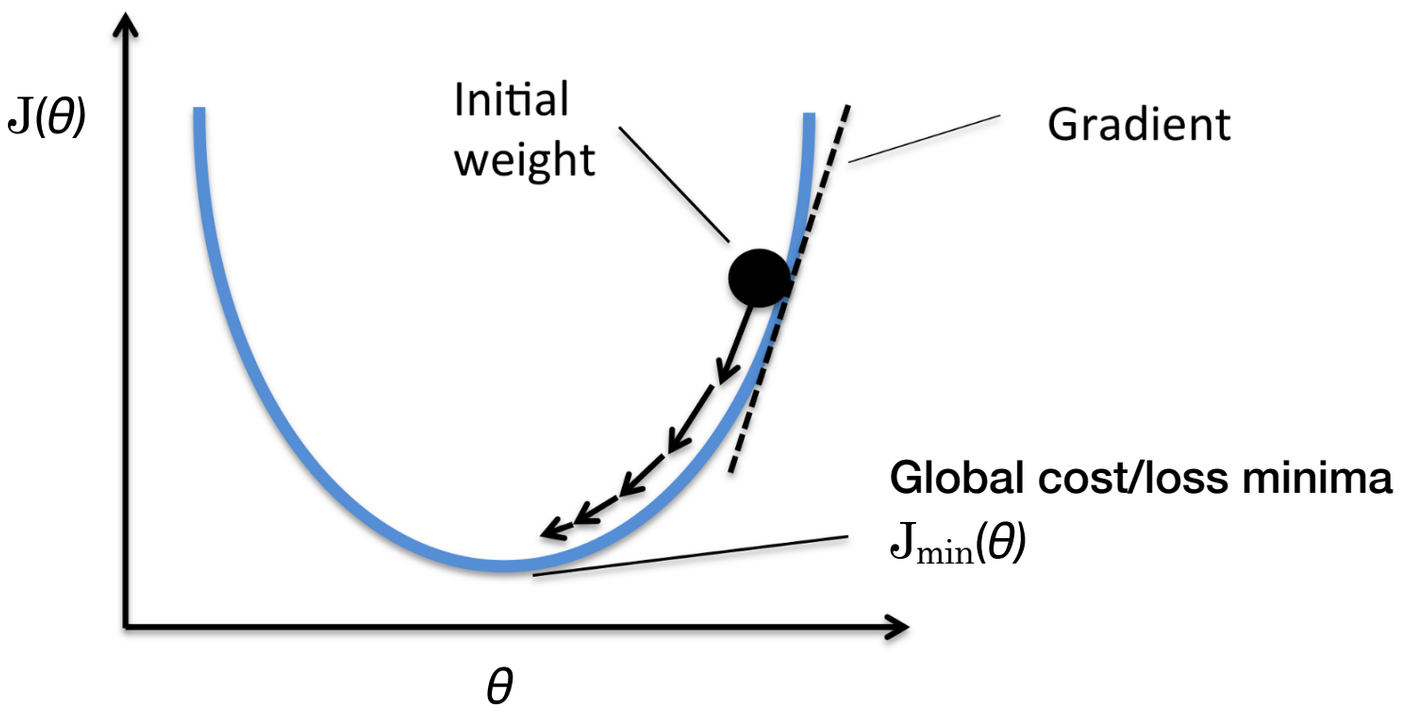


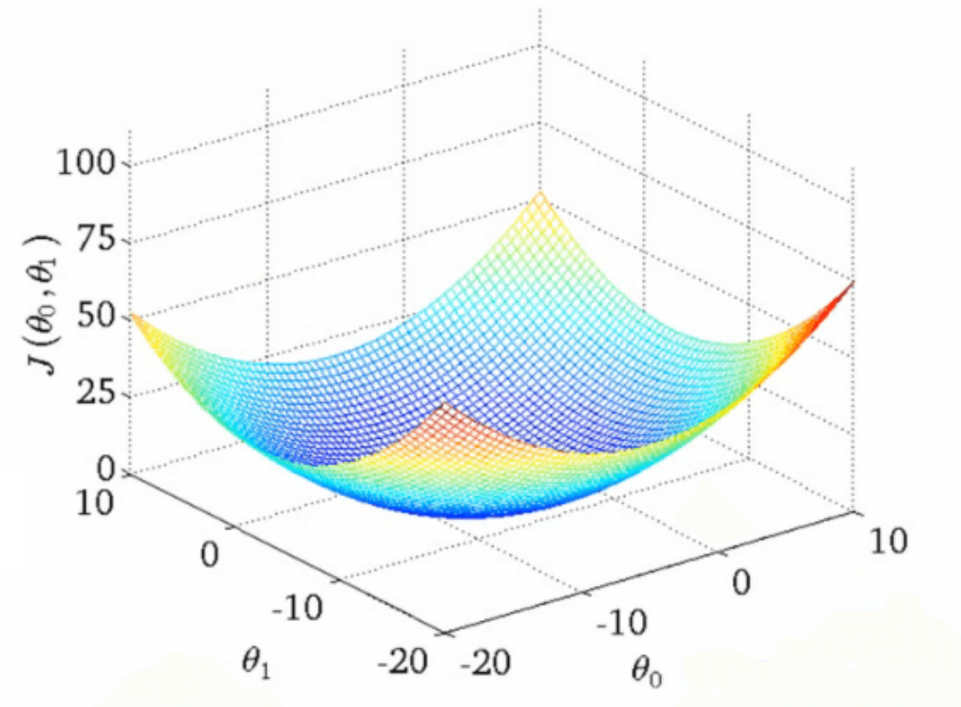
1) OLS {ordinary least squares}

Let θ_0 and θ_1 be your linear model (parameters, previously we called them β_0, β_1)

Gradient descent algorithm	Linear Regression Model

repeat until convergence {
$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$
(for $j = 1$ and $j = 0$)
}
	$h_\theta(x) = \theta_0 + \theta_1 x$
	$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$





2) MLE {Maximum Likelihood Estimate}

The Assumptions again!

