

data science for (physical) scientists V

the ABC of regression

dr.federica bianco | fbb.space |  fedhere |  fedhere



Uncertainties

- *types of uncertainties: Statistical and Systematics*

Stochastic vs Systematics

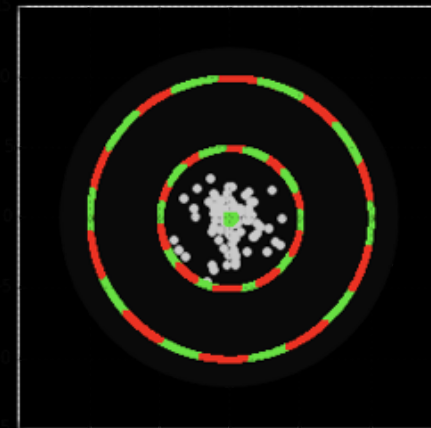
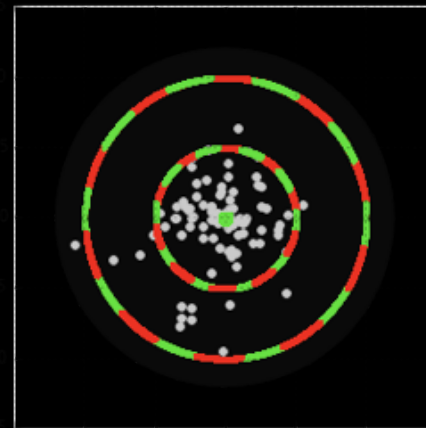
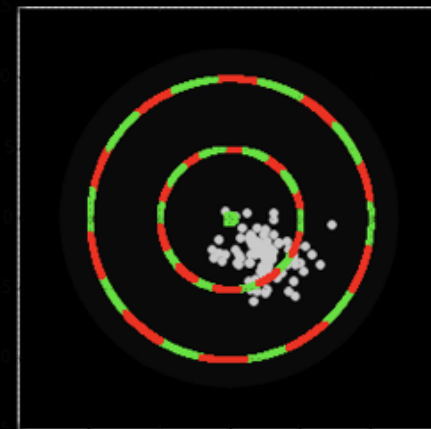
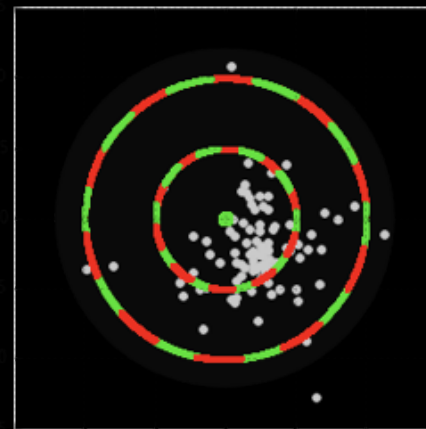
Systematic	Statistical
Biases the measurement <i>in one direction</i>	No preferred direction
Affects the sample regardless of the size	Shrinks with the sample size (typically as N)
Any distribution (usually we use Gaussian though)	Typically Gaussian or Poisson

