Urban Informatics

Fall 2018

dr. federica bianco fbianco@nyu.edu

@fedhere

CUSP

Recap:

- Good practices with data: falsifiability, reproducibility
- Basic data retrieving and munging: APIs, Data formats
- Basic statistics: distributions and their moments
- Hypothesis testing: *p*-value, statistical significance
- Statistical and Systematic errors
- Goodness of fit tests

Recap:

- Good practices with data: falsifiability, reproducibility
- Basic data retrieving and munging: APIs, Data formats
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- Hypothesis testing: *p*-value, statistical significance
- Statistical and Systematic errors
- Goodness of fit tests

Today:

- Residuals minimization
- Likelihood
- model diagnostics
  - Chi^2, R^2, and LR test
- Higher degree regression

Goodness of fit

You have some data, and an idea of how it should look: a *model*

Is it a good model?

Goodness of fit

Tests Cheat Sheet: goodness of fit

	metric (statistic)	compare to	
KS	$D_{n_1,n_2}(x)=max(\lvert F_n(x)-F\ \ (x) \rvert)$	$\frac{K_\alpha}{\sqrt{n}}$	power in the core only
Pearson's chi square	$\chi^2_{red}=\frac{\chi^2}{df}=\frac{1}{df}\sum\frac{(O-E)^2}{\sigma^2}$	scipy.stats.chisquare(f_obs, f_exp=None, ddof=0, axis=0)[	
Anderson-Darling	$A=n\int_{-\infty}^{\infty}\frac{(F_n(x)-F(x))^2}{F(x)\ (1-F(x))}dF(x)$	scipy.stats.anderson(x, dist='norm')	power in the tails
K-L divergence	$D_{KL}\ = -\int_x p(x)\ log(q(x))\ +\ p(x)\ log(p(x))$	scipy.stats.entropy(pk. qk=<not None>)	relates to information entropy
Likelihood ratio	$\frac{L\ (model\ \ 1\mid\ data)}{L\ (model\ \ 2\mid\ data)}$		suitable to bayesian analysis

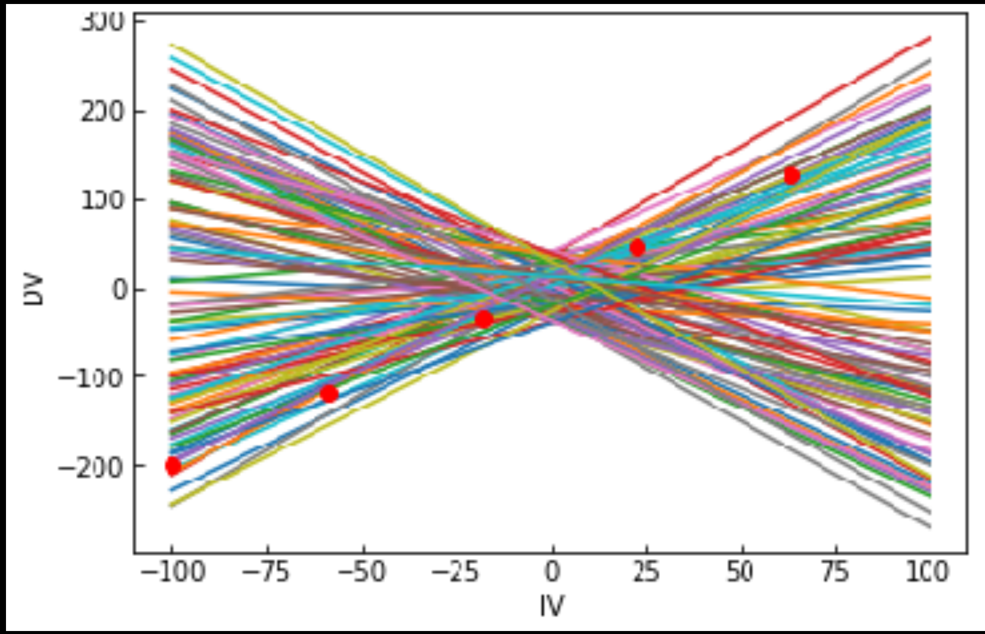
All models are wrong

Since *all models are wrong* the scientist cannot obtain a "correct" one by excessive elaboration. On the contrary following William of Occam he should seek an economical description of natural phenomena. Just as the ability to devise simple but evocative models is the signature of the great scientist so overelaboration and overparameterization is often the mark of mediocrity

George Box (1979),
"Robustness in the strategy of scientific model building",
in Launer, R. L.; Wilkinson, G. N., Robustness in Statistics,

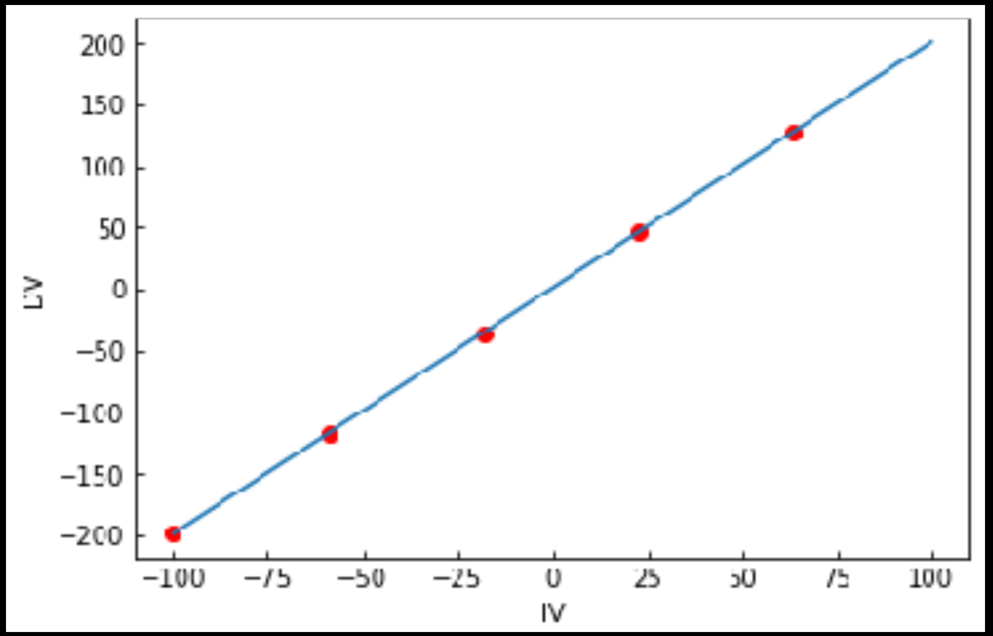
What's a model??

a formula that describes the data ⟶ *a family of models*



What's a model??

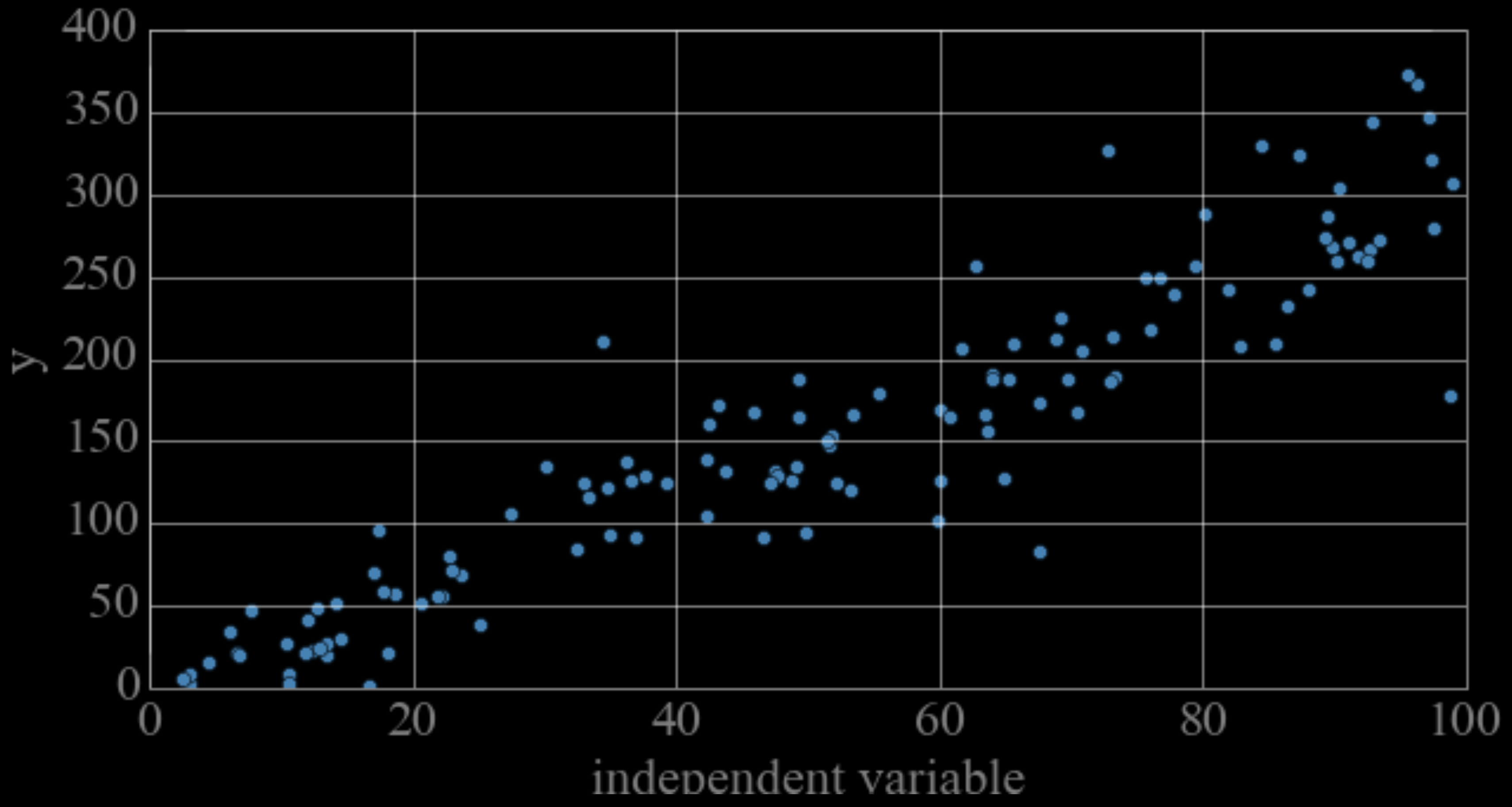
a formula that describes the data → *a family of models*



the best fit chooses within that family
the model that has the
best parameters

What's a model??