1. The distribution of X is arbitrary (and perhaps X is even non-random).
2. If $X = x$, then $Y = \beta_0 + \beta_1 x + \epsilon$, for some constants ("coefficients", "parameters") β_0 and β_1, and some random noise variable ϵ.
3. $\epsilon \sim N(0, \sigma^2)$, and is independent of X.
4. ϵ is independent across observations.

$$P(y_i|X = x_i; \beta_0, \beta_1, \sigma^2)$$

Given any data set $(x_1, y_1), (x_2, y_2), ...(x_n, y_n)$, we can now write down the probability density, under the model, of seeing that data:

$$P(y_i|X = x_i; \beta_0, \beta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-\frac{(y_i - (\beta_0 + \beta_1 x_i))^2}{2\sigma^2}}$$

2) MLE {Maximum Likelihood Estimate}

$$P(y_i|X = x_i; \beta_0, \beta_1, \sigma^2)$$

$$P(y_i|X = x_i; \beta_0, \beta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-\frac{(y_i - (\beta_0 + \beta_1 x_i))^2}{2\sigma^2}}$$

$$\arg\max_{\vec{\beta}} \prod_{i=1}^{N} P(y_i|x_i, \vec{\beta})$$

$$\arg\max_{\vec{\beta}} \sum_{i=1}^{N} \log P(y_i|x_i, \vec{\beta})$$

$$= \log \prod_{i=1}^{n} p(y_i|x_i; b_0, b_1, s^2) \quad (1)$$

$$= \sum_{i=1}^{n} \log p(y_i|x_i; b_0, b_1, s^2) \quad (2)$$

$$= -\frac{n}{2} \log 2\pi - n \log s - \frac{1}{2s^2} \sum_{i=1}^{n} (y_i - (b_0 + b_1 x_i))^2 \quad (3)$$

… "under certain assumptions any learning algorithm that minimizes the squared error between the output hypothesis predictions and the training data will output a maximum likelihood hypothesis." — T. Mitchell Machine Learning [1st Ed.], 1997.

Simple linear regression

Solving for the fit: least-squares regression

Assuming that this is actually how the data $(x_1, y_1), \ldots, (x_n, y_n)$ we observe are generated, then it turns out that we can find the line for which the probability of the data is highest by solving the following optimization problem [*]:

$$\min_{\beta_0,\beta_1} : \sum_{i=1}^{n} \left[y_i - (\beta_0 + \beta_1 x_i)\right]^2, \tag{1}$$

where $\min_{\beta_0,\beta_1}$ means "minimize over β_0 and β_1". This is known as the **least-squares linear regression problem**. Given a set of points, the solution is:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} x_i y_i - \frac{1}{n}\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n}(\sum_{i=1}^{n} x_i)^2} \rightarrow \boxed{\frac{cov(x,y)}{s_x^2}} \tag{2}$$

$$= r\frac{s_y}{s_x}, \tag{3}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}, \tag{4}$$

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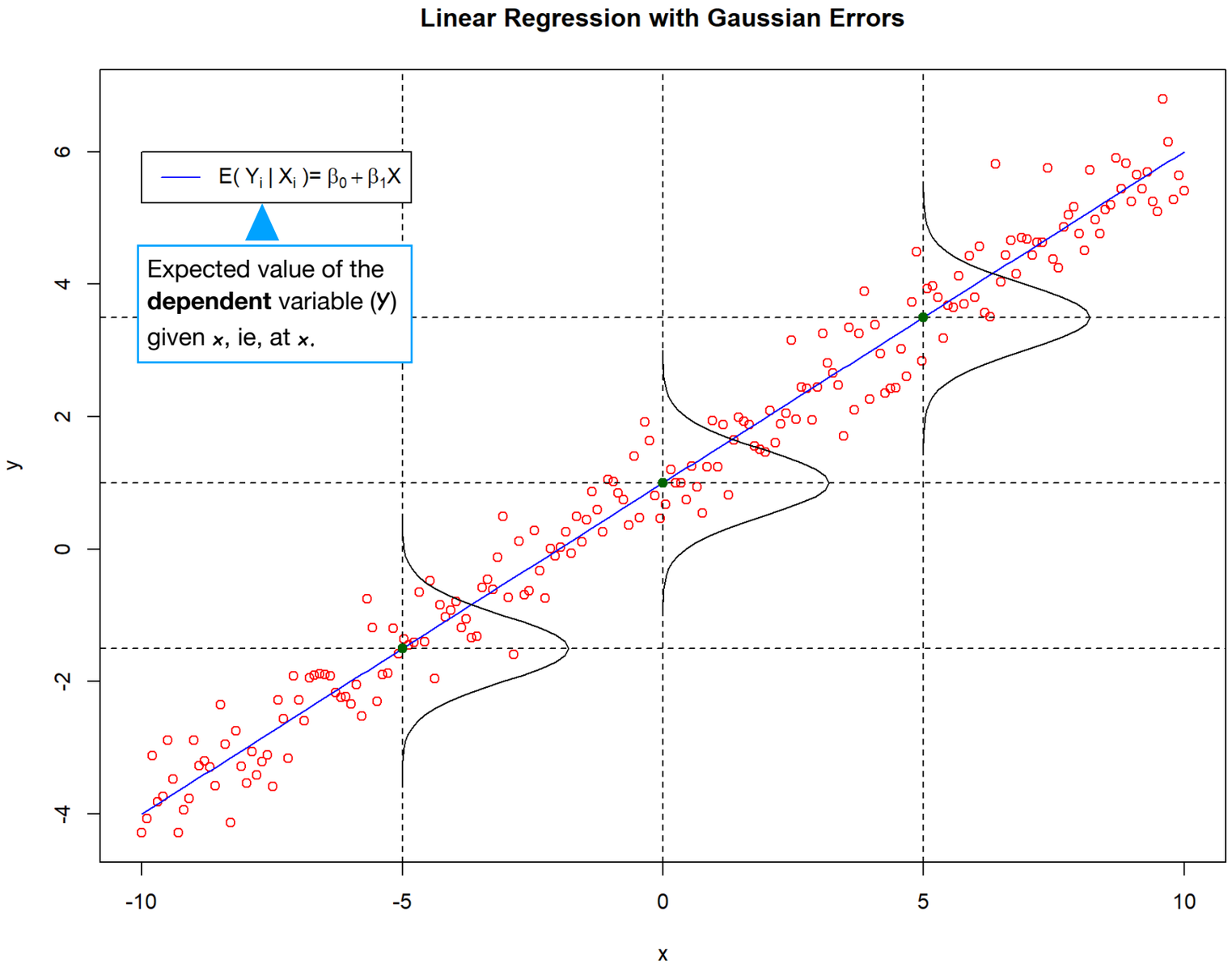
[*] This is an important point: the assumption of Gaussian noise leads to squared error as our minimization criterion.