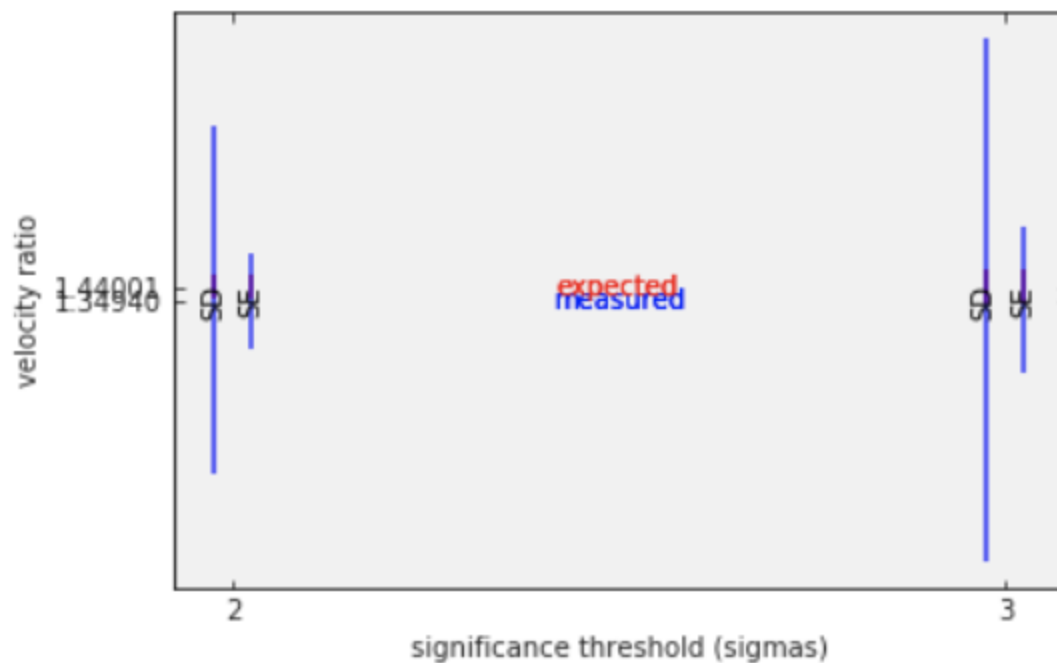
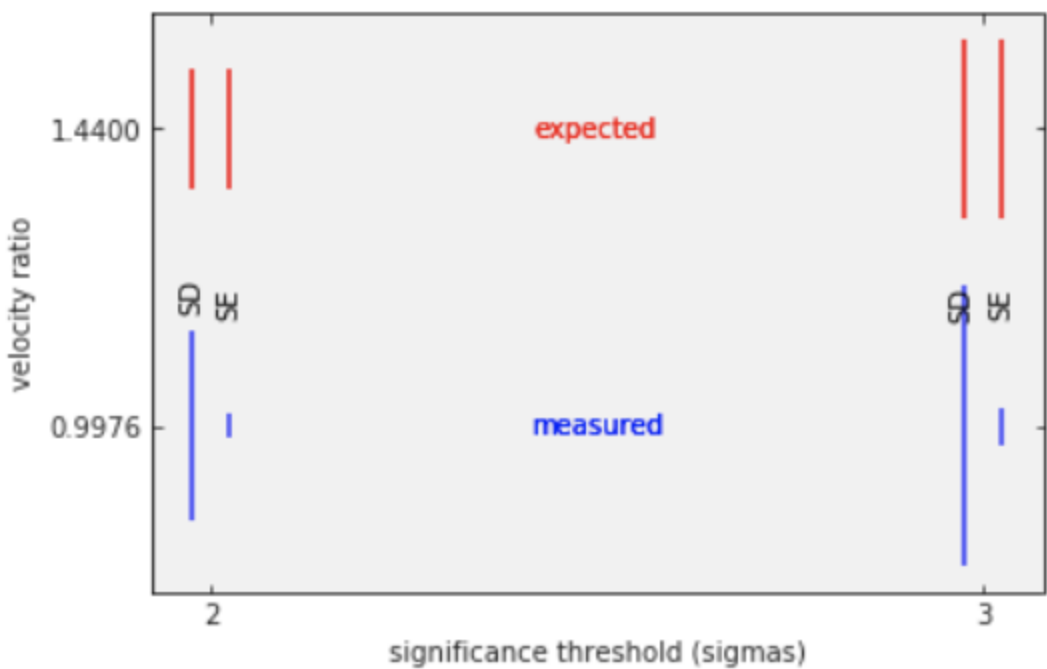
