Classical statistical inference

Regression and Model fitting

Associated notebook:

05-MLE_and_regression/Regression_short.ipynb

Regression and model fitting

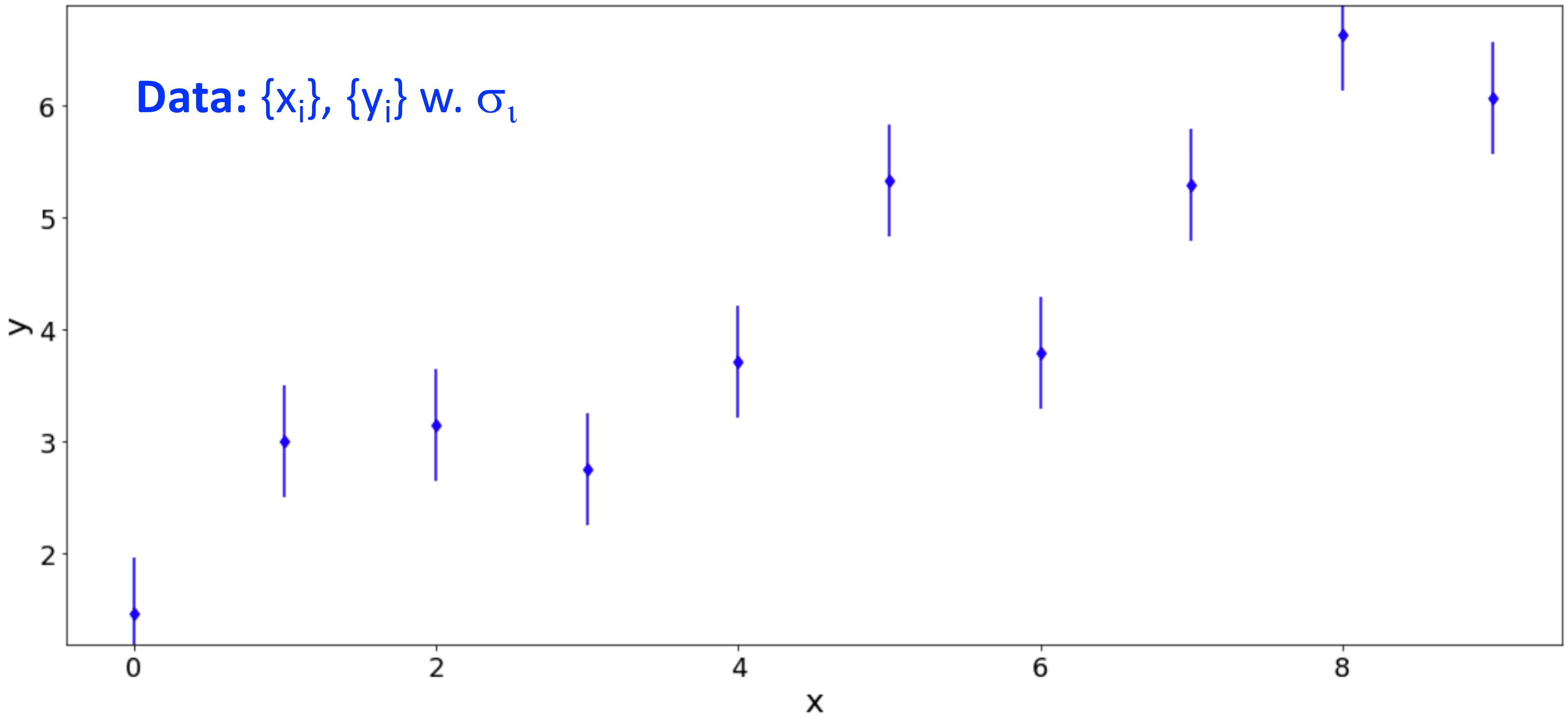
Problem: the quantities of interest are parameters of a model, not the RV that you measure

Examples

Observation	**Quantity of interest**	**Model**
Position of a star: **x**(t)	Proper motion (velocity) of the star	V = f(**x**, t, …)
Photometry of an asteroid: mag(t)	P (period of rotation)	mag = f(t, P, …)
Transit of a planet: mag(t)	P (period), e (eccentricity), D (dist to star)	Δ m = f (t, P, e, D, …)
Spectrum of a QSO: F (λ)	M_{BH} (Black hole mass of QSO)	FWHM = f(M_{BH}, L, …)