What to takeaway!



$$E(Y \mid x) = \beta_0 + \beta_1 x$$

The structural model underlying a linear regression analysis is that the explanatory (x) and outcome variables (y) are linearly related such that the population mean of the outcome for any x value is $\beta_0 + \beta_1 x$.

What to takeaway!

➡ Explanatory (independent) and Response (dependent) Variables are *Numeric.*

➡ Relationship between the ***mean*** of the response variable and the values of the explanatory variable assumed to be approximately linear (straight line)

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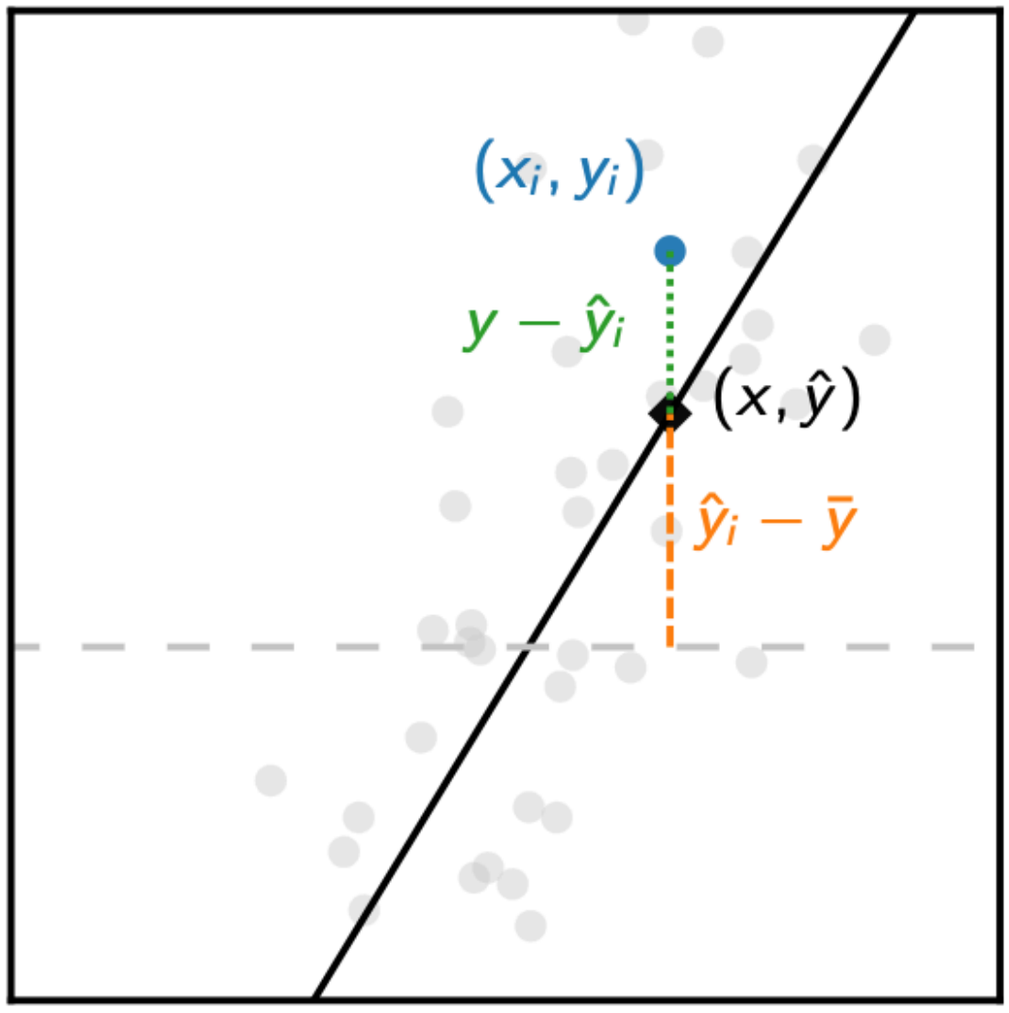
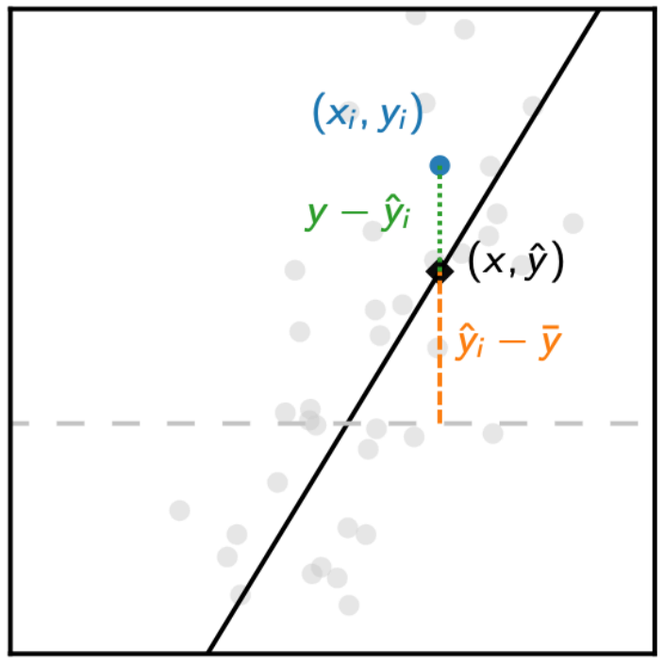
Evaluating LR model

Total LR square error



How much (what %) of the variation in ***y*** (orange and green) is NOT explained by the variation in ***x*** (as in LR model)***?*** — ***green left out*** (ie, unexplained by the model).