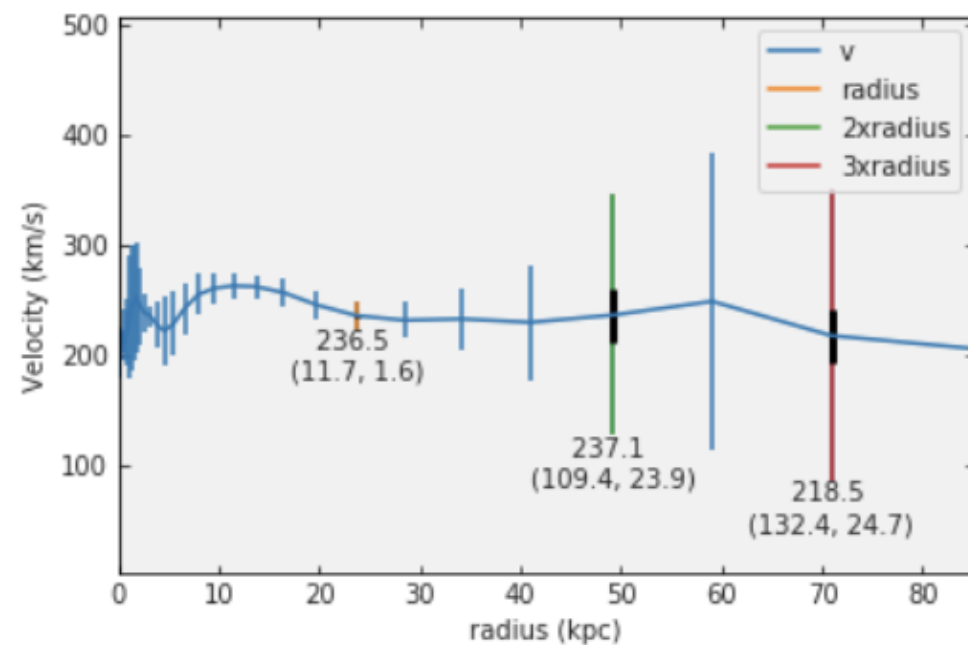
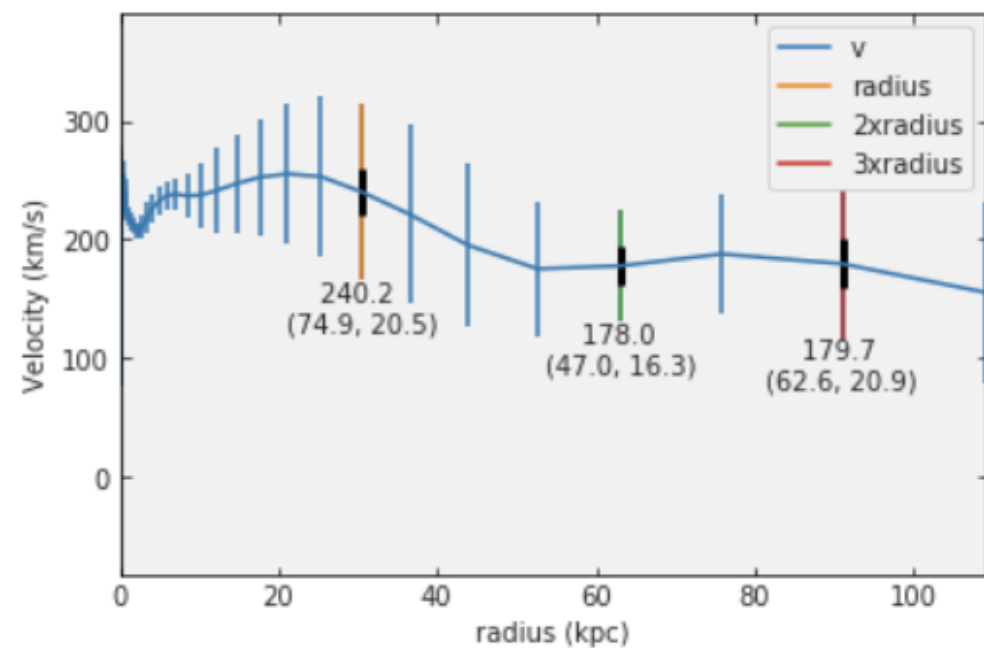
Precision vs Accuracy