How do we fit a model to data?


400
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y
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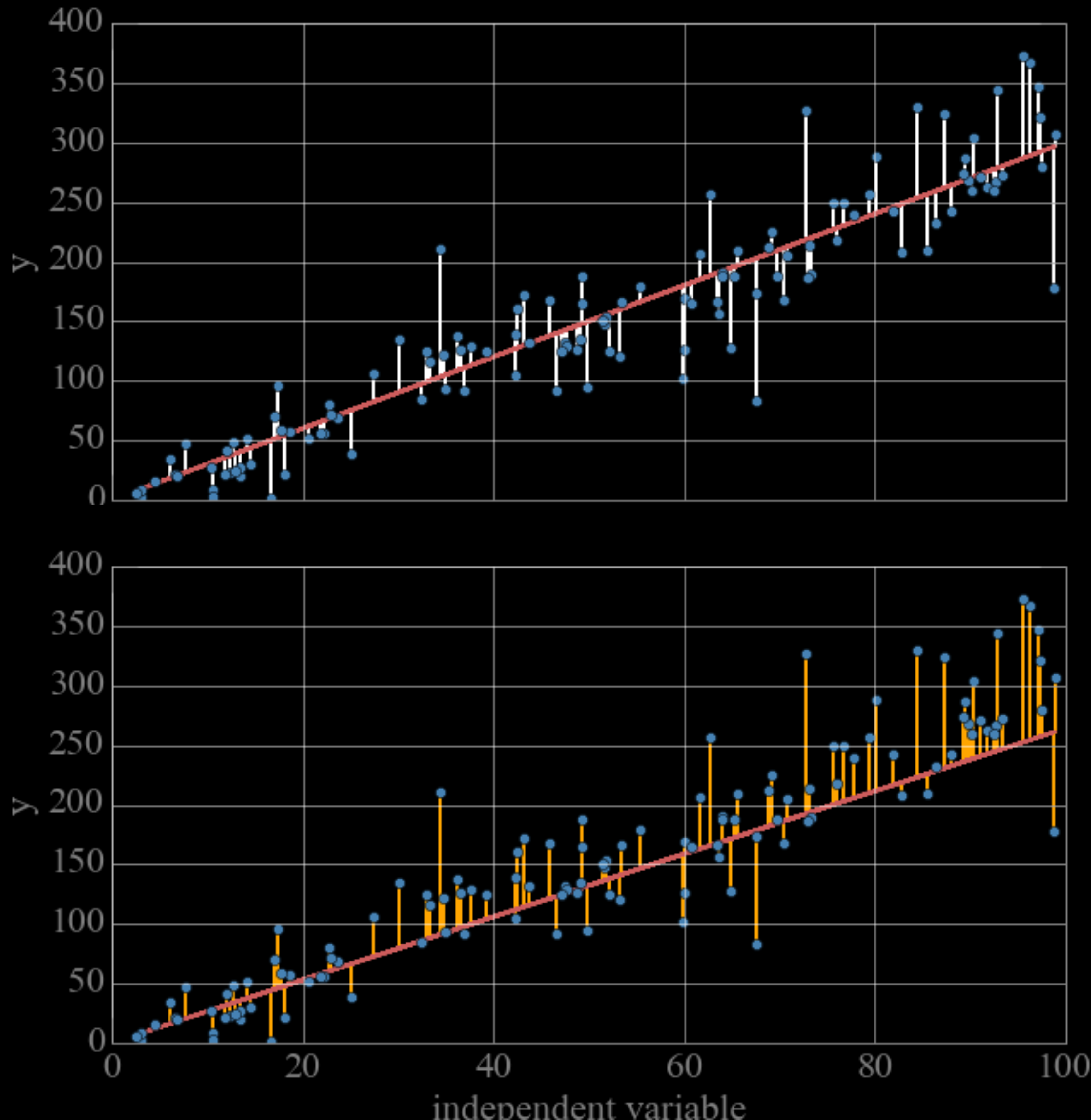
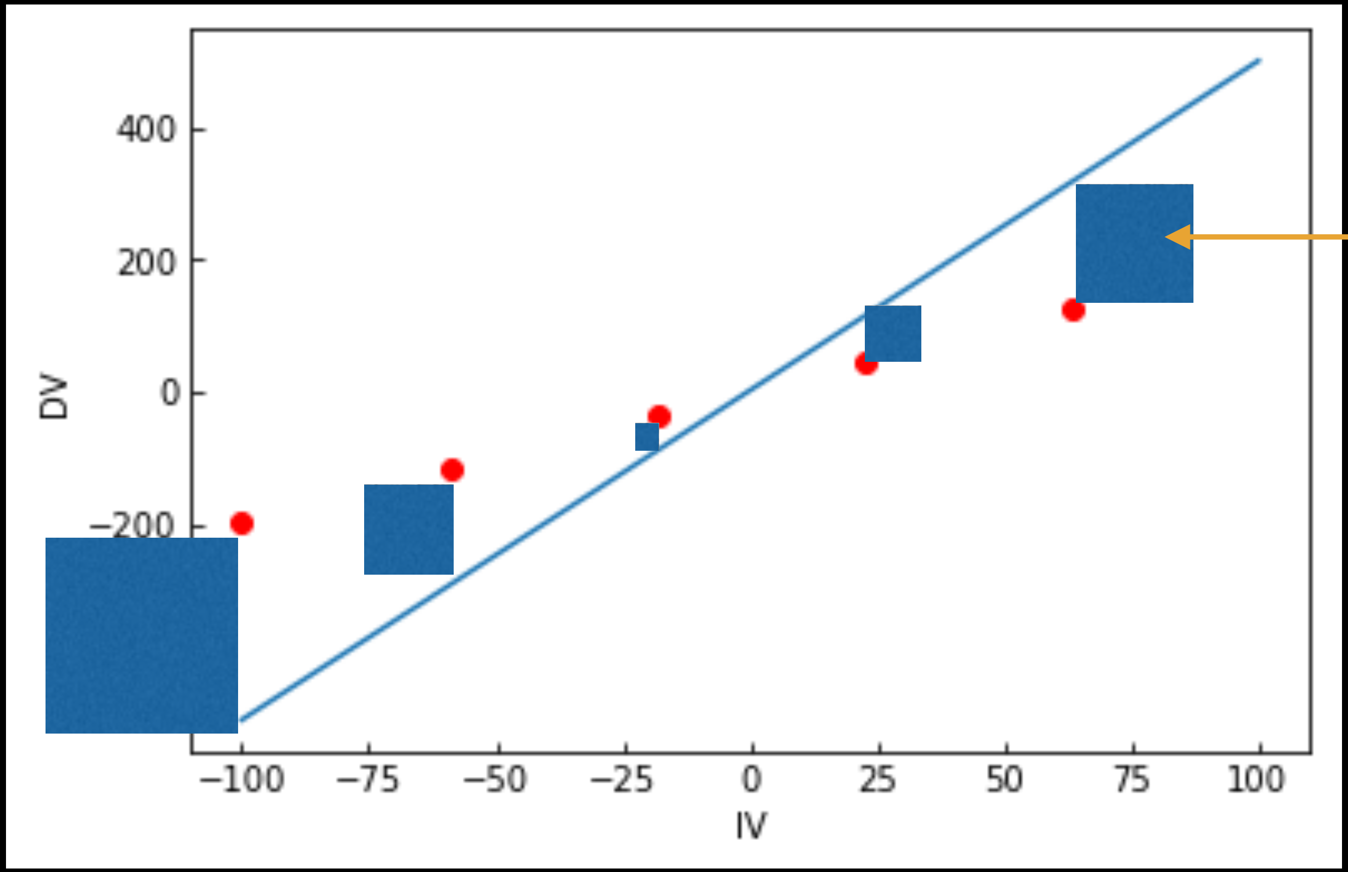
independent variable


400
350
300
250
200
150
100
50
0
y
0
20
40
60
80
100
independent variable

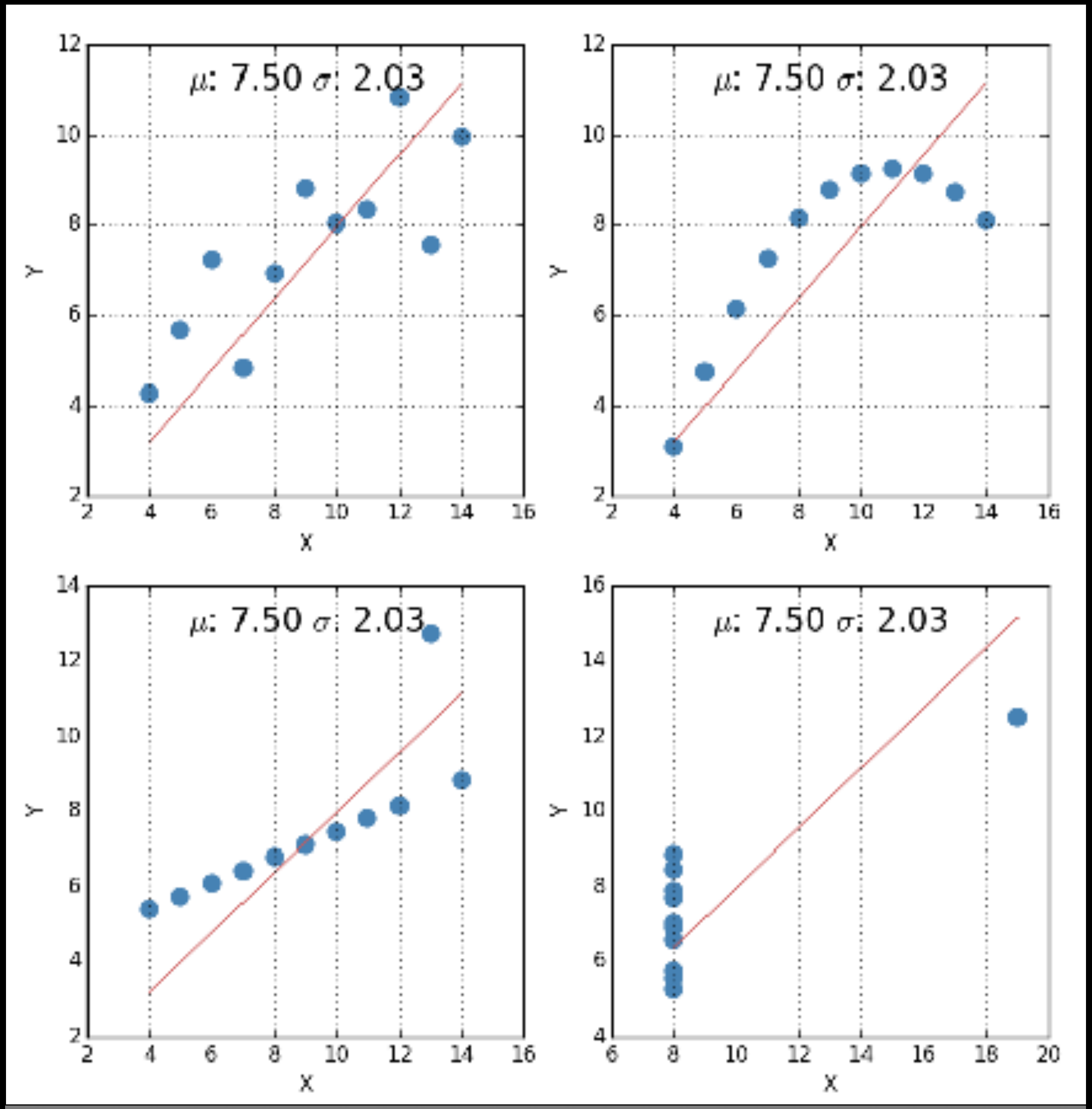
$$\sum_i (y_i - (ax_i + b))^2$$



These are the residuals squared

R^2: measures the amount (fraction)

