Analyzing Astrophysical Data with Python: Statistical Methods and Applications-I

Workshop on Python Programming in Astronomy, Astrophysics & Cosmology

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Organized by

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Why do we study statistics in Astrophysics & Cosmology?

Astrophysics & Cosmology in the Era of Big Data

- **Motivations:**
  - Availability of vast and precise data
  - Different kinds of Statistical techniques
- **Goal:**
  - To understand the universe with high accuracy,
  - To extract the maximum amount of information from the observational data.
- **Methodology used:**
  - Frequentist Statistics: Likelihood or Chi-square.
  - Bayesian Statistics: Markov Chain Monte Carlo.

Outline

1. Introduction to Statistics
2. Least Square Fitting
    a). Maximum Likelihood Estimator (MLE)
    b). Minimum Chi-square Statistics
    c). Example: Hand-on Session
3. Bayesian Statistics
    a). Markov Chain Monte Carlo
    b). Metropolis Hasting Algorithm
    c). Example

Introduction to Statistics

Problem: Making the Decision to Pursue a Career in Astrophysics and Cosmology After Completing Your Bachelor's or Master's Degree

- Collect data: *Based on salary range, job satisfaction, and career growth*
- Analyze data: *Identify patterns and comparison with other fields*
- Interpret data: *Potential benefits and drawbacks of pursuing a career in this*
- Present data: *Data & analysis in a concise manner: graphs, charts, & tables*

Statistics: *Study of collecting, analyzing, interpreting, and presenting numerical data.*

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Basic form of Statistics:

- Descriptive Statistics: *Summarizing and describing the data*
  - mean, median, mode
  - standard deviation, variance
  - achieved with the help of charts, graphs, tables, etc.
- Inferential Statistics: *Generalizations or draw conclusions about a larger dataset.*
  - testing hypotheses
  - estimating parameters
  - achieved by probability.

Descriptive Statistics:

1	2	1	1	3	4	100

- Mean: *Average of observed values*: 16
- Median: *Value which divides the dataset into half* : 2 [Data should be in Ascending order]
- Mode: *Value which occurs with greatest frequency*: 1

outlier: 100

- Mean: 2
- Median: 1.5
- Mode: 1

Descriptive Statistics:

1	2	1	1	3	4

- Standard Deviation: *Dispersion of data points from the mean of a dataset.*

$$\sigma = \sqrt{\sum_{i=0}^{n} \frac{(x_i - \mu)^2}{n}} = 1.155$$

- Variance: *Average of the squared differences from the mean.*

$$\sigma^2 = \sum_{i=0}^{n} \frac{(x_i - \mu)^2}{n} = 1.334$$

Inferential Statistics: *Generalizations or draw conclusions about a larger dataset.*

1. Hypothesis Testing:

Year	2018	2019	2020	2021	2022
Rainfall (inches)	8	5	7	5	6

$\Rightarrow$ Test the hypothesis that the average rainfall in a given area is 8 inches?

- Null Hypothesis (H_0): *The average annual rainfall from 2018-2022 is the same as the overall average annual rainfall of 8 inches.*
- Alternative Hypothesis (H_A): *The average annual rainfall from 2018-2022 is the same not as the overall average annual rainfall of 8 inches*

Inferential Statistics:

1. Hypothesis Testing:

Year	2018	2019	2020	2021	2022
Rainfall (inches)	8	5	7	5	6

$\Rightarrow$ Test the hypothesis that the average rainfall in a given area is 8 inches?

Sample mean $(\bar{x}) = 6.2$, sample size $(n) = 5$

Sample Standard Deviation $(\sigma) = 1.30$, Population mean $(\mu) = 8$

t-test:

$$t_{obs} \equiv \frac{\bar{x} - \mu}{\sigma / \sqrt{n}} = -3.10$$

Degree of freedom: $d \equiv N - 1 = 4$

Inferential Statistics:

1. Hypothesis Testing:

Year	2018	2019	2020	2021	2022
Rainfall (inches)	8	5	7	5	6

$\Rightarrow$ Test the hypothesis that the average rainfall in a given area is 8 inches?