Coefficient of Determination



$$y_i - \bar{y} = \underbrace{(\hat{y}_i - \bar{y})}_{\text{difference explained by model}} + \underbrace{(y_i - \hat{y}_i)}_{\text{difference not explained by model}}$$

$$\underbrace{\sum_i (y_i - \bar{y})^2}_{\text{SS}_{\text{total}} \,=\, \text{SS}_{yy}} = \underbrace{\sum_i (\hat{y}_i - \bar{y})^2}_{\text{SS}_{\text{model}}} + \underbrace{\sum_i (y_i - \hat{y}_i)^2}_{\text{SS}_{\text{error}}},$$

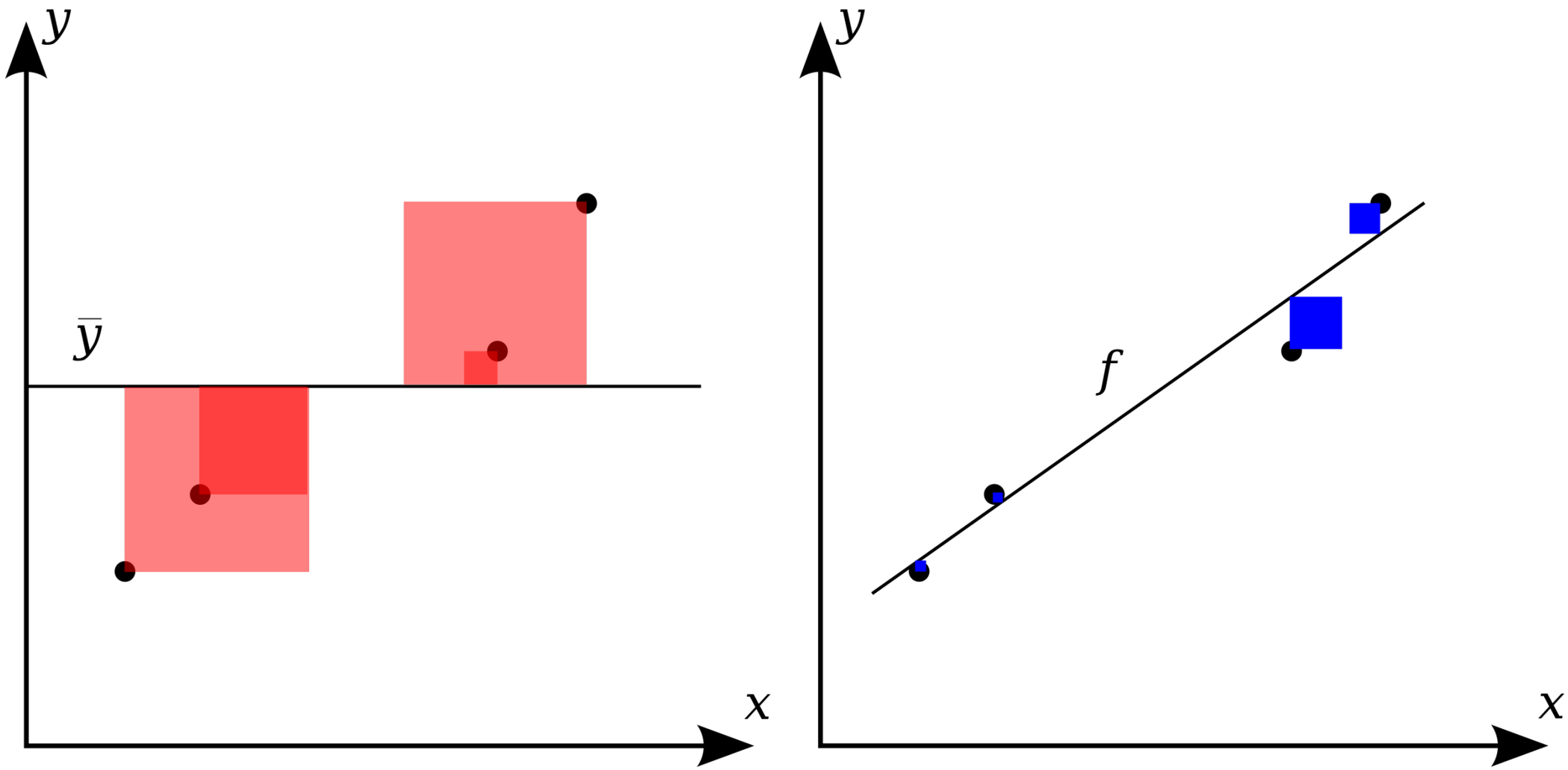
Coefficient of Determination [0,1]

the higher, the best

$$R^2 = (R)^2 = 1 - \frac{SSE}{SS_{yy}}$$

Note that $SS_{yy} = \sum_{i=1}^{n} (y_i - \overline{y})^2$ represents the total variation in the response variable, while $SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ represents the variation in the observed responses about the fitted equation (after taking into account x). This is why we sometimes say that R^2 is "proportion of the variation in y that is 'explained' by x."

Coefficient of Determination



$$R^2 = (R)^2 = 1 - \frac{SSE}{SS_{yy}}$$

The better the linear regression (on the right) fits the data in comparison to the simple average (on the left graph), the closer the value of is to 1. The areas of the blue squares represent the squared residuals with respect to the linear regression. The areas of the red squares represent the squared residuals with respect to the average value (mean of observations). — *From Wikipedia on Coefficient of determination.*

Exercise!

What is the Adjusted R^2 — explore and apply on tasks B2 of the Tutorial.