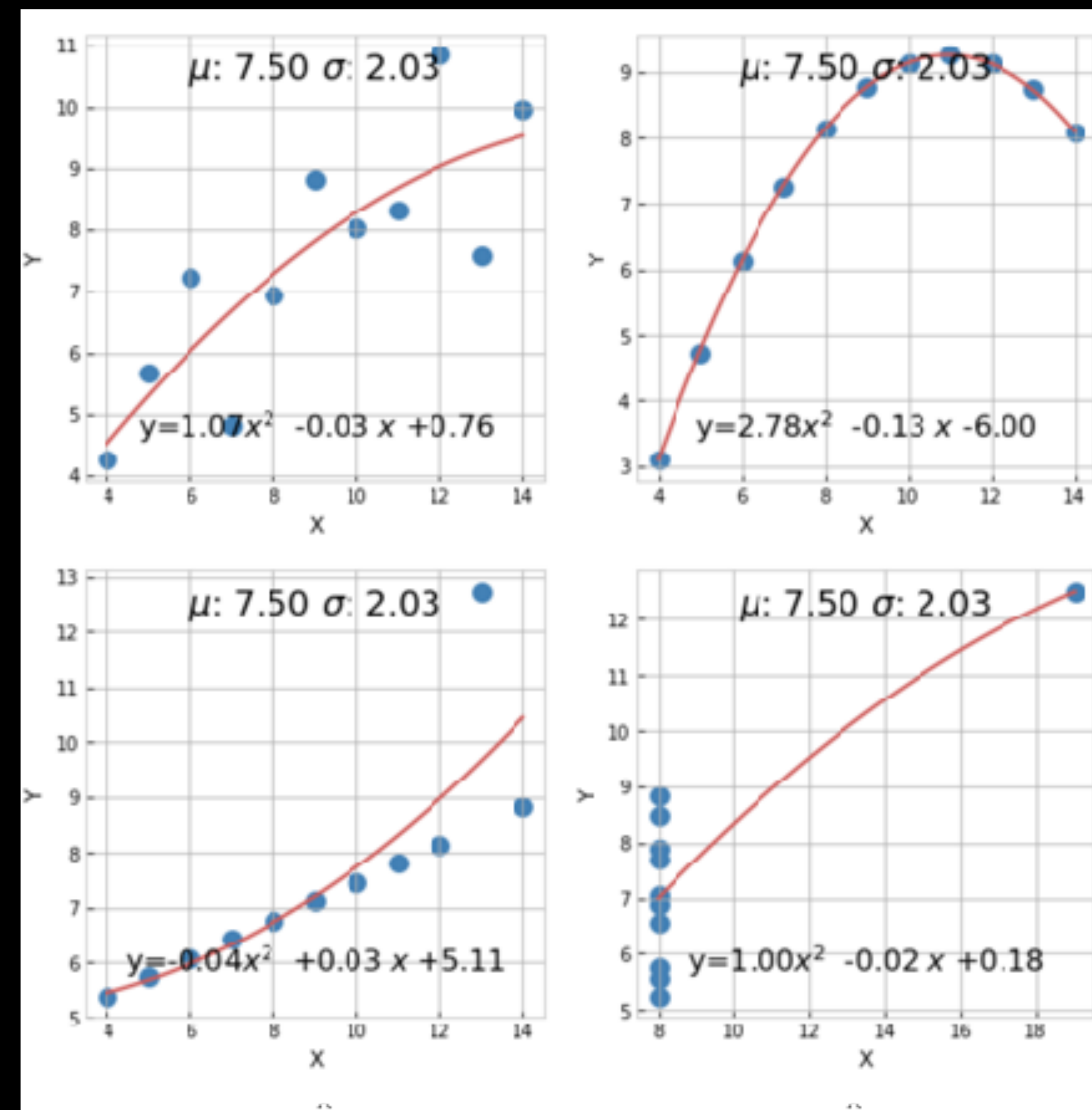
of variance in data explained by the model https://github.com/fedhere/UInotebooks/blob/master/Anscombe's%20Quartet.ipynb



Model residuals

https://github.com/fedhere/UInotebooks/blob/master/Anscombe's%20Quartet.ipynb

Model residuals



How good is a model?

Model diagnostics:

Chi^2, R^2, and LR test

Ok, you came up with a model, and fond the best fit parameters. Now what? How good is your model??
There are a lot of model diagnostics you should consider!

Regression diagnostics

This example file shows how to use a few of the `statsmodels` regression diagnostic tests in a real-life context. You can learn about more tests and find out more information abou the tests here on the Regression Diagnostics page.

http://www.statsmodels.org/dev/examples/notebooks/generated/regression_diagnostics.html

Ok, you came up with a model, and fond the best fit parameters. Now what? How good is your model?? There are a lot of model diagnostics you should consider!

QUESTIONS YOU SHOULD ASK ABOUT YOUR MODEL:

- Are my model predictions close enough to the observations? (R^2)
- Are my model predictions close enough to the observations accounting for uncertainties in the data? (chi^2)
- Is my model complete? (are the residuals randomly distributed?)
- Is my model overfitting? (chi^2 - or better compare to a simpler models- LR ratio)