$t_{obs} < t_{tab}$

Reject the null hypothesis.

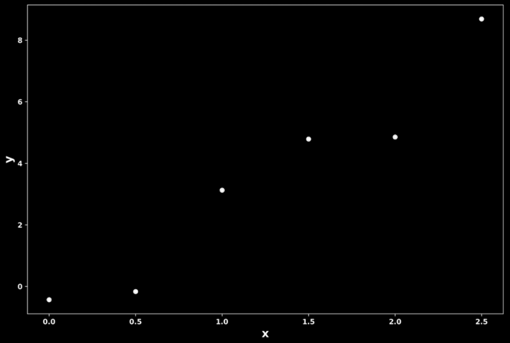
Difference is not purely due to the random error.

Inferential Statistics:

2. Parameter Estimation:

Observational Dataset

i	x	y
1	0.0	-0.4326
2	0.5	-0.1656
3	1.0	3.1253
4	1.5	4.7877
5	2.0	4.8535
6	2.5	8.6909



Least Square Fitting

Parameter Estimation

i	x	y
1	0.0	-0.4326
2	0.5	-0.1656
3	1.0	3.1253
4	1.5	4.7877
5	2.0	4.8535
6	2.5	8.6909

- $y_{\rm obs}$: Observational dataset
- $y_{\rm th}$: Theoretical Model: $y = a + bx$
- AIM: $a =?$ and $b =?$

Least Square Fit: *Minimizing the sum of the squares of the residuals.*

- Observable quantity: $y^{\rm obs}$
- Theoretical quantity: $y^{\rm th}(x_i; a, b)$

$$\min_{a,b} : \sum_{i=1}^{n} \left[y_i^{\rm obs} - y^{\rm tr}(x_i; a, b) \right]^2$$

$$\text{Residuals} = \sum_{i=1}^{n} \left[y_i^{\rm obs} - (a + b x_i) \right]^2$$

Least Square Fitting

Least Square Fit: *Minimizing the sum of the squares of the residuals.*

- Observable quantity: y^{obs}
- Theoretical quantity: $y^{\mathrm{th}}(x_i; a, b)$

$$\frac{\partial \text{Residuals}}{\partial a} = 0 \qquad \frac{\partial \text{Residuals}}{\partial b} = 0$$

$$\Rightarrow aN + b\sum x_i = \sum y_i^{\mathrm{obs}} \qquad \Rightarrow a\sum x_i + b\sum x_i^2 = \sum x_i y_i^{\mathrm{obs}}$$

Least Square Fit: *Minimizing the sum of the squares of the residuals.*

$$\boxed{\begin{aligned} a &= \frac{\sum x^2 \sum y - \sum x \sum xy}{N \sum x^2 - (\sum x)^2} \\ b &= \frac{N \sum xy - \sum x \sum y}{N \sum x^2 - (\sum x)^2} \end{aligned}}$$

$$\begin{bmatrix} N & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum (x_i y_i) \end{bmatrix}$$

$$X \cdot P = Y \quad \Rightarrow P = X^{-1} \cdot Y$$

i	1	2	3	4	5	6
x	0	0.5	1.0	1.5	2.0	2.5
y	-0.4326	-0.1656	3.1253	4.7877	4.8535	8.6909