Residual Plots

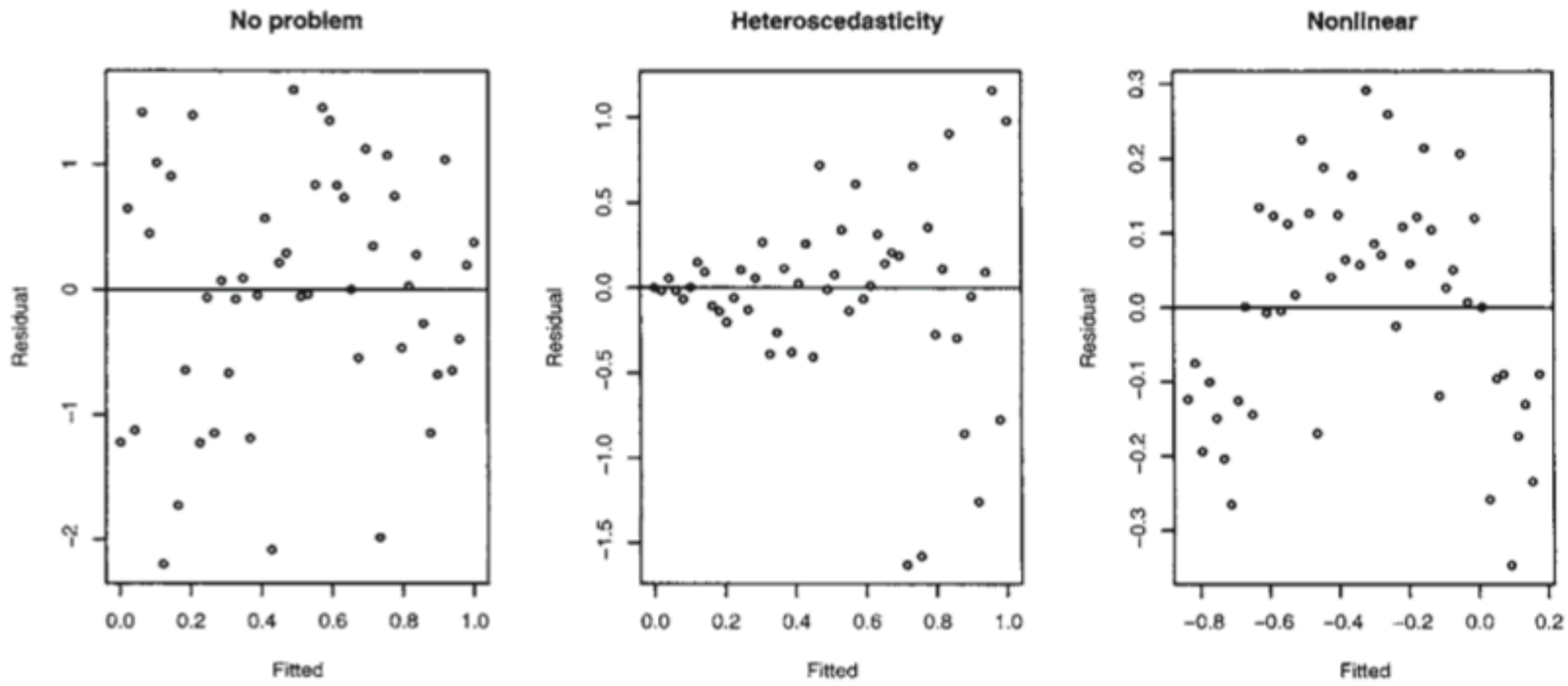
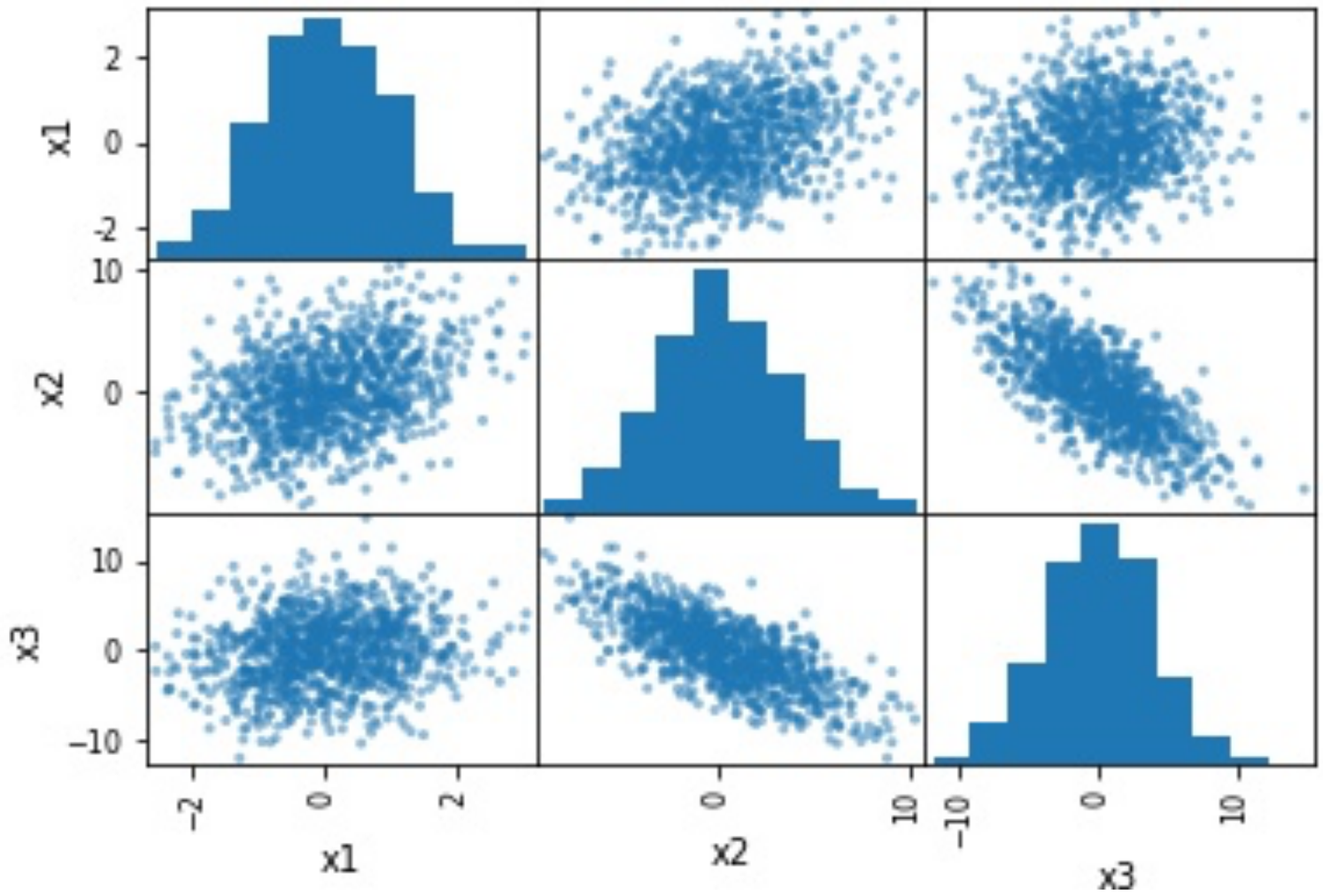


Figure 4.1 *Residuals vs. fitted plots—the first suggests no change to the current model while the second shows nonconstant variance and the third indicates some nonlinearity, which should prompt some change in the structural form of the model.*

```
from yellowbrick.regressor import ResidualsPlot
```

Excerpt from Faraway's Linear Models with R (2005, p. 59)

Choosing independent variables - Predictors!