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      Y   R-squared:                       0.687
Model:                            OLS   Adj. R-squared:                  0.609
Method:                 Least Squares   F-statistic:                     8.793
Date:                Tue, 11 Oct 2016   Prob (F-statistic):            0.00956
Time:                        06:14:52   Log-Likelihood:                -16.487
No. Observations:                  11   AIC:                             38.97
Df Residuals:                       8   BIC:                             40.17
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
```

adjusted R^2

$$\overline{R}^2 = R^2 - (1 - R^2)\frac{p}{n-p-1}$$

adjusts for the number of *explanatory terms* (parameters) in a model relative to the number of data points

χ^2 (chi²)

$$\chi^2_F = \sum_i \frac{(m_i - x_i)^2}{\sigma_i^2}$$

how well model explains data *including uncertainties*

Uncertainties in the measurement (errorbar)

m : model prediction

x: observation

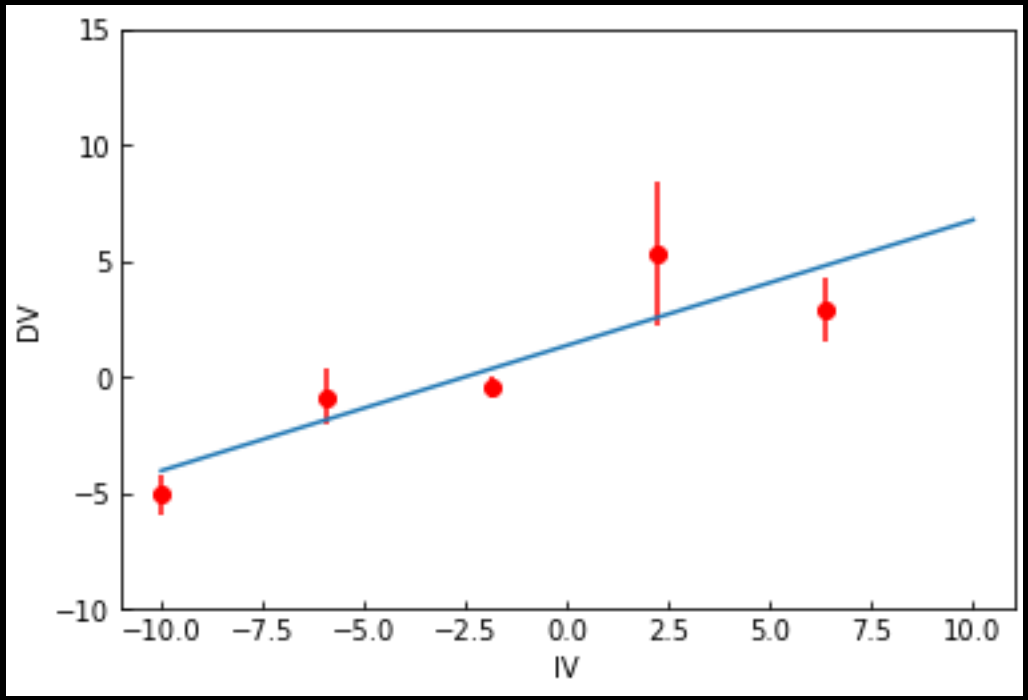
σ: uncertainty in the observation

χ^2 (chi²)

$$\chi^2_{/DOF} = \frac{1}{DOF} \sum_i \frac{(m_i - x_i)^2}{\sigma_i^2}$$

$R^2 = 0.8$

$\chi^2 = 2.5$

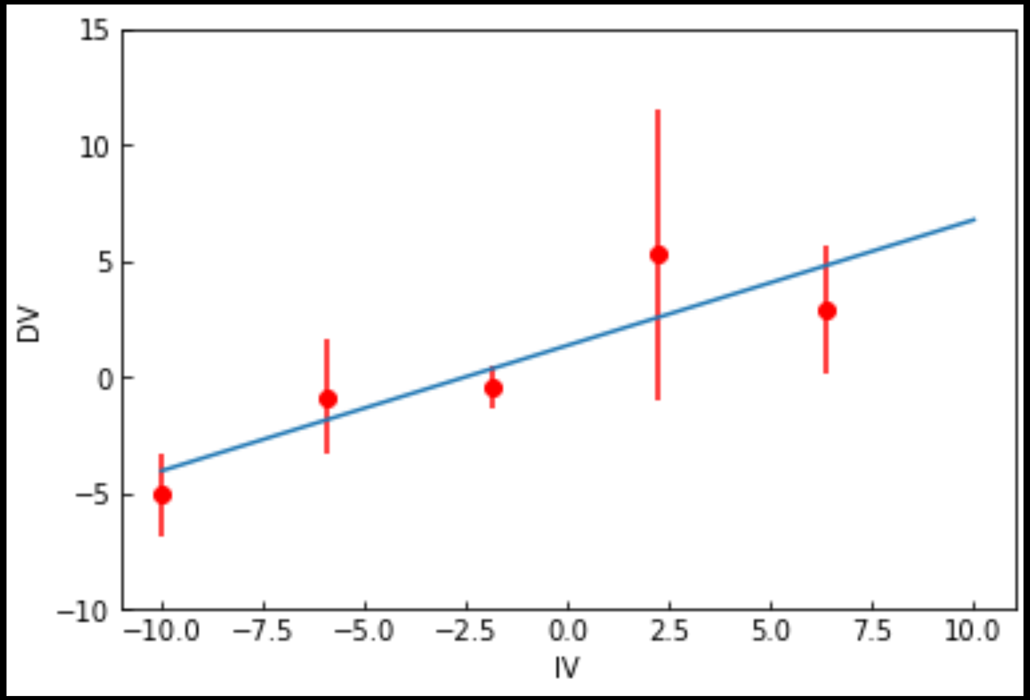


χ^2 (chi²)

$$\chi^2_{/DOF} = \frac{1}{DOF} \sum_i \frac{(m_i - x_i)^2}{\sigma_i^2}$$

$R^2 = 0.8$

$\chi^2 = 0.6$



The χ^2/DOF (reduced χ^2 or χ^2 per degree of freedom of your model) is a *statistics* (a measurable number) that follows a χ^2 *distribution* with mean 1.

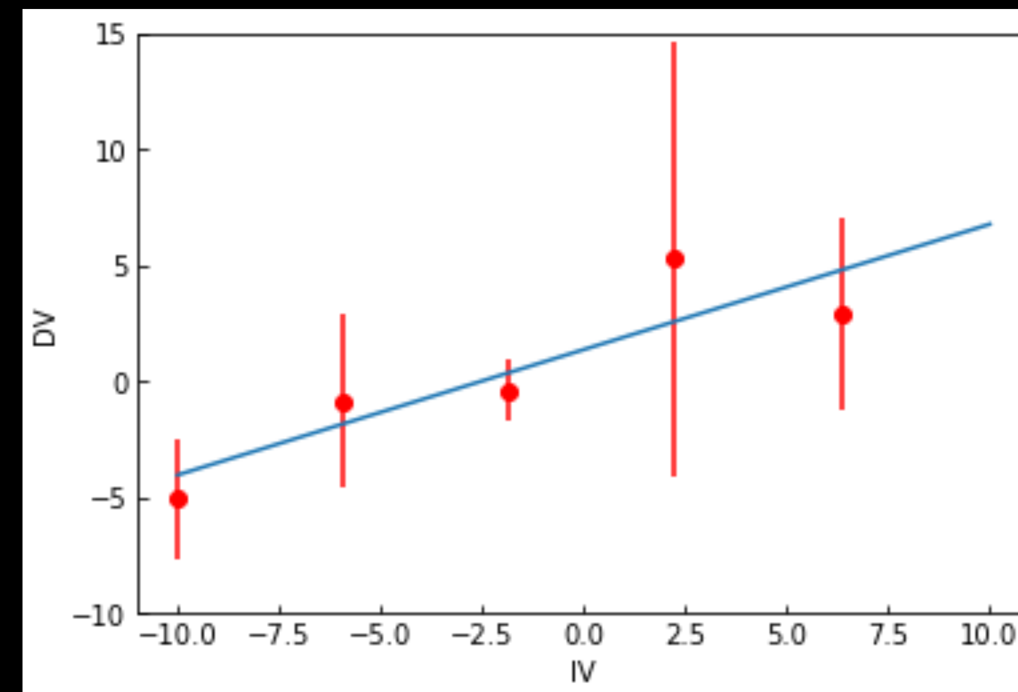
The larger the χ^2 the “worse” your model.

χ^2 (chi²)

$$\chi^2_{/DOF} = \frac{1}{DOF} \sum_i \frac{(m_i - x_i)^2}{\sigma_i^2}$$

$R^2 = 0.8$

$\chi^2 = 0.3$



The χ^2 /DOF (reduced χ^2 or χ^2 per degree of freedom of your model) is a *statistics* (a measurable number) that follows a χ^2 *distribution* with mean 1.

The larger the χ^2 the "worse" your model.

But be suspicious of χ^2<1!! It may indicate overfitting (or overestimation of the uncertainties)

(χ^2 assumes gaussian-distributed uncertainties)

Likelihood

Data given model

Probability $P(\ x \mid \theta\ )$

Likelihood

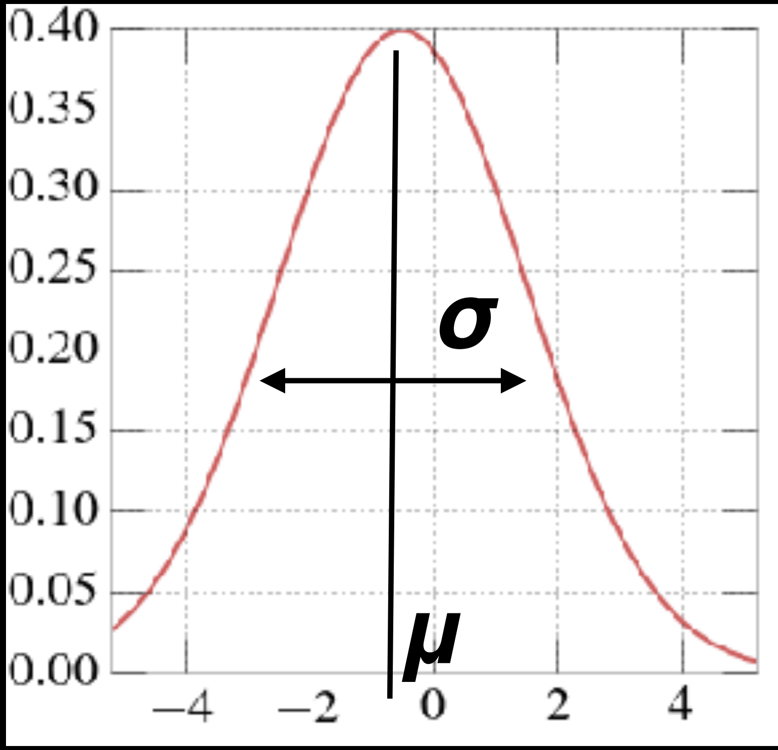