Regression and model fitting

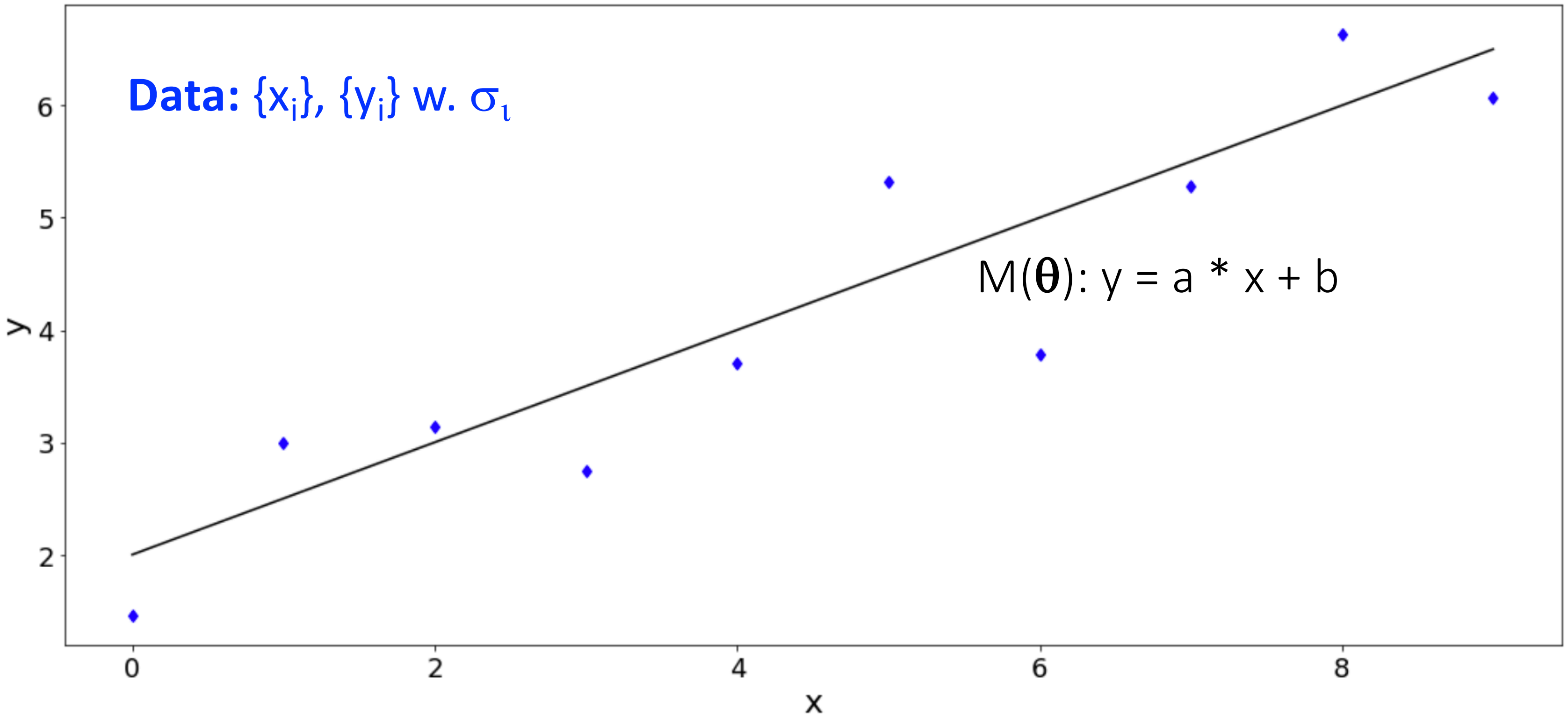
Problem: You measure D ≡ ($\{y_i\}$, $\{x_i\}$)



Model: M(θ)

Regression and model fitting

Problem: You measure D ≡ ({y_i}, {x_i})