Precision



Accuracy





$$z = x \pm y \sim | \quad \sim dz = \sqrt{dx^2 + dy^2} \quad (1)$$

$$z = x * y \sim | \quad \sim dz = |xy| \sqrt{\left(\frac{dx}{x}\right)^2 + \left(\frac{dy}{y}\right)^2} \quad (2)$$

$$z = x / y \sim | \quad \sim dz = \left|\frac{x}{y}\right| \sqrt{\left(\frac{dx}{x}\right)^2 + \left(\frac{dy}{y}\right)^2} \quad (3)$$

$$z = x^n \sim | \quad \sim dz = |n| x^{n-1} dx \quad (4)$$

$$z = cx \sim | \quad \sim dz = |c| dx \quad (5)$$

$$z = f(x, y) \sim | \quad \sim dz = \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 dx^2 + \left(\frac{\partial f}{\partial y}\right)^2 dy^2} \quad (6)$$

1 what is a model

2 the principle of parsimony

3 fitting a model to data *epistemology*

line fit

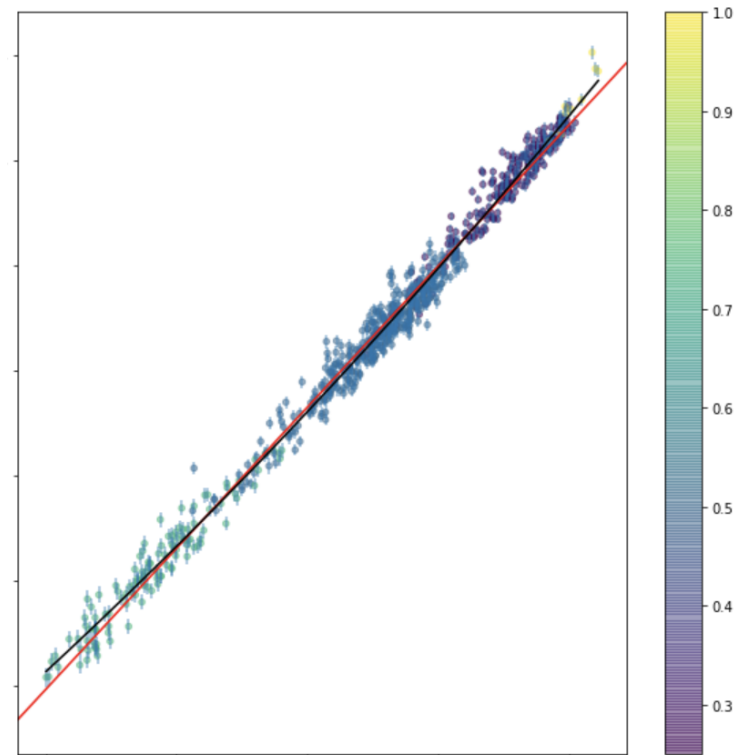
standard linear fit

higher order equation

uncertainties in the fit parameters

generative models

4 cross-validation



O

what is machine learning?

what is machine learning?

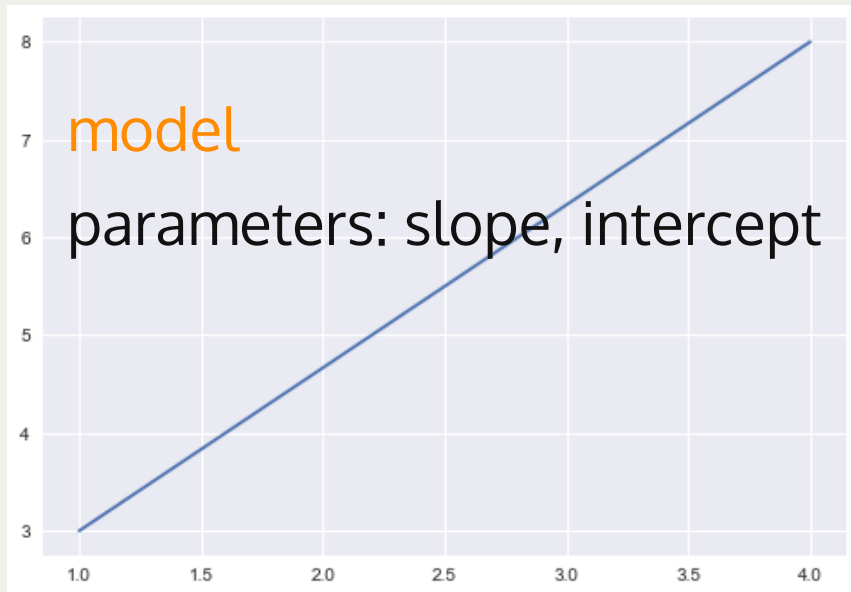
[Machine Learning is the] field of study that gives computers the ability to learn without being explicitly programmed.