Probability $P(\vec{x} \mid \mu, \sigma)$

Likelihood

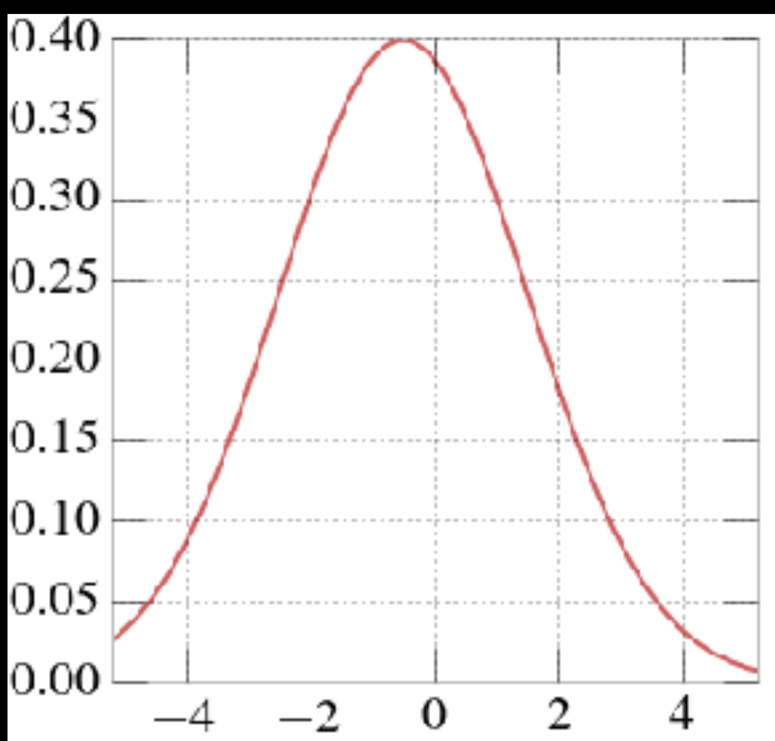
Probability $P(\vec{y} \mid \vec{x}, \mu, \sigma)$

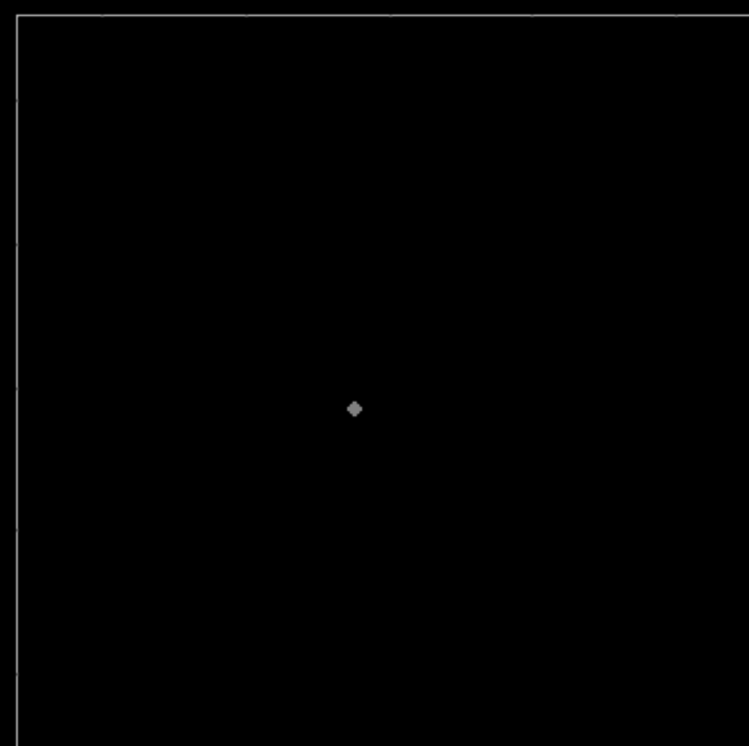
Likelihood

Probability $P(\vec{x} \mid \mu, \sigma)$

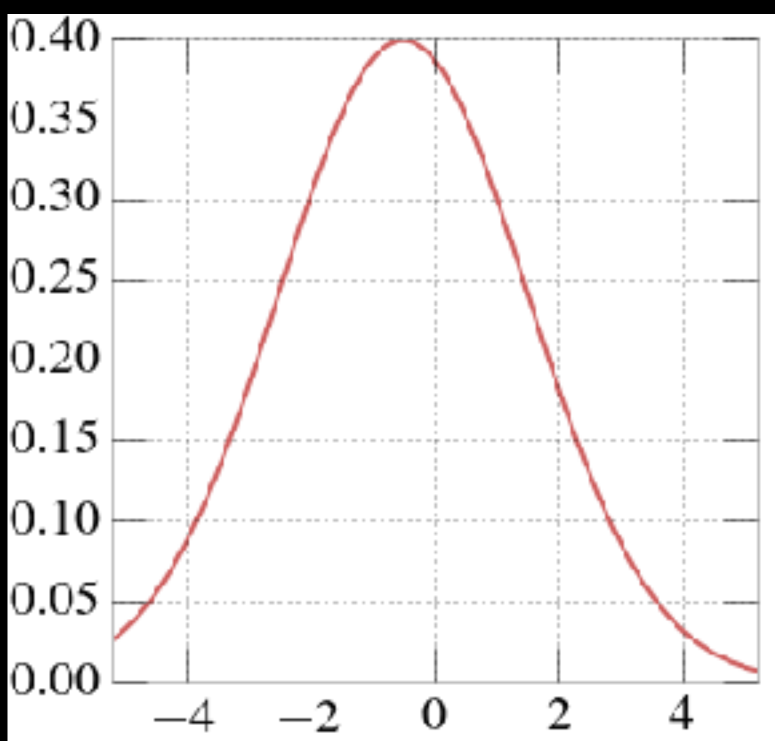


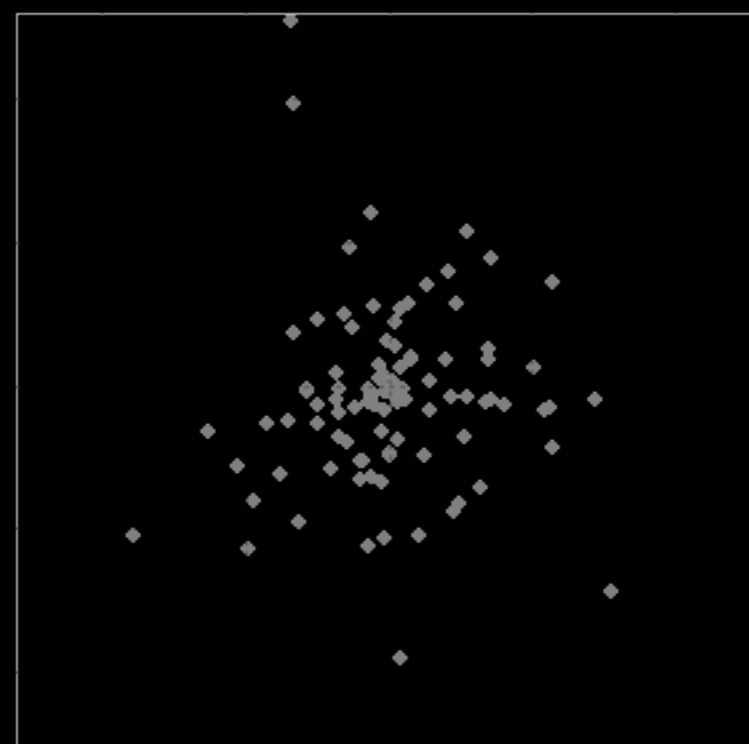
Probability $P(\vec{x} \mid \vec{\theta})$

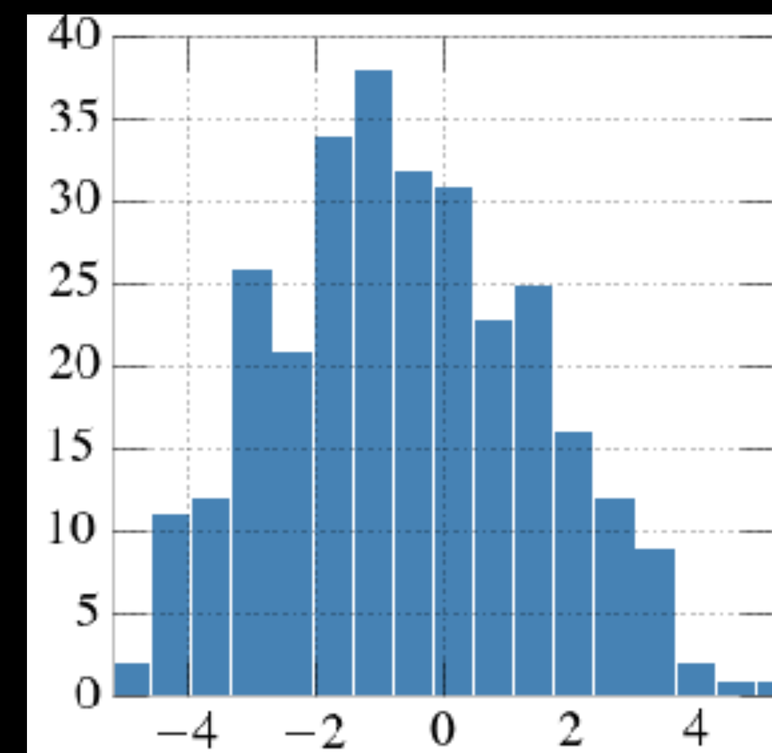




Probability $P(\vec{x} \mid \vec{\theta})$



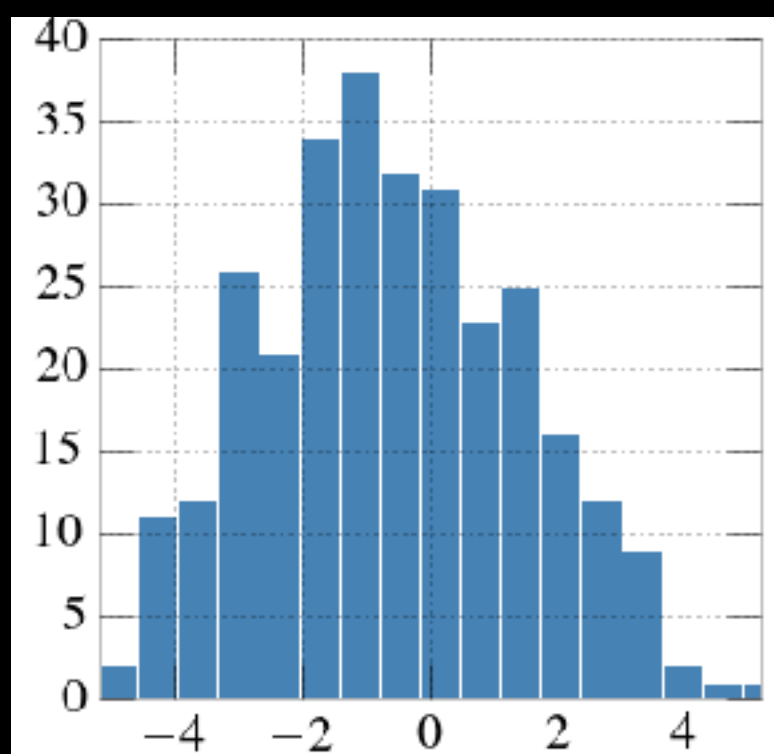




Probability $P(\vec{x} \mid \vec{\theta})$

Model given data

Likelihood $P(\vec{\theta} \mid \vec{x})$

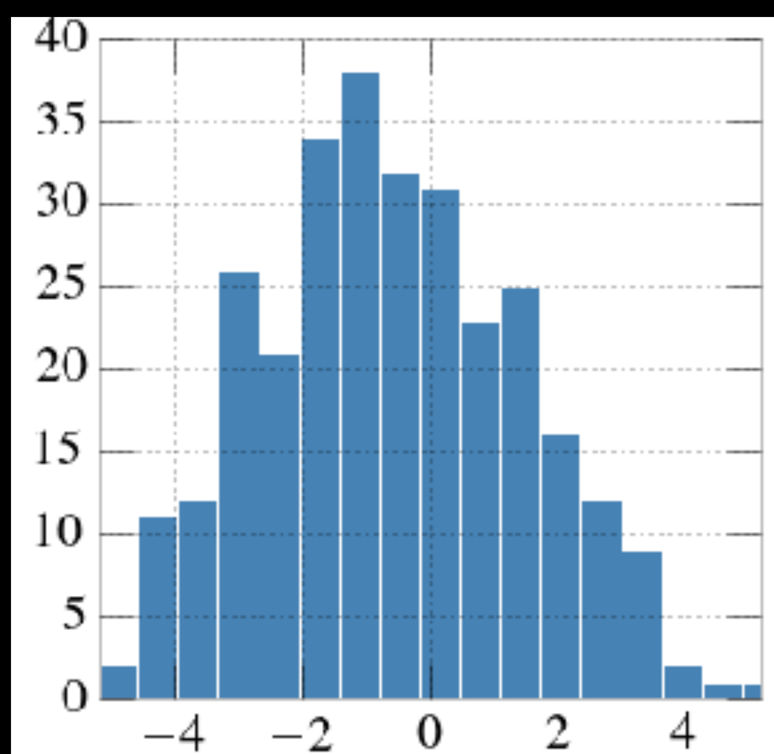


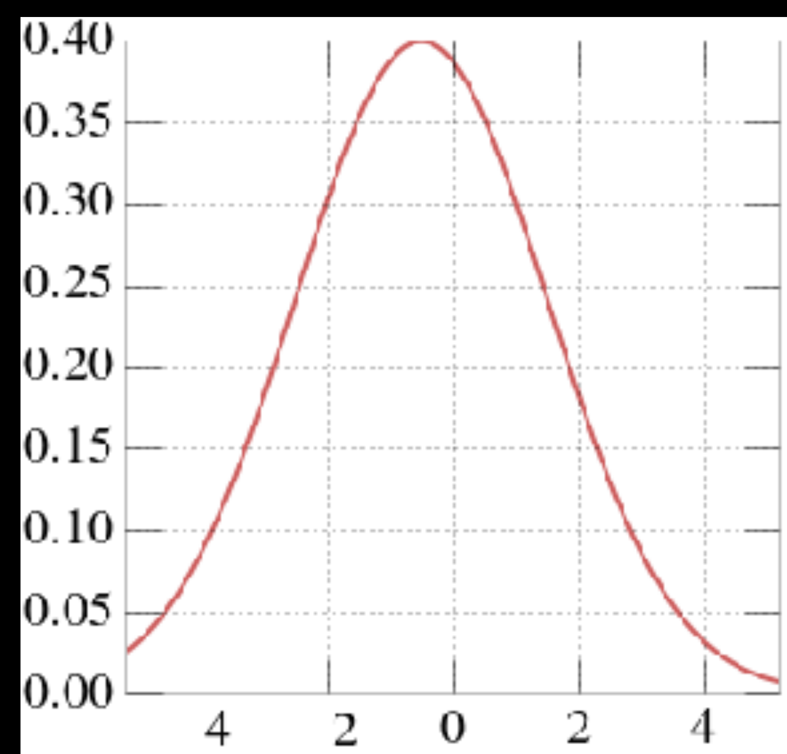
The likelihood is the probability of a model given the data

- given what I measured (my observations) what is the probability that the data I observed is generated by a process such as the one described by my model

Probability $P(\vec{x} \mid \vec{\theta})$

Likelihood $P(\vec{\theta} \mid \vec{x})$





Assume the data is generated in a Gaussian distribution

My model is a gaussian w/ mean μ and standard deviation σ

Probability $$N(\mu,\sigma) \sim \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Likelihood

Assume the data is generated in a Gaussian distribution

Probability of μ,σ given that 1 observations

Probability $$N(\mu,\sigma) \sim \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathscr{L}_{(\mu,\sigma)}(x) \sim \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Assume the data is generated in a Gaussian distribution

Probability of *n* independent observations

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood

Assume the data is generated in a Gaussian distribution

Probability of *μ,σ* given those n observations

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Assume the data is generated in a Gaussian distribution

(some algebraic transformations to simplify things)

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} \Pi_i e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Assume the data is generated in a Gaussian distribution

(some algebraic transformations to simplify things)

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i(x_i-\mu)^2}{2\sigma^2}}$$