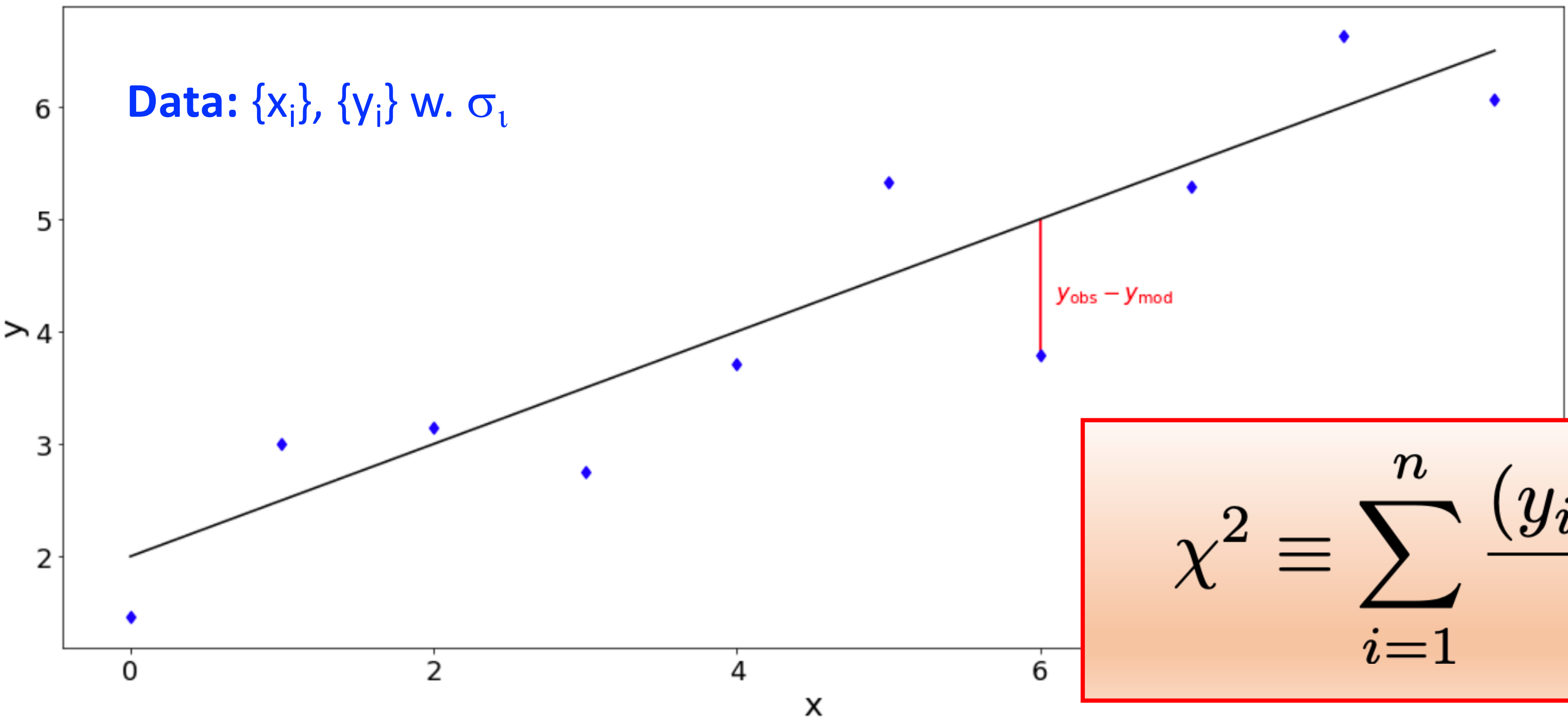
Model: M($\boldsymbol{\theta}$)

y = a * x + b

$\boldsymbol{\theta}$ = a, b

Regression and model fitting

How to find a good model?



Model: M(**θ**)

y = a * x + b
= f(x | **θ**)

θ = a, b

Minimize

$$\chi^2 \equiv \sum_{i=1}^{n} \frac{(y_i - y_{i,mod})^2}{\sigma_i^2}$$

Regression and model fitting

$$\chi^2 \equiv \sum_{i=1}^{n} \frac{(y_i - y_{i,mod})^2}{\sigma_i^2}$$

If $\sigma_i = 1$: Least square regression

If $\sigma_i \neq 1$: chi-square regression

The χ^2 is called a **merit** function

When uncertainties between variables are correlated, the χ^2 is expressed:

$$\chi^2 = \sum_{i=1}^{n} \sum_{l=1}^{n} (y_i - y_{i,mod}) F_{i,l} \, (y_l - y_{l,mod})$$

Where *F* is the Fisher matrix

$$[F]^{-1} = [C] = \begin{bmatrix} \sigma_k^2 & \sigma_{kl} \\ \sigma_{kl} & \sigma_l^2 \end{bmatrix}$$

Link between χ^2 and likelihood

$$\boxed{L \;=\; p(D\,|\,M(\boldsymbol{\theta}))}$$

Case of a straight line: $y_i = \theta_0 + \theta_1\, x_i + \epsilon_i$ with $\epsilon_i \sim N(0, \sigma_i)$

For each y_k we have: $p(y_k\,|\,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\,\pi}} \exp\left[-0.5\left(\frac{y_k-\mu}{\sigma}\right)^2\right]$

Hence, we have for our data set D:

$$L \;\equiv\; p(\{y_i\}\,|\,\{x_i\},\boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sigma_i\sqrt{2\,\pi}} \exp\left[\left(\frac{-(y_i-(\theta_0+\theta_1\,x_i))^2}{2\,\sigma_i^2}\right)\right]$$

Link between χ^2 and likelihood

Hence, we have for our data set D:

$$L \equiv p(\{y_i\} \,|\, \{x_i\}, \boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sigma_i \sqrt{2\,\pi}} \exp\left[\left(\frac{-(y_i - (\theta_0 + \theta_1\, x_i))^2}{2\,\sigma_i^2}\right)\right]$$