Arthur Samuel, 1959

what is machine learning?

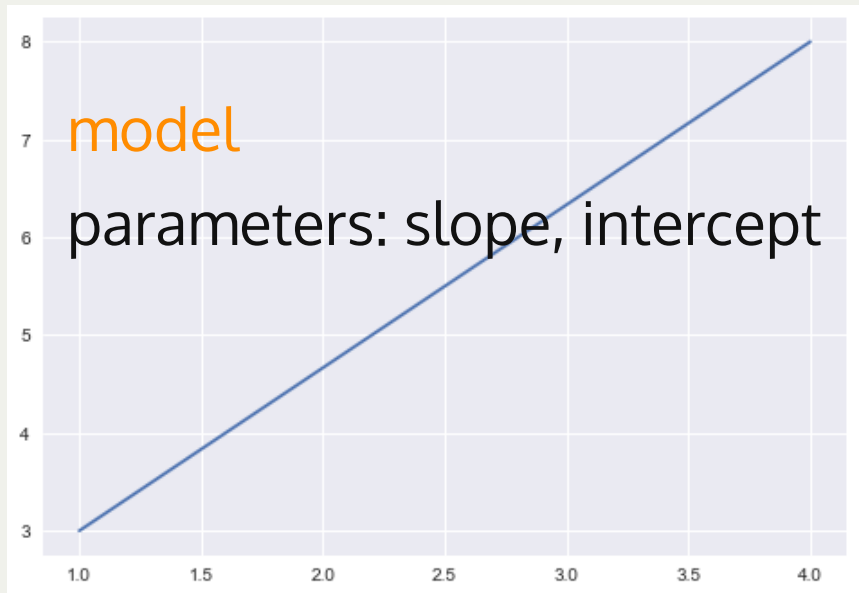
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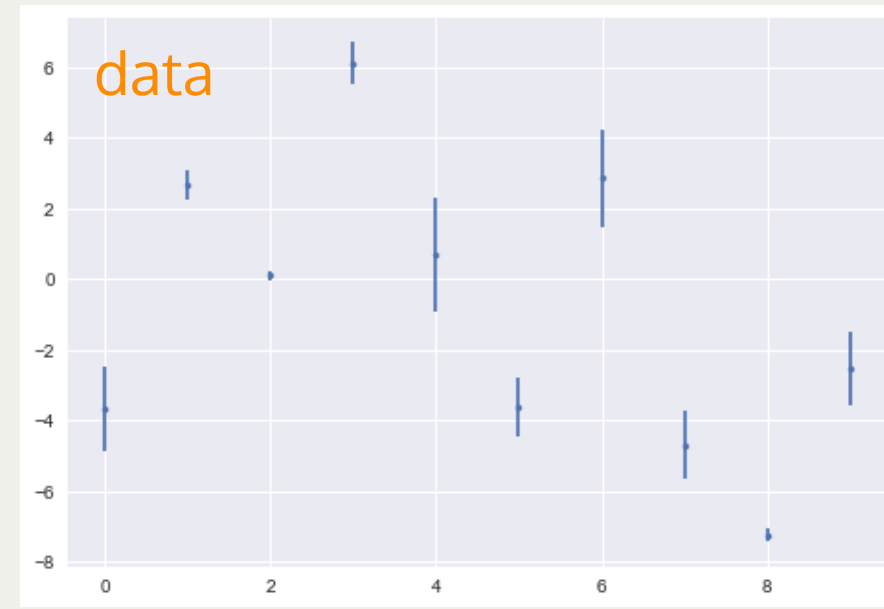