USING LIKELIHOOD FOR PARAMETER OPTIMIZATION:

Given a model functional form the optimal set of parameters is the set that maximized the likelihood

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i (x_i-\mu)^2}{2\sigma^2}}$$

Essentially the same as OLS

Probability $N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

Likelihood $\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i(x_i-\mu)^2}{2\sigma^2}}$

Given some observations $\vec{x}$ we want to model them with the best function: the one that is MAXIMALLY LIKELY.

Probability $N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

Likelihood $\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i (x_i-\mu)^2}{2\sigma^2}}$

Given some observations $\vec{x}$ we want to model them with the best function: the one that is MAXIMALLY LIKELY. After we choose a functional form (N) for the model we want to choose the parameters (μ,σ) that maximiz $\mathscr{L}_{(\mu,\sigma)}(\vec{x})$

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Likelihood $$\mathcal{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i(x_i-\mu)^2}{2\sigma^2}}$$

$$\boxed{\text{FIND } \mu^*, \sigma^* \mid \mathcal{L}_{(\mu^*,\sigma^*)} = \max(\mathcal{L}_{(\mu,\sigma)}(\vec{x}))}$$

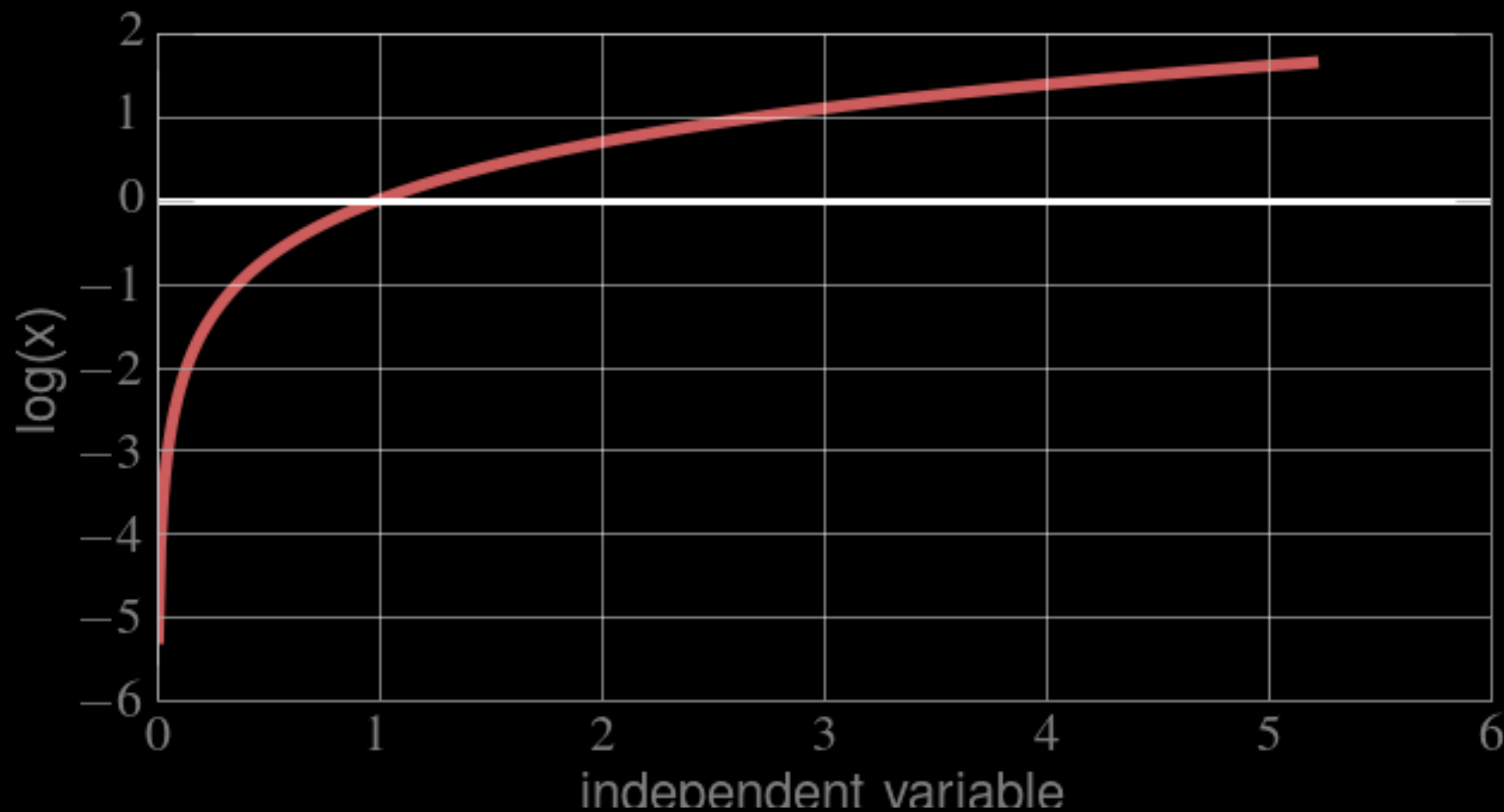
Probability $N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

Likelihood $\mathscr{L}_{(\mu,\sigma)}(\vec{x}) \sim \frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i(x_i-\mu)^2}{2\sigma^2}}$

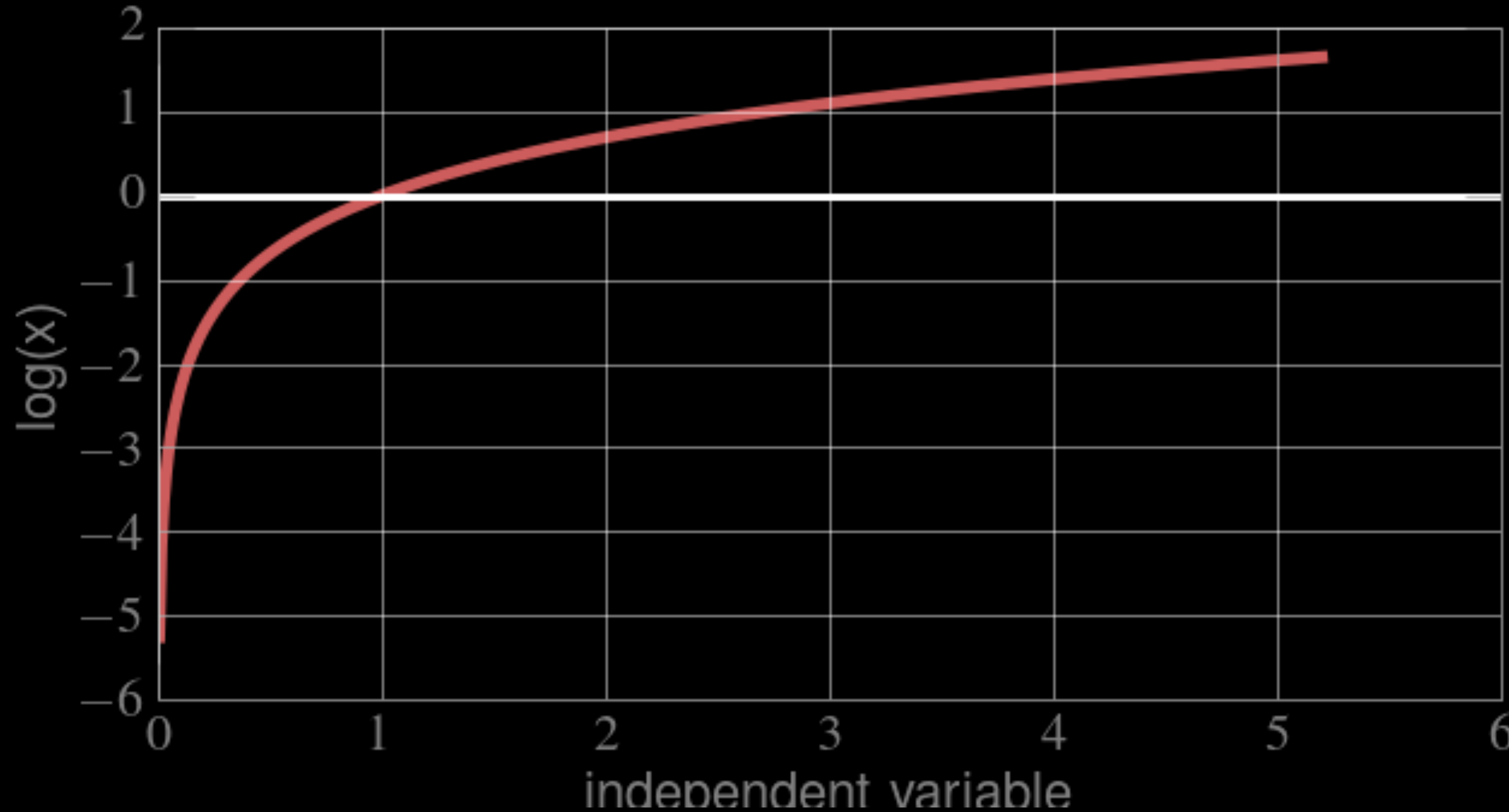
$$\boxed{\text{FIND } \mu^*, \sigma^* \mid -\log(\mathscr{L}_{(\mu^*,\sigma^*)}) = \min(-\log(\mathscr{L}_{(\mu,\sigma)}(\vec{x})))}$$

But, because it is mathematically convenient, instead of maximizing the likelihood we often MINIMIZE *-log(likelihood)…*

Logarithm:



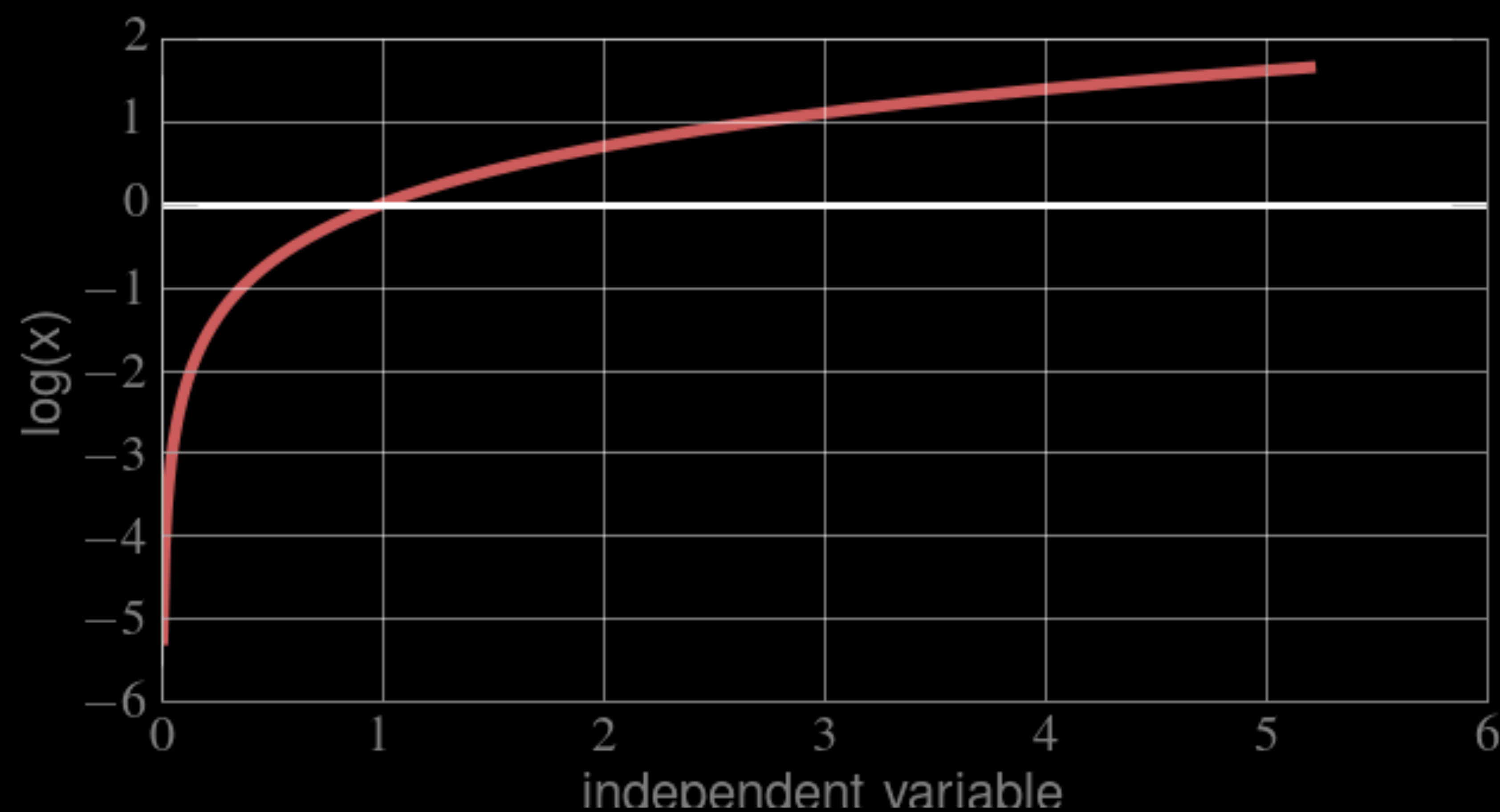
Logarithm: MONOTONICALLY INCREASING



Logarithm: MONOTONICALLY INCREASING

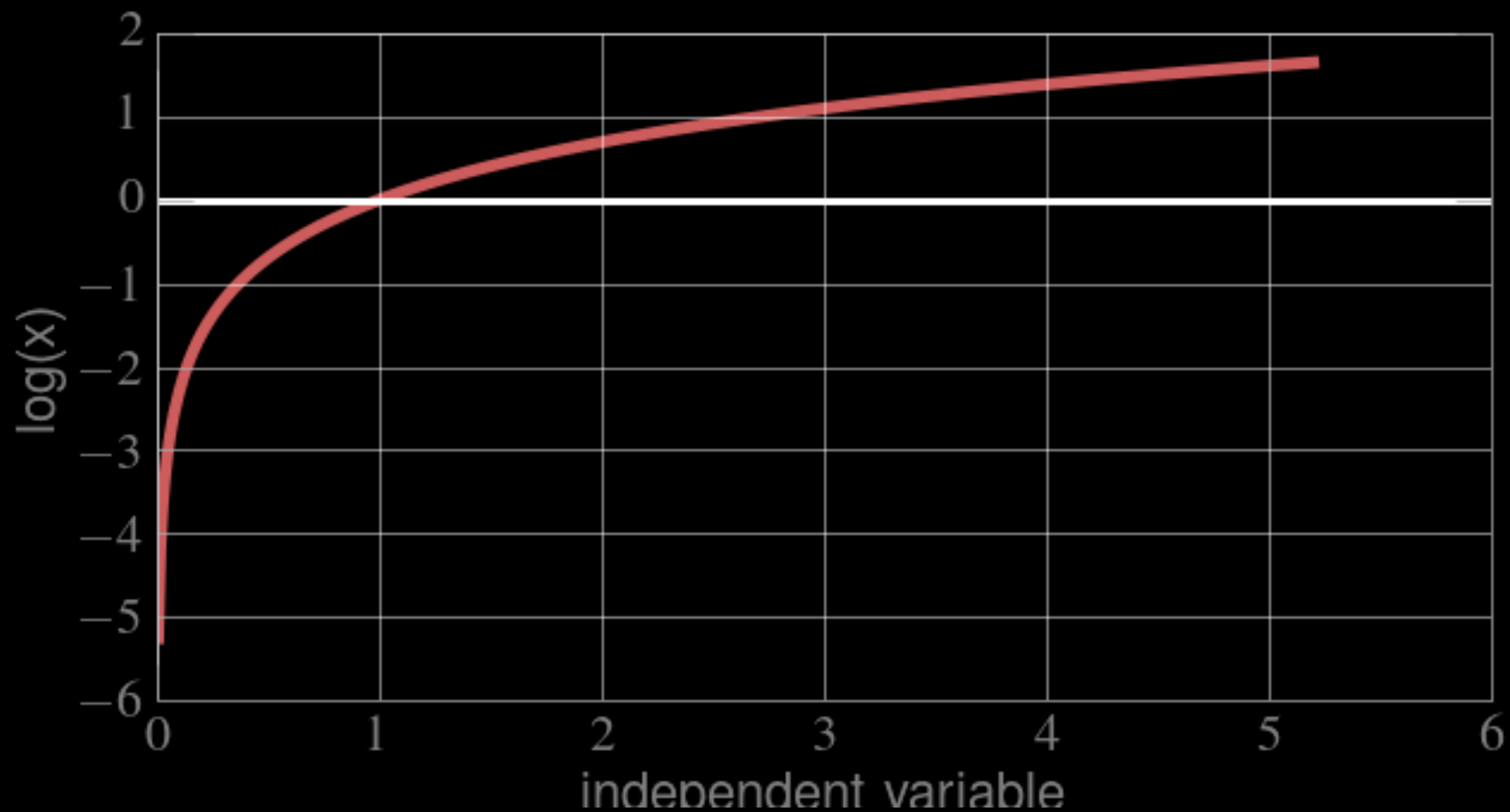
if x grows, log(x) grows, if x decreases, log(x) decreases

the location of the maximum is the same!



Logarithm: MONOTONICALLY INCREASING

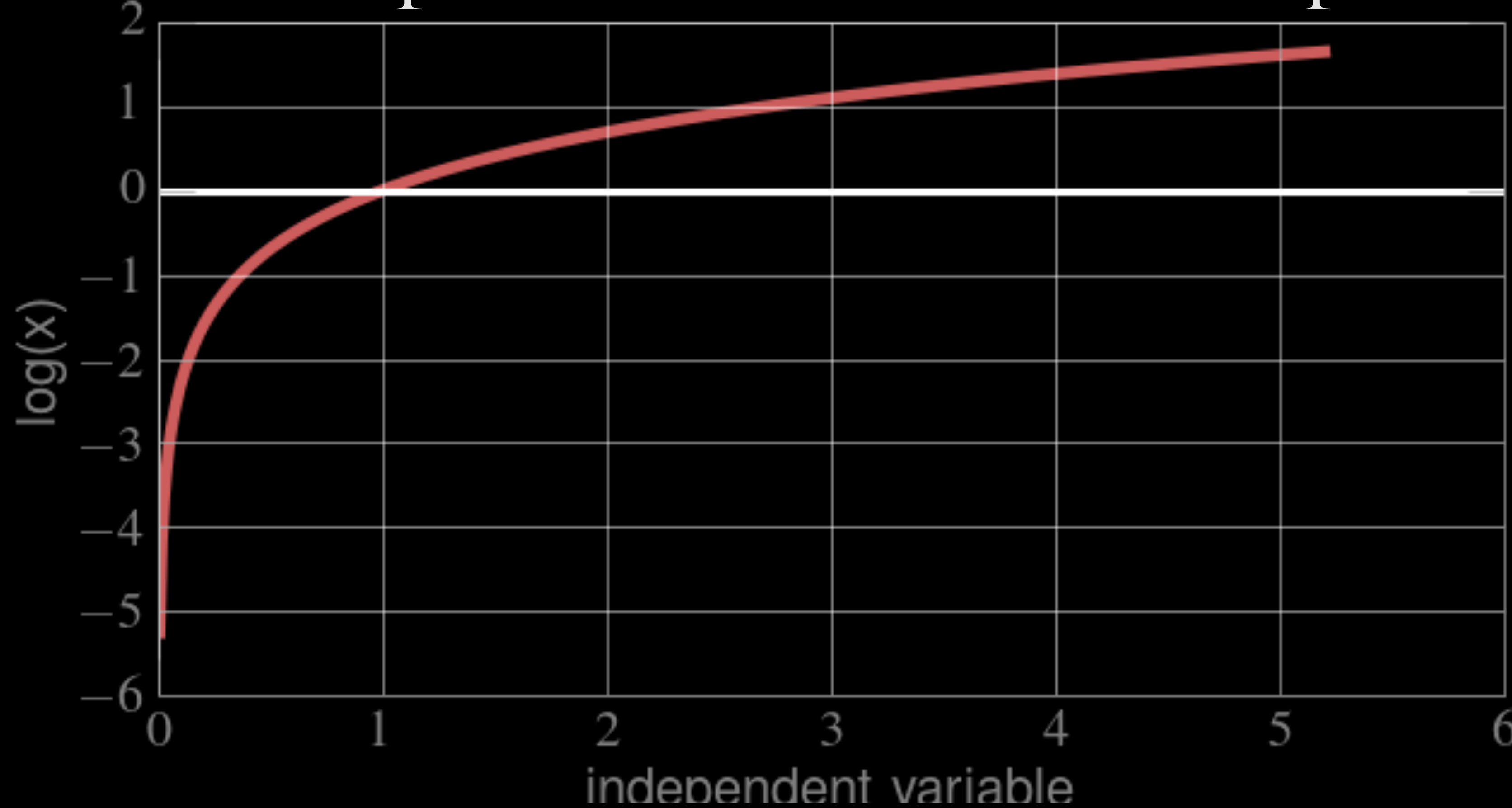
SUPPORT : (0: ∞]



Logarithm: MONOTONICALLY INCREASING