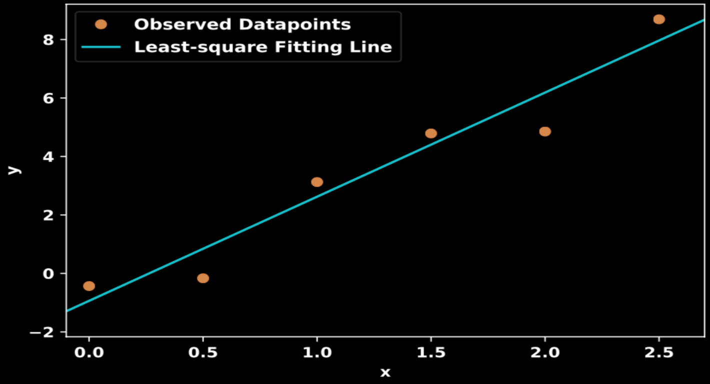
- $n = 6 \quad \sum x_i = 7.5, \quad \sum y_i = 20.8593, \quad \sum x_i^2 = 13.75, \quad \sum x_i y_i = 41.6584$

$$\begin{bmatrix} 6 & 7.5 \\ 7.5 & 13.75 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 20.8593 \\ 41.6584 \end{bmatrix} \Rightarrow \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 6 & 7.5 \\ 7.5 & 13.75 \end{bmatrix}^{-1} \times \begin{bmatrix} 20.8593 \\ 41.6584 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} -0.975 \\ 3.561 \end{bmatrix}$$

Least Square Fitting

$$y = -0.975 + 3.561x$$



What if uncertainties or errors are associated with the observed data?

- Key-points of Error Bars:
  - How far the reported value is from the true (error-free) value?
  - Errors introduced by random fluctuations in the measurement: random errors.
  - Errors due to a faulty calibration of equipment or observer biasing: systematic errors.
- Total Error Estimation:
  - Sum and Difference: $q_o = x_o \pm y_o$ $\qquad \sigma_q = \sigma_x + \sigma_y$
  - Products and Quotients: $q_o = x_o.y_o$ & $q_o = x_o/y_o$ $\qquad \sigma_q = |q_o| \left[\frac{\sigma_x}{x_o} + \frac{\sigma_y}{y_o}\right]$

Observational dataset:

x	y	σ_{y}
1.0	2.3	0.08
2.0	4.1	0.12
3.0	6.2	0.20
4.0	8.1	0.16
5.0	10.0	0.28

Assumptions: Observed data are normal distributed with center y and width σ_y

Theoretical Model: $y^{\mathrm{th}} = a + bx$

- Theoretical Term: $y^{\rm th} = a + bx$
- Observational Term: $y_i^{\rm obs}, \quad \sigma_{y_i}$

The probability of obtaining the observed value $(y_i^{\rm obs})$ is

$$\text{Prob}_{a,b}\left(y_i\right) = \frac{1}{\sqrt{2\pi\sigma_y^2}} e^{-\left(y_i^{\rm obs} - a - bx_i\right)^2/2\sigma_y^2}$$

$$\mathcal{L}(x_i; a, b) = \prod_{i=1}^{n} \text{Prob}_{a,b}\left(y_i\right) \Rightarrow \text{Maximise it}$$

...... gives the parameters values for which observed data have the highest probability

Least Square Fitting

a). Maximum Likelihood Estimator (MLE)

The probability of obtaining the observed value (y_i^{obs}) is

$$\mathcal{L}(x_i; a, b) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_{y_i}^2}} \exp\left\{ -\frac{1}{2} \left[\frac{\left(y_i^{\mathrm{obs}} - a - bx_i\right)^2}{\sigma_{y_i}^2} \right] \right\}$$

$$-2 \ln \mathcal{L}(x_i; a, b) = \sum_{i=1}^{N} \frac{\left(y_i^{\mathrm{obs}} - a - bx_i\right)^2}{\sigma_{y_i}^2} \equiv \chi^2$$

To estimate parameters: either maximize the likelihood or minimise the Chi-square

..... log *makes math easier, doesn't change answer (monotonic)!*

- Chi-square:

$$\chi^2 = \sum_{i=1}^{N} \frac{\left(y_i^{\mathrm{obs}} - a - bx_i\right)^2}{\sigma_{y_i}^2}$$