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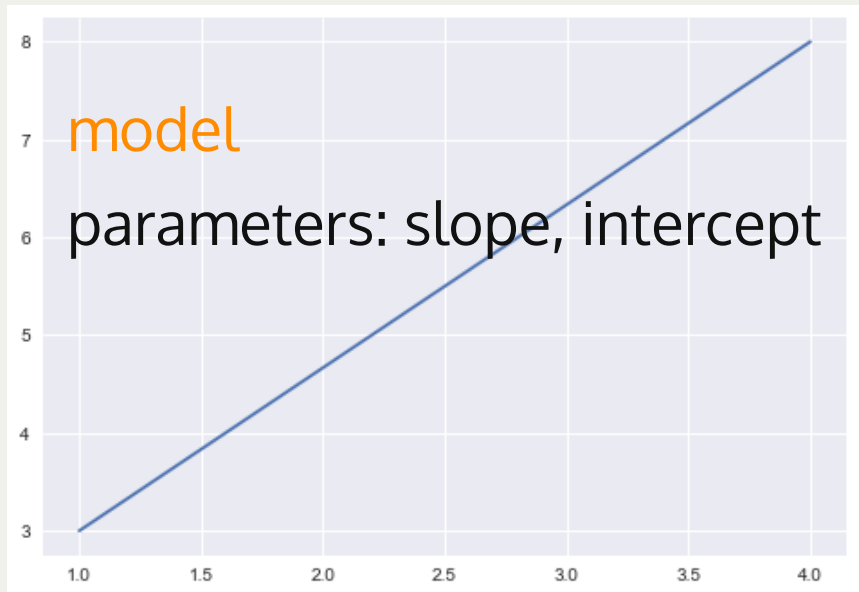


Arthur Samuel, 1959



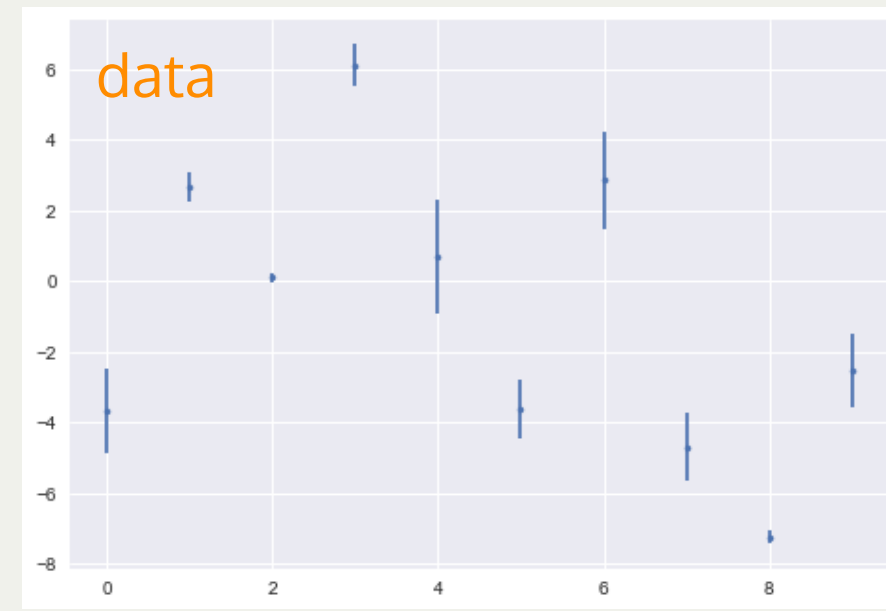
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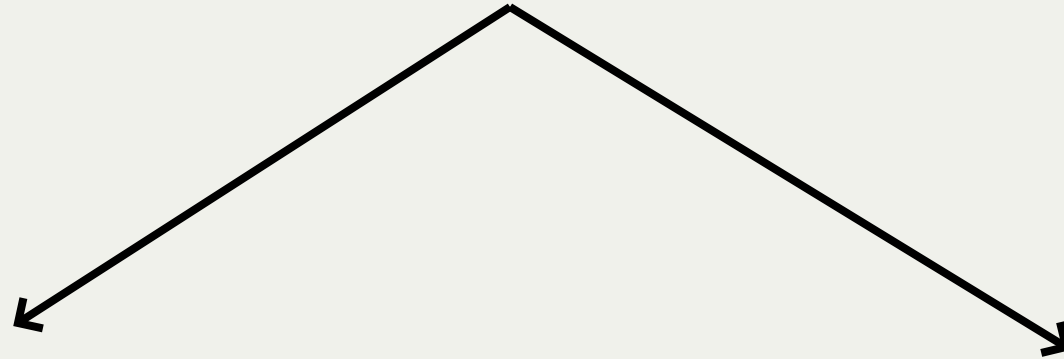


ML: any model
with parameters
learnt from the
data

Arthur Samuel, 1959



what is machine learning?



supervised learning

extract features and create models
that allow prediction where the
correct answer is known for a subset
of the data

unsupervised learning

identify features and create
models that allow to understand
structure in the data

what is machine learning?