SUPPORT : (0: ∞]

Not a problem cause L like P is positive defined



(some algebraic transformations to simplify things)

Probability $N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

log Likelihood $\log(\mathscr{L}_{(\mu,\sigma)}(\vec{x})) \sim \log\left(\frac{1}{(\sigma\sqrt{2\pi})^n} e^{-\frac{\Sigma_i(x_i-\mu)^2}{2\sigma^2}}\right)$

(some algebraic transformations to simplify things)

Probability
$$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

log Likelihood
$$\log(\mathscr{L}_{(\mu,\sigma)}(\vec{x})) \sim$$
$$\log\left((2\pi\sigma^2)^{-\frac{n}{2}} exp\left(-\frac{1}{2\sigma^2}\sum_1^n (x_i-\mu)^2\right)\right)$$

(some algebraic transformations to simplify things)

Probability

$$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

log Likelihood

$$\ell(\mu,\sigma)(\vec{x}) \sim$$

$$-\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_1^n (x_i-\mu)^2$$

(some algebraic transformations to simplify things)

Probability

$$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

log Likelihood

$$\ell(\mu,\sigma)(\vec{x}) \sim$$

$$-\frac{n}{2}\log(2\pi)-\frac{n}{2}\log(\sigma^2)-\frac{1}{2\sigma^2}\sum_1^n (x_i-\mu)^2$$

(some algebraic transformations to simplify things)

Probability

$$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

log Likelihood

$$\ell(\mu,\sigma)(\vec{x}) \sim$$

$$\cancel{-\frac{n}{2}\log(2\pi)} - \frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{1}^{n}(x_i-\mu)^2$$

(some algebraic transformations to simplify things)

Probability $N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

max log Likelihood $\ell(\mu,\sigma)(\vec{x}) \sim$

$$\cancel{-\frac{n}{2}\log(2\pi)} - \frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{1}^{n}(x_i-\mu)^2$$

(some algebraic transformations to simplify things)

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

max log Likelihood $$\ell_{(\mu^*,\sigma^*)}(\vec{x}) = max(\ell_{(\mu,\sigma)}(\vec{x}))$$

(some algebraic transformations to simplify things)

Probability $$N(\mu,\sigma) \sim \Pi_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

max log Likelihood $$\frac{d\ell_{(\mu,\sigma)}(\vec{x})}{d(\mu,\sigma)} = 0$$

USING LIKELIHOOD TO COMPARE MODELS