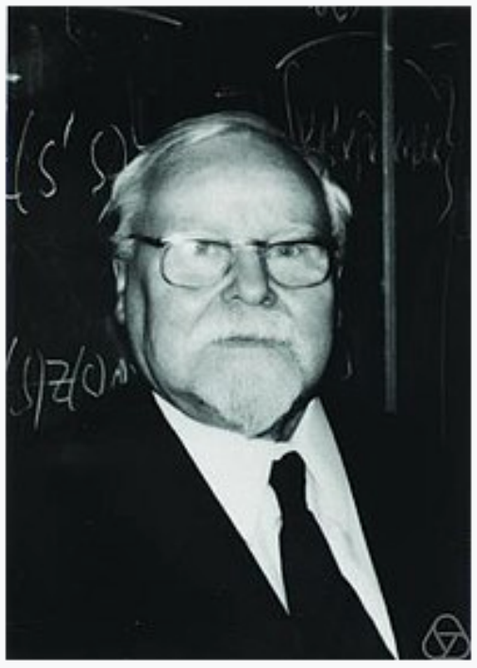


Correlation Matrix

Multicollinearity

Ridge and Lasso

Andrey Tikhonov



Born	30 October 1906 Gzhatsk, Russian Empire
Died	October 7, 1993 (aged 86) Moscow, Russia

Weight Decay method

L2 Regularisation

Added constraint: minimise $\beta_1, \beta_2, ..., \beta_n$

Ie, minimise SSE with slopes <u>close</u> to zero.

‘Least absolute shrinkage and selection operator’

L1 Regularisation

Added constraint: minimise $\beta_1, \beta_2, ..., \beta_n$

Ie, minimise SSE with slopes <u>close or equal</u> to zero.

Robert Tibshirani

Born	July 10, 1956 (age 61)
Nationality	Canada, American
Alma mater	University of Waterloo, Stanford University
Known for	LASSO method