- Minimize the Chi-square: $\dfrac{\partial \chi^2}{\partial a}$ $\dfrac{\partial \chi^2}{\partial b}$

$$a = \frac{\sum wx^2 \sum wy - \sum wx \sum wxy}{\Sigma w \sum wx^2 - (\sum wx)^2} \qquad b = \frac{\sum w \sum wxy - \sum wx \sum wy}{\Sigma w \sum wx^2 - (\sum wx)^2}$$

$$\sigma_a = \sqrt{\frac{\sum wx^2}{\Sigma w \sum wx^2 - (\sum wx)^2}} \qquad \sigma_b = \sqrt{\frac{\Sigma w}{\Sigma w \sum wx^2 - (\sum wx)^2}}$$

$$w = 1/\sigma_{y_i}^2$$

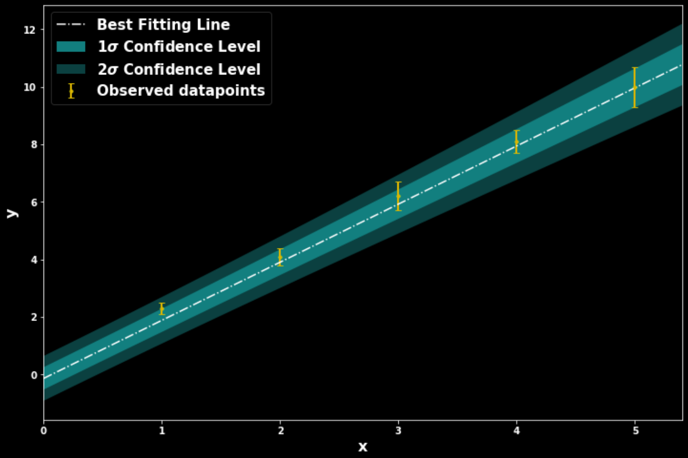
Observational dataset:

x	y	σ_{y}
1.0	2.3	0.08
2.0	4.1	0.12
3.0	6.2	0.20
4.0	8.1	0.16
5.0	10.0	0.28

Theoretical Model: $y^{\mathrm{th}} = a + bx$

Best Fit values: $a = 0.22 \pm 0.14, \quad b = 2.03 \pm 0.07$

Maximum Likelihood Method



Revise:

- Observational dataset: $x_i^{\rm obs}$, $y_i^{\rm obs}$, σ_{y_i}
- Theoretical model: $y = f(x; a_0, a_1, \cdot\cdot, a_j)$
- Likelihood: Maximise or Chi-square: Minimise
- Solve:

$$\begin{bmatrix} N & \sum x_i & \sum x_i^2 & \cdots & \sum x_i^j \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \cdots & \sum x_i^{j+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \cdots & \sum x_i^{j+1} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \sum x_i^j & \sum x_i^{j+1} & \sum x_i^{j+2} & \cdots & \sum x_i^{j+n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_j \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum (x_i y_i) \\ \sum (x_i^2 y_i) \\ \vdots \\ \sum \left(x_i^j y_i\right) \end{bmatrix} \Rightarrow \text{Inverse} = ...?$$

Least Square Fitting

b). Minimum Chi-square Statistics

Chi-square Test: describes the goodness-of-fit of the data to the model.

$$\chi^2 = \sum_i \frac{(\text{ observed } - \text{ expected })^2}{\text{expected}} = \sum_i \frac{(O_i - E_i)^2}{E_i}$$

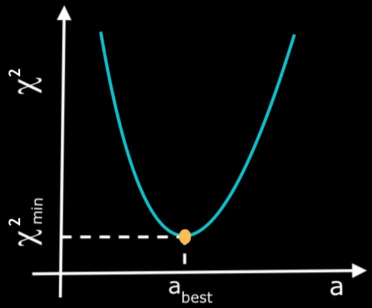
- Observational dataset: $x_i,\ y_{\rm obs}(x_i),\ \sigma_{y_i}$
- Theoretical model: $y_{\rm th}(x_i; a, b) = f(x_i; a, b)$
- Define

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_{\rm obs}(x_i) - y_{\rm th}(x_i; a, b)}{\sigma_{y_i}} \right)^2$$