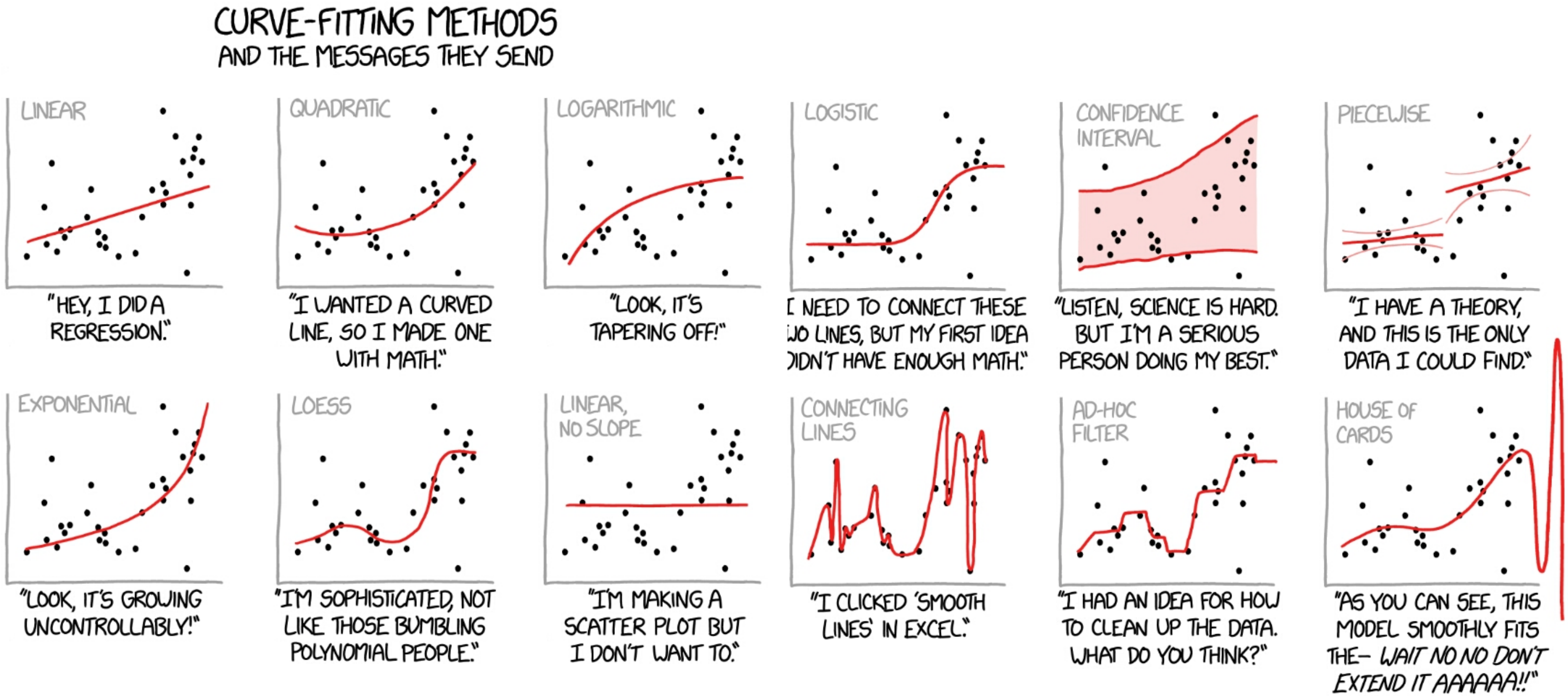
$$\ln(L) \propto \sum_{i=1}^{N} \left(\frac{-(y_i - (\theta_0 + \theta_1\, x_i))^2}{2\,\sigma_i^2}\right)$$

$$\chi^2 \equiv \sum_{i=1}^{n} \frac{(y_i - y_{i,mod})^2}{\sigma_i^2}$$

$$\Rightarrow \quad \boxed{L \propto \exp(-\chi^2/2)}$$

Minimizing χ^2 is equivalent to maximizing L

Regression and model fitting



https://xkcd.com/2048/

How to choose a suitable regression method ?

The way you will tackle a regression problem may depend on:

- **Linearity:** is the model linear *in its parameters*? $f(x \mid \boldsymbol{\theta}) = \sum_{p=1}^{k} \theta_p g_p(x)$

- **Complexity:** large number of parameters increase complexity and covariance matrix on uncertainties

- **Error behaviour:** uncertainties on dependent and independent variable and their correlation.

How to choose a suitable regression method ?

Frequentist: (this lecture)	***Bayes (future lecture):***
Optimization with some merit function	*Sampling* of the likelihood
Search for *best* (fit) model *parameters*	PDF on parameters
Often when *simple* error behaviour	More *complex* error behaviour

Linear vs non linear regression

A model is **linear** if: $$f(x\,|\,\boldsymbol{\theta}) = \sum_{p=1}^{k} \theta_p g_p(x)$$

$g_p(x)$ can be a non linear function of *x* BUT does not depend on any free parameter

In this case, the values of the parameters that yield $\frac{\partial \ln(L)}{\partial \theta_i} = 0$ (max. likelihood) can be found "analytically"

When the model is **not linear** , the minimization of the χ^2 has to be performed *numerically* xkcd.co/1725/