Ridge and Lasso

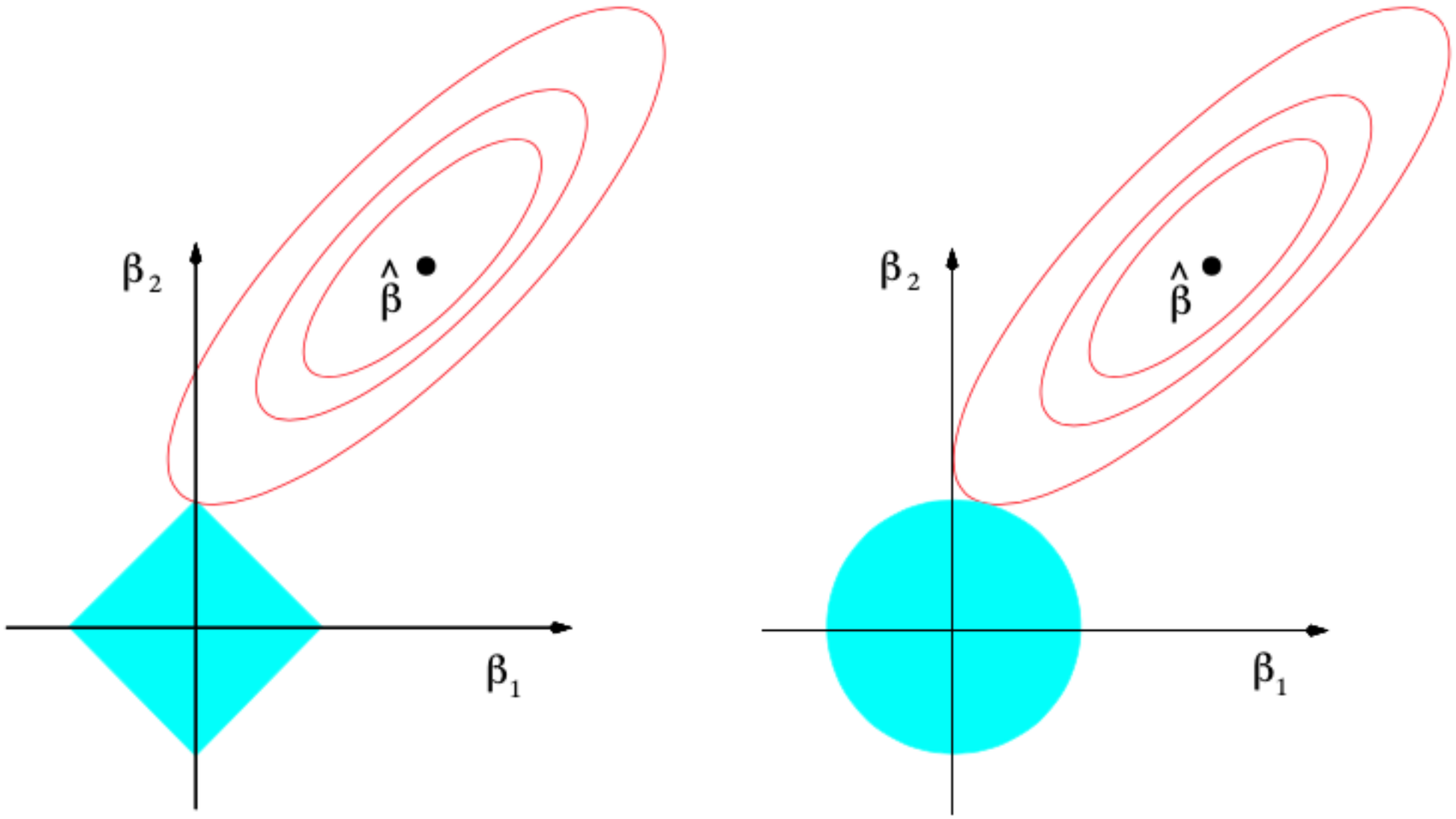
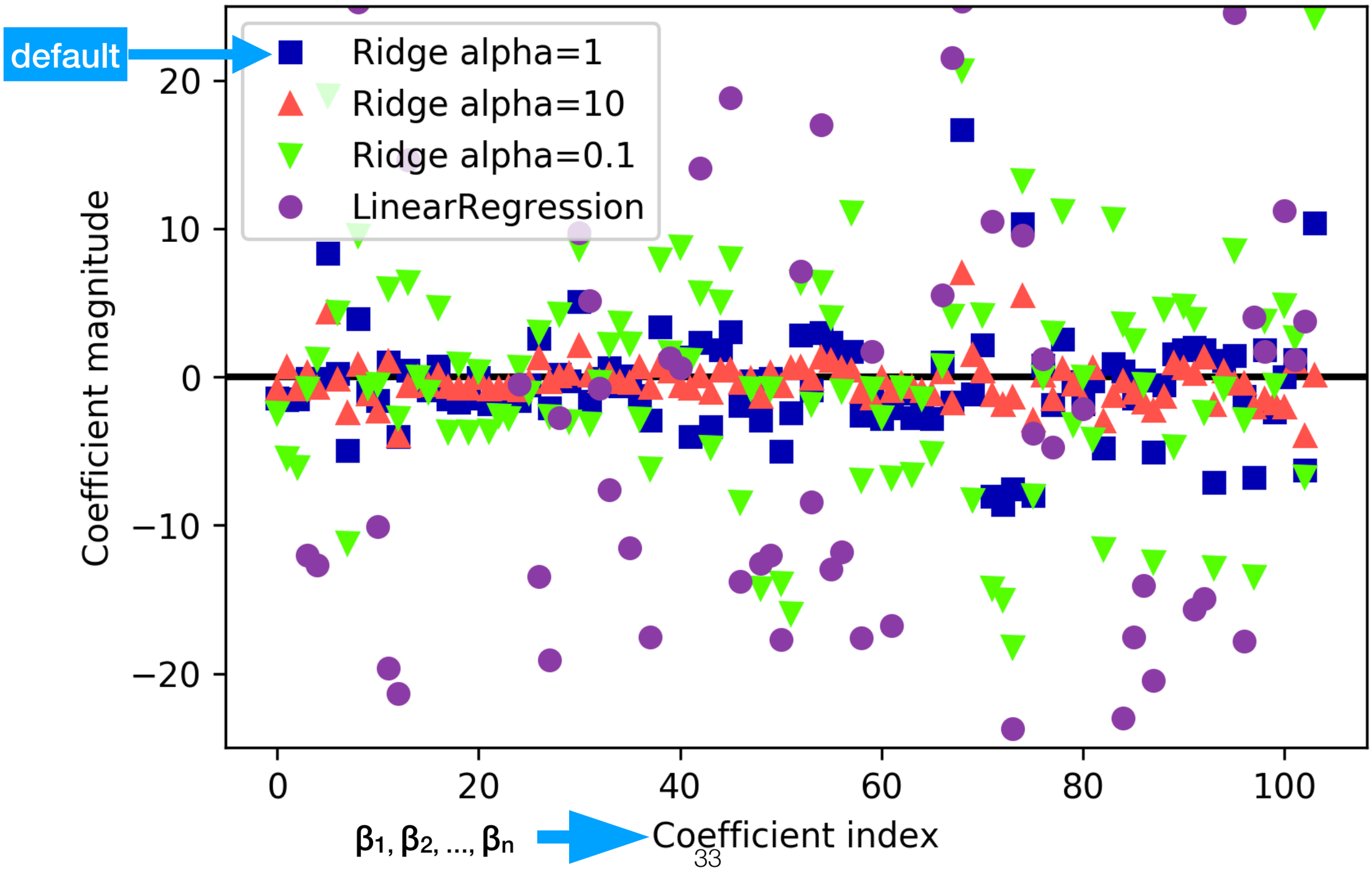


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

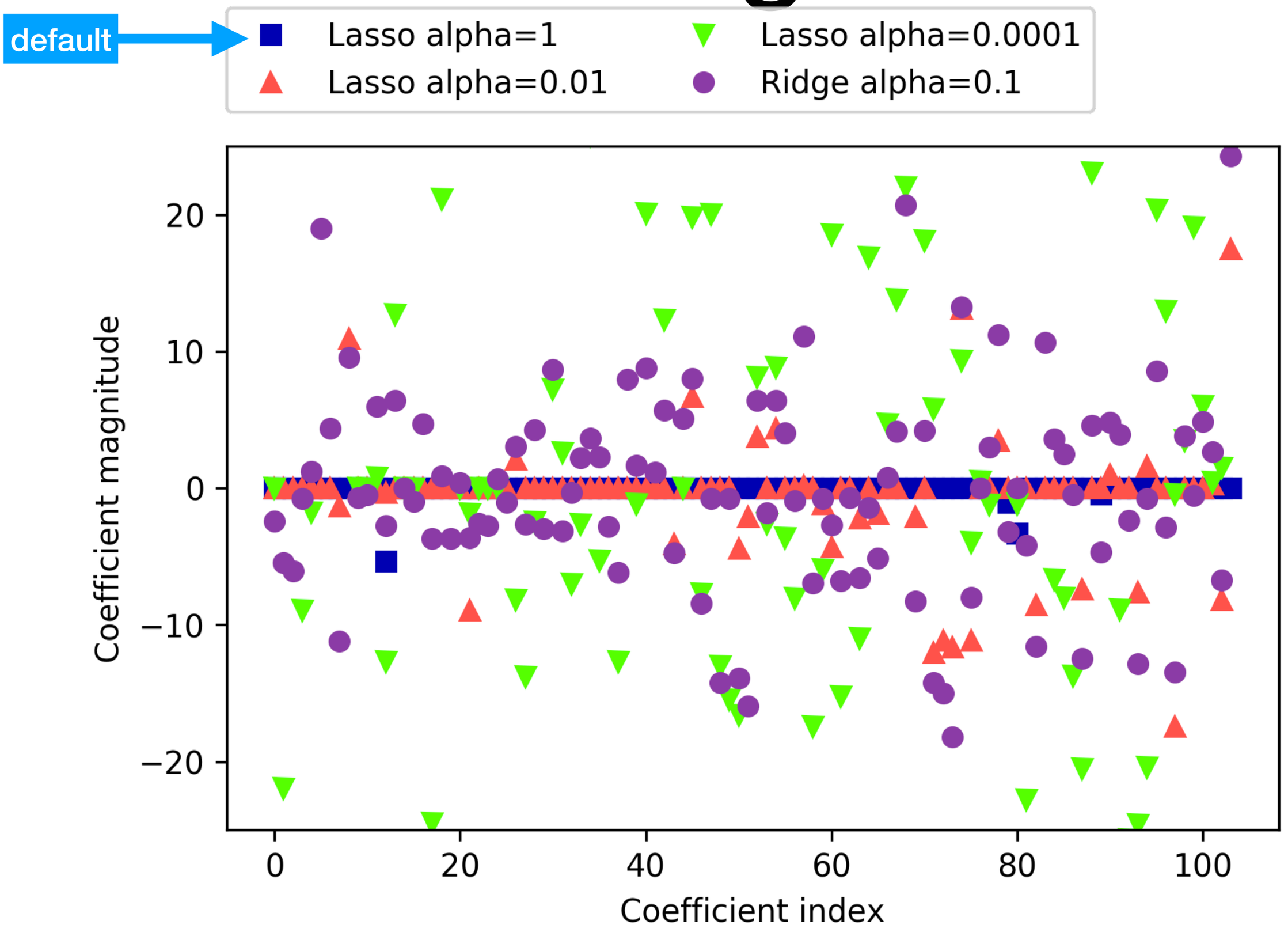
excerpt from “The Elements of Statistical Learning - Data Mining, Inference and Prediction - 2nd Edition. PP. 71