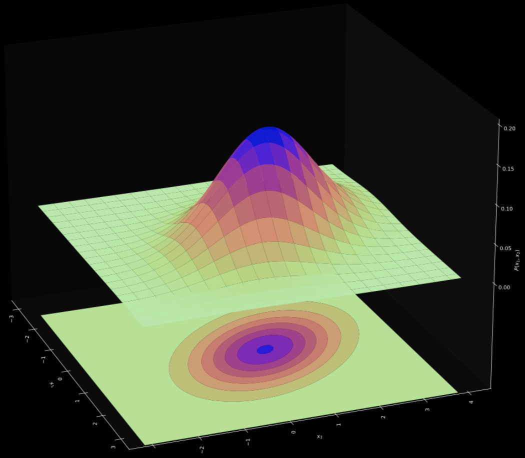
Chi-square:

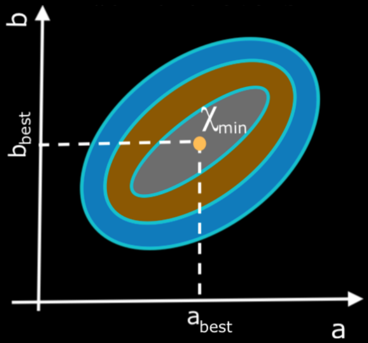
$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_{\rm obs}(x_i) - y_{\rm th}(x_i; a, b)}{\sigma_{y_i}} \right)^2 \Rightarrow \chi^2_{\rm min} \rightarrow \text{Best fit value of parameter}$$

Case:1 One Parameter Model:



Case:2 Two Parameters Model:





Question: *Why should we trust our model?*

→ *Fitting can be* `overfit` *or* `underfit`*..*

→ *Model can be* `linear`*,* `quadratic` *or so..*

- Chi-squared probability distribution:

$$P\left(\chi^2\right) \propto \left(\chi^2\right)^{\frac{\nu-2}{2}} \exp\left(-\chi^2/2\right);\qquad \nu : \text{d.o.f.=N-p}$$

- Mean: $\overline{\chi^2} = \nu$ Variance: $\mathrm{Var}\left(\chi^2\right) = 2\nu$

$\Rightarrow$ we expect $\boxed{\chi^2 \sim \nu \pm \sqrt{2\nu}}$

Reduced Chi-square:

$$\chi^2_\nu = \frac{\chi^2}{\nu}$$

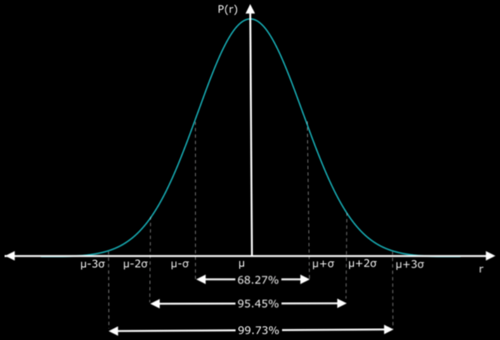
Goodness-of-fit:

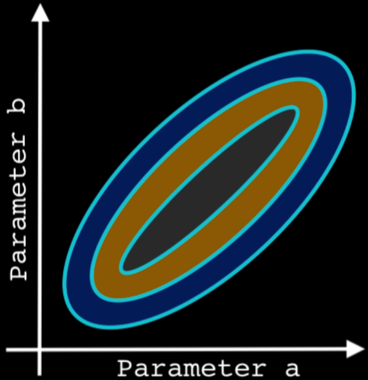
- $\chi^2_\nu < 1 \rightarrow$ over-fitting of the data.
- $\chi^2_\nu > 1 \rightarrow$ poor model fit
- $\chi^2_\nu \simeq 1 \rightarrow$ good match between data and model