Linear vs non linear regression

Linear model fitting: See Sect. IV.1

Python implementation: `numpy.polyfit(x, y, deg=1, w=1/sigma)`

NON Linear model fitting: See Sect. IV.3

Python implementation: `scipy.optimize.curvefit()`

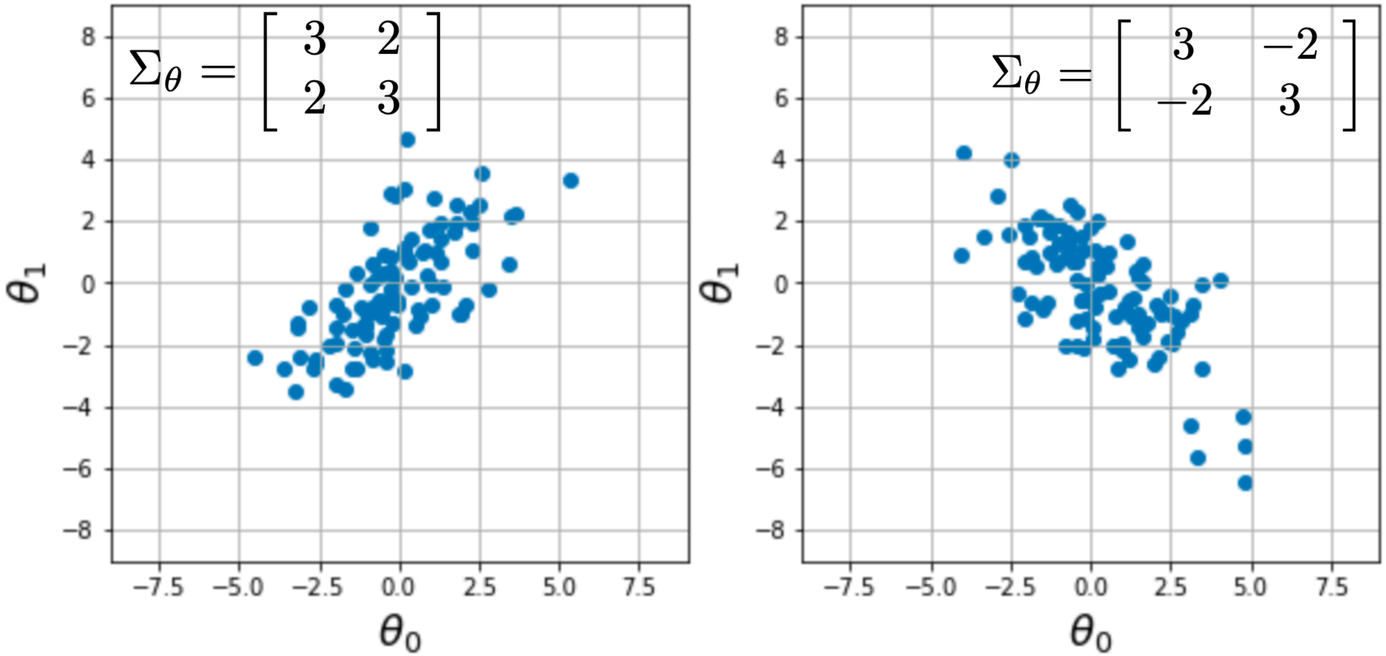
Go to Sect. IV.1.1 of the Notebook for practical example

Uncertainty on the fitted parameters

The python functions return a covariance matrix (Warning : use arg. cov=True)

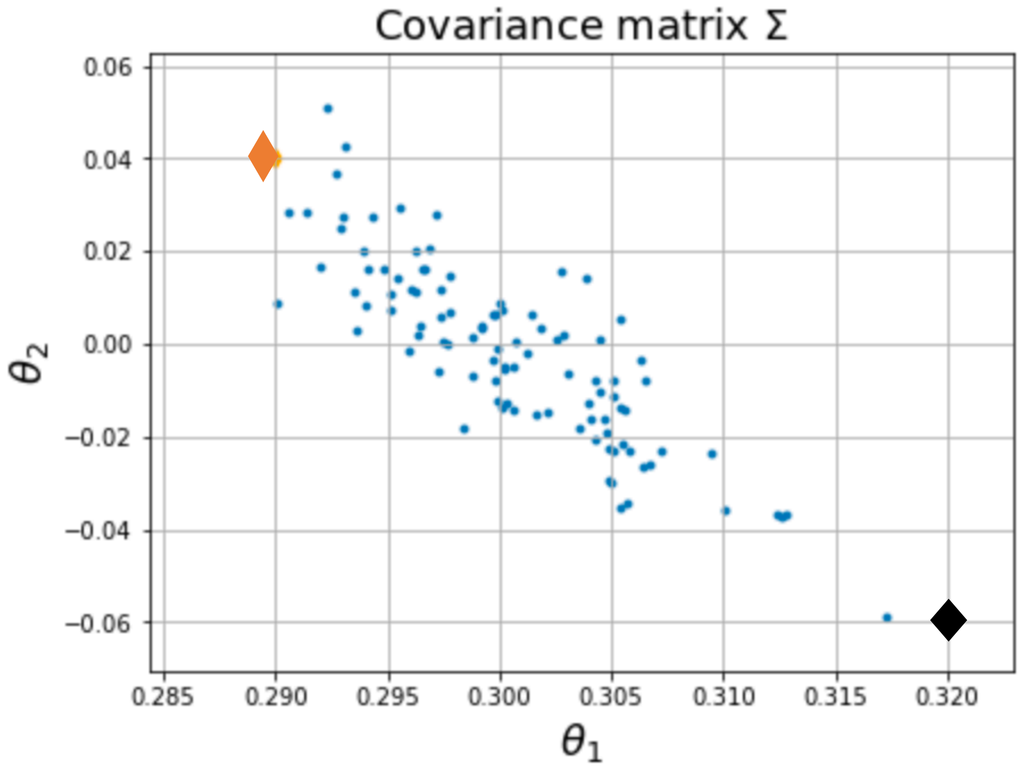
The diagonal elements of the matrix give the variance on the parameters (uncertainty^2)