Ridge Regression

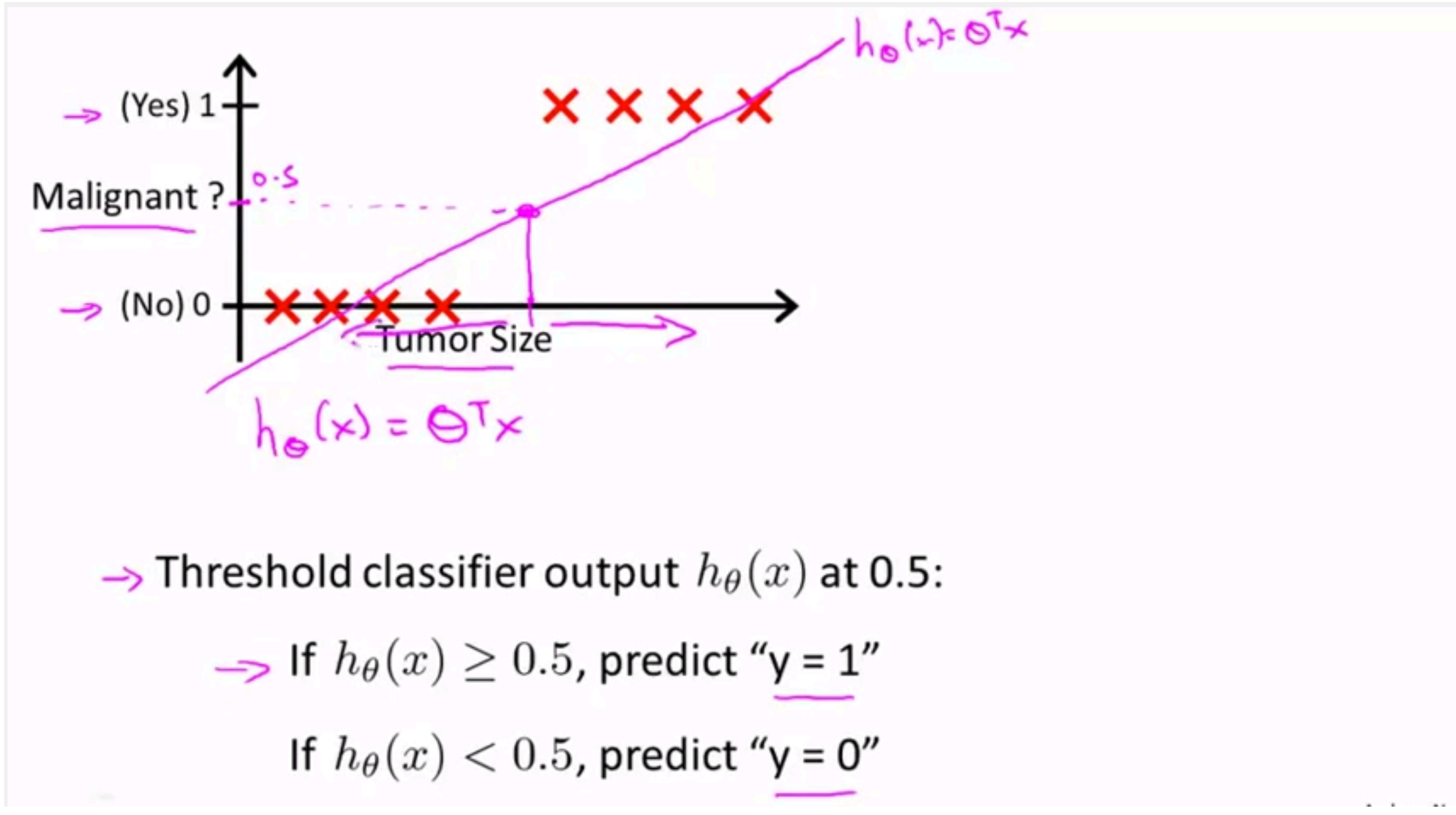


Lasso Regression

default



For Classification: Don't you ever consider! — wait until we get to log regression)



Source: Coursera online course on LR by Andrew NG

Reading

➡ See recommended reading provided in BB - Linear Regression Folder

➡ J Grus, Data Science from Scratch, ch. 14 and 15, pp.173 —188.

Tutorial

➡ Wish Russ a happy 25th Birthday!

- كل عام و أنت بخير (علي و هشام) :)

➡ See Tutorial Tasks Document