Model Comparison: Linear model: M_L or Quadratic model: M_Q

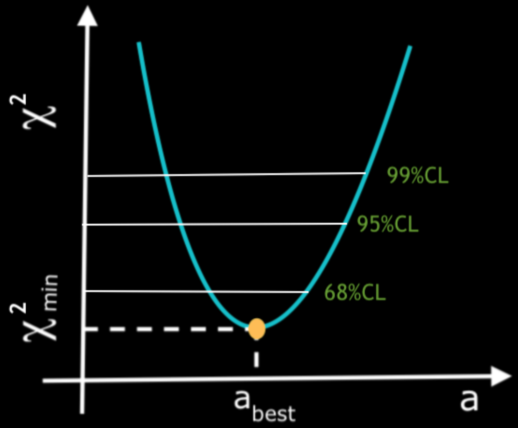
Best model is one whose value of χ^2_ν is closest to one!

Confidence Intervals: Range of estimates for an unknown parameter.





Chi-squared Distribution with Sigma Values: $\chi^2_{n\sigma} = \chi^2_{\text{min}} + \Delta\chi^2_{n\sigma}$

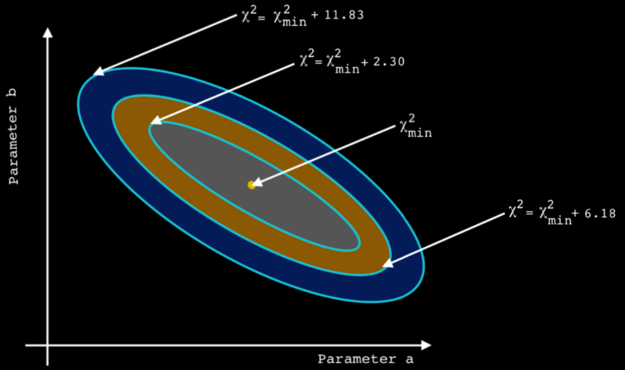


Dimensionality	1σ	2σ	3σ
1	1.00	4.00	9.00
2	2.30	6.18	11.83
3	3.53	8.02	14.16
4	4.72	9.72	16.25
5	5.89	11.31	18.21

Chi-squared distribution $\Delta\chi^2_{n\sigma}$ upto 5 parameters (5D).

Chi-squared Distribution with Sigma Values: $\chi^2_{n\sigma} = \chi^2_{\min} + \Delta\chi^2_{n\sigma}$

Two-parameters model:



Parameter error estimation:

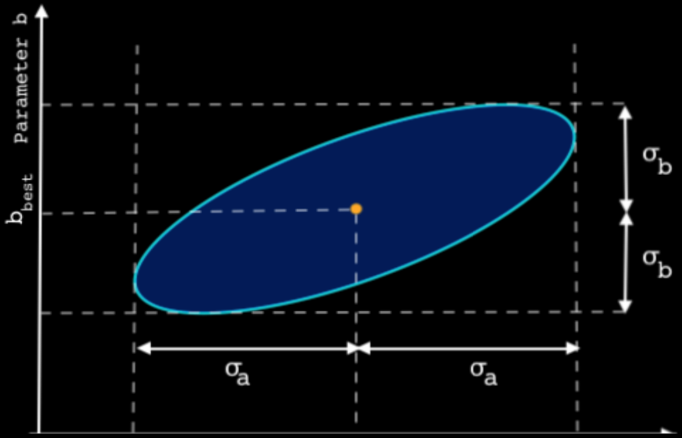
$$\sigma_{a_o} = \sqrt{\frac{\mathscr{B}}{\mathscr{C}^2 - \mathscr{A}\mathscr{B}}}, \quad \sigma_{b_o} = \sqrt{\frac{\mathscr{A}}{\mathscr{C}^2 - \mathscr{A}\mathscr{B}}}, \quad \sigma_{a_o b_o} = \sqrt{\frac{-\mathscr{C}}{\mathscr{C}^2 - \mathscr{A}\mathscr{B}}}$$

where $\mathscr{A} < 0, \quad \mathscr{B} < 0, \quad \mathscr{A}\mathscr{B} > \mathscr{C}^2$ and defined as