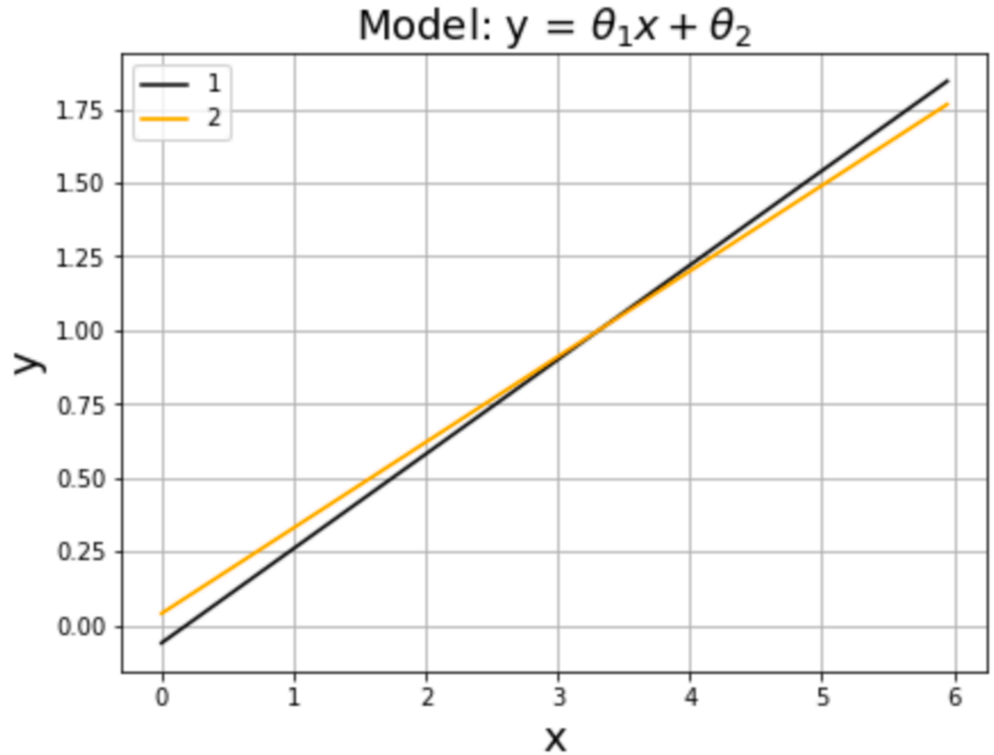
$$\Sigma_\theta = \begin{bmatrix} \sigma^2_{\theta_0} & \sigma_{\theta_0\theta_1} \\ \sigma_{\theta_0\theta_1} & \sigma^2_{\theta_1} \end{bmatrix}$$



Uncertainty on the fitted parameters

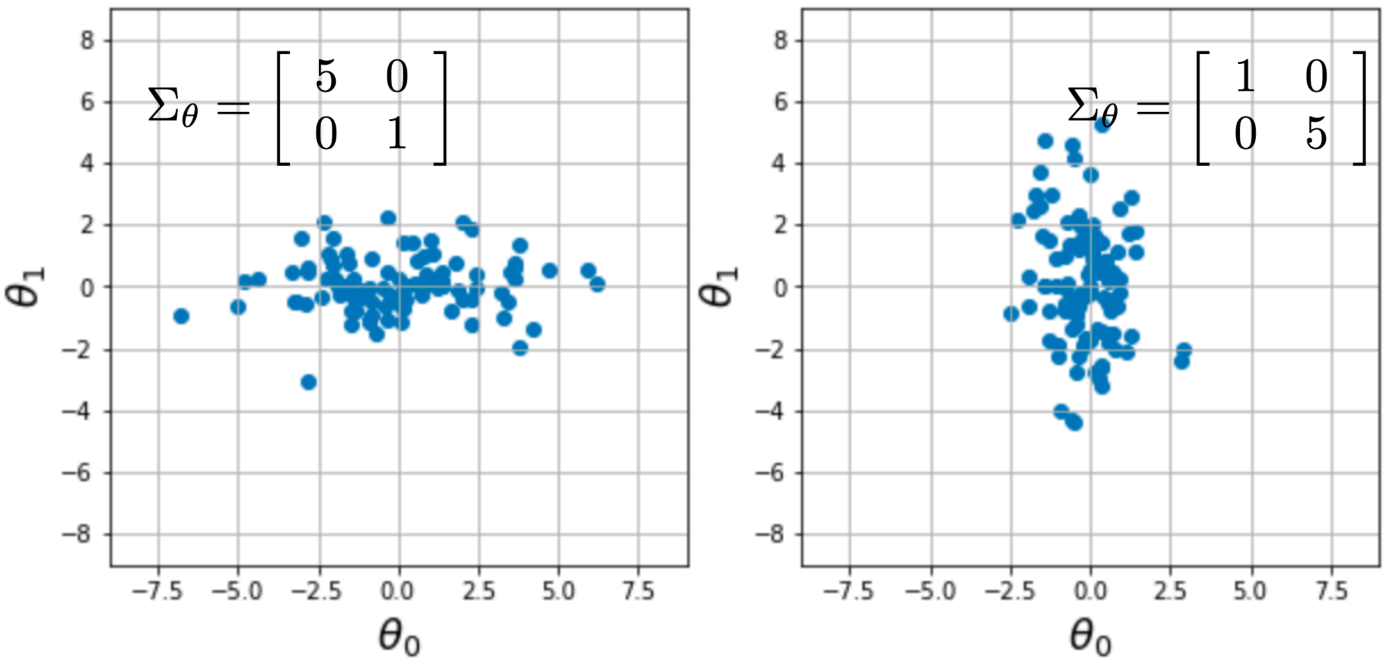
$$\Sigma_\theta = \begin{bmatrix} + & - \\ - & + \end{bmatrix}$$