Given two models which is preferable.
A *rigorous* answer (in terms of NHST) can be obtained for *2 nested* models thus answering "is my more complex model *overfitting* the data?"

Likelihood-ratio tests

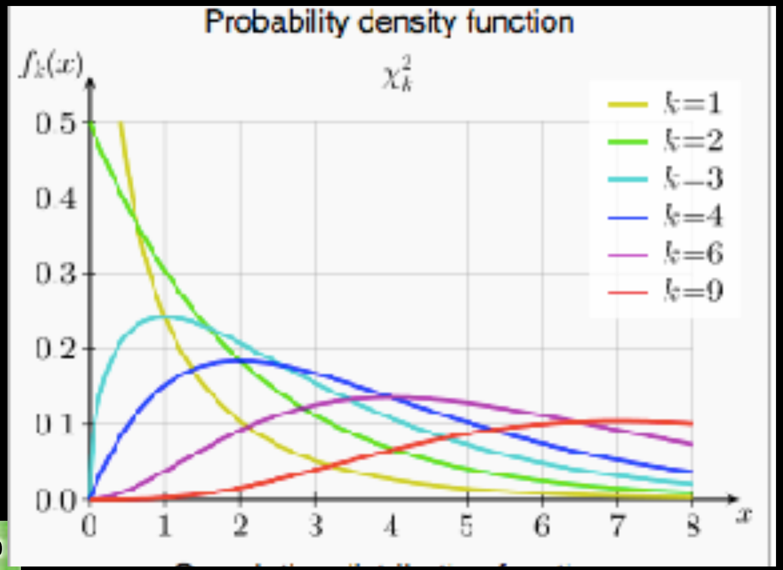
USING LIKELIHOOD TO COMPARE MODELS

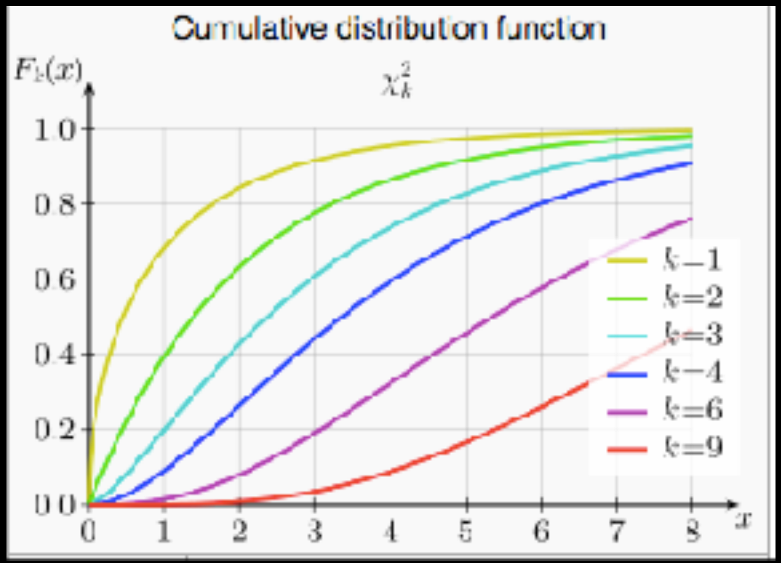
Measure the *likelihood ratio* statistics LR

L: Likelihood

$$LR = -2 \log_e \frac{L(\text{model 1})}{L(\text{model 2})}$$

This statistic is chi-squared distributed





$$LR = -2 \log_e \frac{L(\text{model 1})}{L(\text{model 2})}$$

This statistic is chi-squared distributed with degrees of freedom equal to the difference in the number of degrees of freedom between the two models (i.e., the number of variables and parameters added to the model).

Maximizing Likelihood

$$LR = -2 \log_e \frac{\max L(\text{model } 1)}{\max L(\text{model } 2)}$$

$$= -2 \log(\max(L(\text{model1})) - \log(\max(L(\text{model2})))$$

This statistic is chi-squared distributed

$$LR = -2 \log_e \frac{\max L(\text{model } 1)}{\max L(\text{model } 2)}$$

This statistic is chi-squared distributed with degrees of freedom equal to the difference in the number of degrees of freedom between the two models (i.e., the number of variables added to the model).

Note: there is another test also called likelihood ratio test…

$$LR = \frac{\text{False Negative}}{\text{True Negative}}$$

	H_0 is True	H_0 is False
H_0 is falsified	Type I error False Positive important message gets spammed	True Positive
H_0 is not falsified	True Negative	Type II error False negative Spam in your Inbox

nrg buildings notebook

Homework:

ENERGY - SIZE building modeling:
follow in class instructions

MUST KNOWS:

- How to minimize fit parameters (OLS, WLS)
- goodness of fit tests
- R^2 , χ^2 , adjusted R^2 , reduced χ^2 , likelihood, Likelihood ratio test

Assigned Reading

"Robustness in the strategy of scientific model building", in Launer, R. L.; Wilkinson, G. N., *Robustness in Statistics*, Academic Press, pp. 201–236.

Resources:

Sarah Boslaugh, Dr. Paul Andrew Watters, 2008
Introduction to General Linear Regression (Chap 12 in most versions)
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