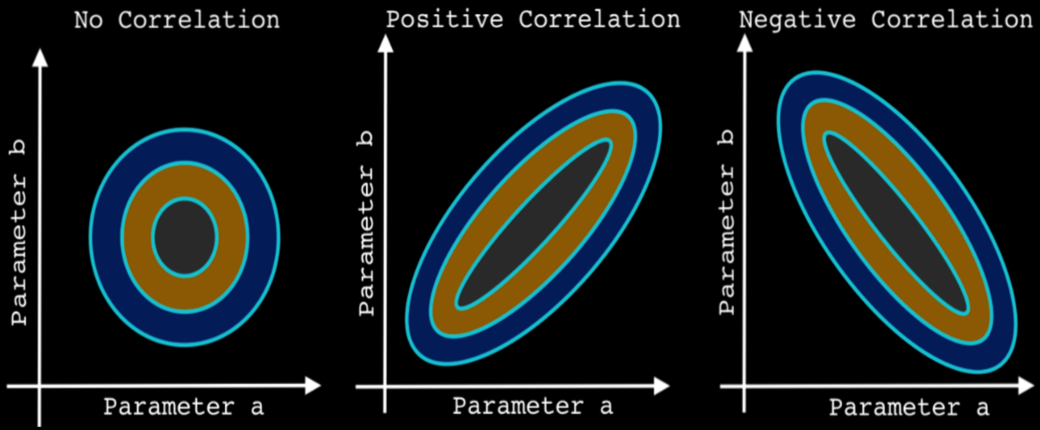
$$\mathscr{A} = \left.\frac{\partial^2 \mathcal{L}}{\partial a^2}\right|_{a_o, b_o}, \quad \mathscr{B} = \left.\frac{\partial^2 \mathcal{L}}{\partial b^2}\right|_{a_o, b_o}, \quad \mathscr{C} = \left.\frac{\partial^2 \mathcal{L}}{\partial a \partial b}\right|_{a_o, b_o}$$

where a_o and b_o : best fit value of a and b parameters, and
$\mathcal{L}$: log-likelihood function.

Parameter error estimation:



Correlation among parameters:



Least Square Fitting

c). Example: Hand-on Session

Example-1: Hand-on Session

Mock dataset:

x	y	σ_{y}
1.0	2.3	0.08
2.0	4.1	0.12
3.0	6.2	0.20
4.0	8.1	0.16
5.0	10.0	0.28

Theoretical Model: $y^{\mathrm{th}} = a + bx$

Best Fit values: $a = ---\pm---, \quad b = ---\pm---$

Example-2: Hand-on Session

Astro-Observational dataset: Hubble parameter measurements of 30 datapoints

z	H(z)	$\sigma_H(z)$
0.07	69.0	19.6
..	..	..
..	..	..
..	..	..
..	..	..
1.965	186.5	50.4

Theoretical Model: $H^{\rm th}(z) = H_0\sqrt{\Omega_{m0}(1+z)^3 + 1 - \Omega_{m0}}$

Best Fit values: $H_0 = ---\pm---,\quad \Omega_{m0} = ---\pm---$

Key Takeaways

Observational dataset: x_i, $y_{\rm obs}(x_i)$, σ_{y_i}

Theoretical model: $y_{\rm th}(x_i; a, b) = f(x_i; a, b)$

Define Chi-square: $\chi^2 = \sum_{i=1}^{N} \left(\frac{y_{\rm obs}(x_i) - y_{\rm th}(x_i; a, b)}{\sigma_{y_i}} \right)^2$

Minimize Chi-square: $\chi^2_{\rm min}$ $\Rightarrow$ **Best fit value of parameters**

Draw Confidence Level: $\chi^2_{n\sigma} = \chi^2_{\mathrm{min}} + \Delta\chi^2_{n\sigma}$

Error in parameters: $a = a_{\rm best} \pm \sigma_a$ **and** $b = b_{\rm best} \pm \sigma_b$