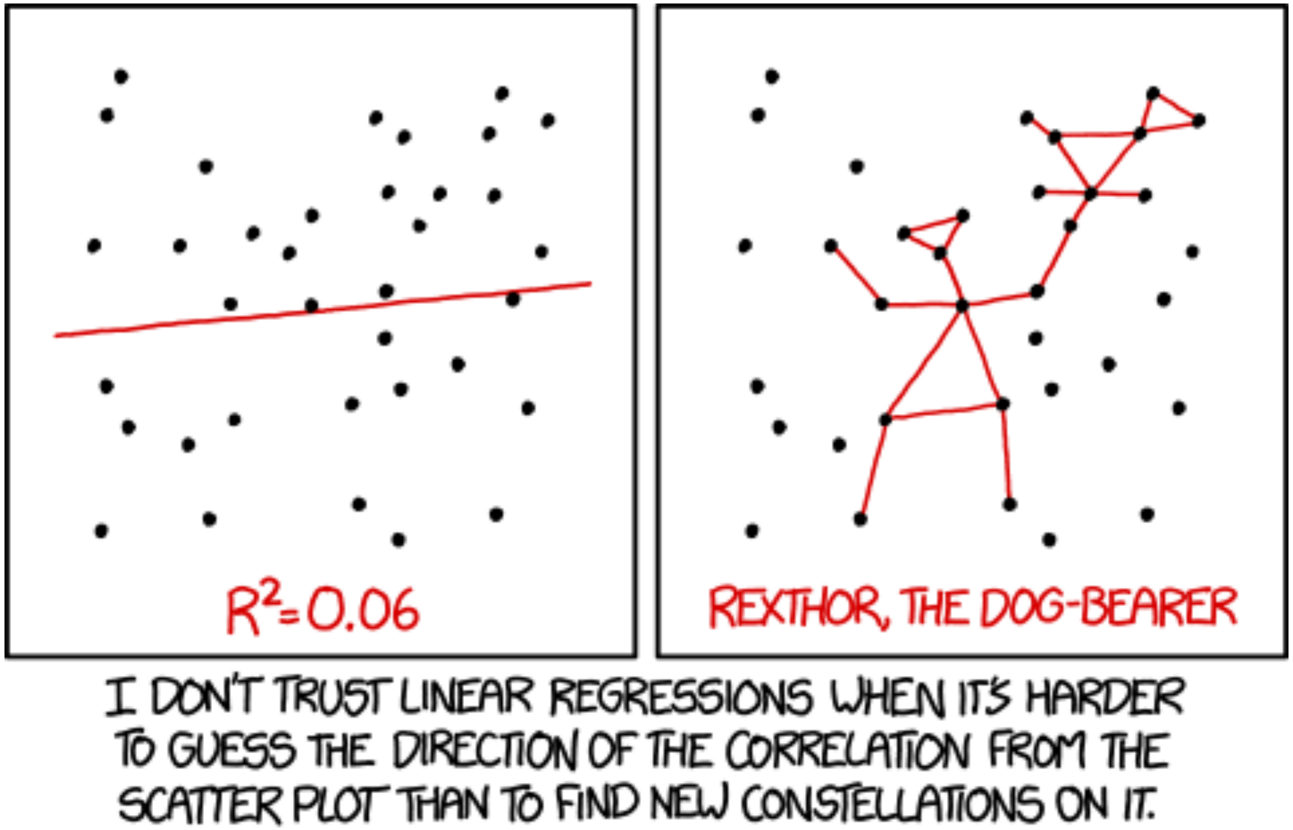


Uncertainty on the fitted parameters

$$\Sigma_\theta = \begin{bmatrix} \sigma^2_{\theta_0} & \sigma_{\theta_0\theta_1} \\ \sigma_{\theta_0\theta_1} & \sigma^2_{\theta_1} \end{bmatrix}$$



Quality of the regression



xkcd.com/1725/

Quality of the regression

Your χ^2 is a random variable !

$$Q = \sum_{i=1}^{k} z_i^2 \;\rightarrow\; p(Q|k) = \frac{1}{(2\,\Gamma(k/2))}(Q/2)^{k/2-1}\exp(-Q/2)$$

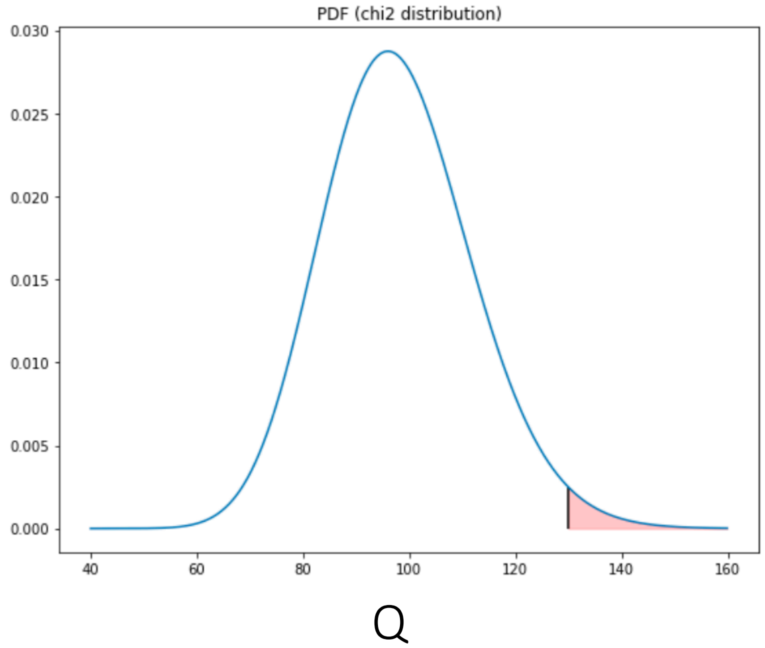
k = **d**egree **o**f **f**reedom = N *points* – n *parameters*

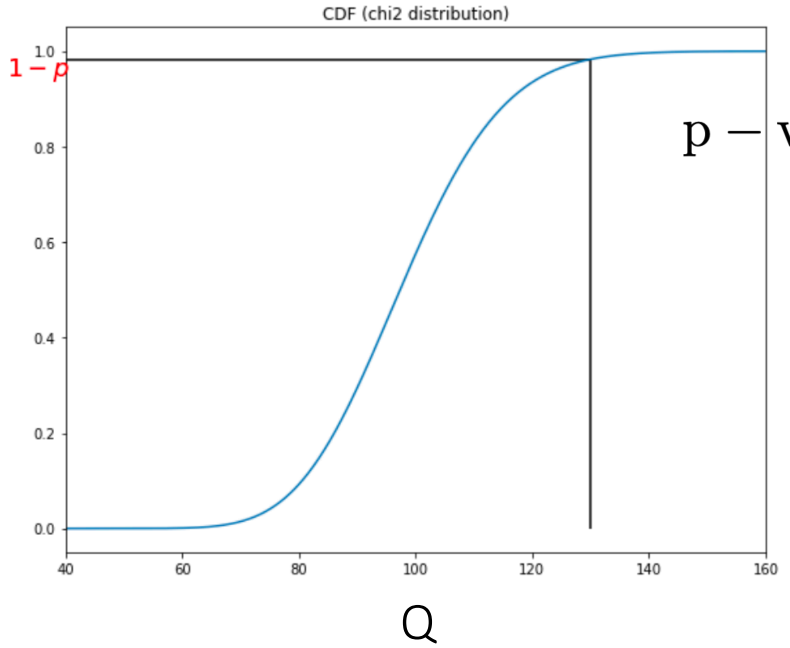
If you fit a model with 2 parameters on a set of 100 points => 98 d.o.f.
Expectation $E(\chi^2) = 100 - 2 = 98$
Reduced χ^2 : $\chi^2_{red} = \chi^2_{dof} /$ d.o.f. $\Rightarrow$ Reduced $\chi^2 \equiv 1.$ if good fit

See also the Notebook 03-Basic_statistics_and_proba_concepts/Descriptive_statistics_02.ipynb

Quality of the regression

$$p(Q|k) = \frac{1}{(2\,\Gamma(k/2))}(Q/2)^{k/2-1}\exp(-Q/2)$$





$$\mathrm{p-value} = \mathrm{p}(\mathrm{Q} \geq \chi^2_{\mathrm{obs}})$$

$$= 1 - p(Q \leq \chi^2_{\mathrm{obs}})$$

CDF

Typically:
p-value < 0.05 : ☹️
0.05 < p-value < 1: 😀
p-value close to 1 : 😕

```
1-scipy.stats.chi2.cdf(chi2_data, df= len(data)-nparam)
```

Go to Sect. IV.1.1 of the Notebook for practical example