- k-Nearest Neighbors
- Regression
- Support Vector Machines
- Neural networks
- Classification/Regression Trees

supervised learning

extract features and create models
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correct answer is known for a subset
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- clustering
- Principle Component Analysis
- Apriori (association rule)

unsupervised learning

identify features and create
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what is machine learning?

- k-Nearest Neighbors
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supervised learning

classification

prediction

feature selection

- clustering
- Principle Component Analysis
- Apriori (association rule)

unsupervised learning

understanding structure

organizing + compressing data

anomaly detection

dimensionality reduction

1

what is a model?

what is a model?

it's always a simplification

what is a model?

a *mathematical* representation of reality

In applying mathematics to subjects such as physics or statistics we make tentative assumptions about the real world which we know are false but which we believe may be useful nonetheless.

George Box, 1976

- no model is right
- some models are useful

what is a model?

why do we model?

1

[https://www.youtube.com/embed/Tk2v1UaTgmk?
enablejsapi=1](https://www.youtube.com/embed/Tk2v1UaTgmk?enablejsapi=1)

1. to understand

what is a model?

why do we model?

1

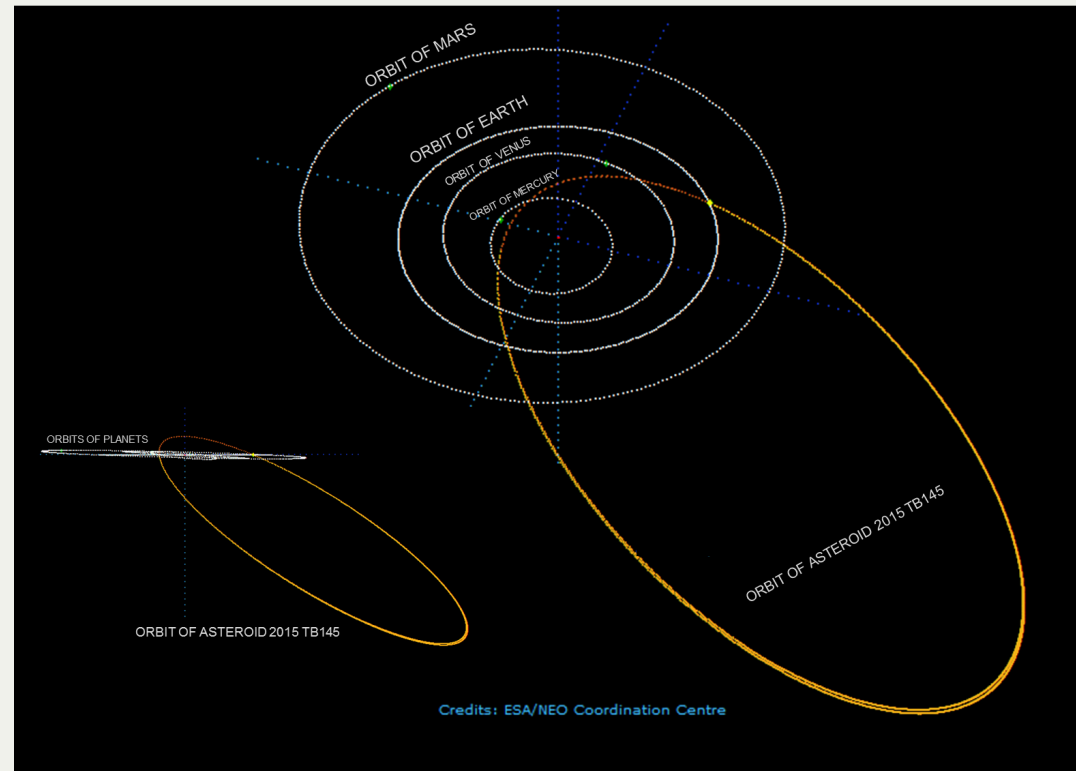
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1. to understand

$$h(t + t_0) = v_0 t - \frac{1}{2} g t^2$$

what is a model?

why do we model?

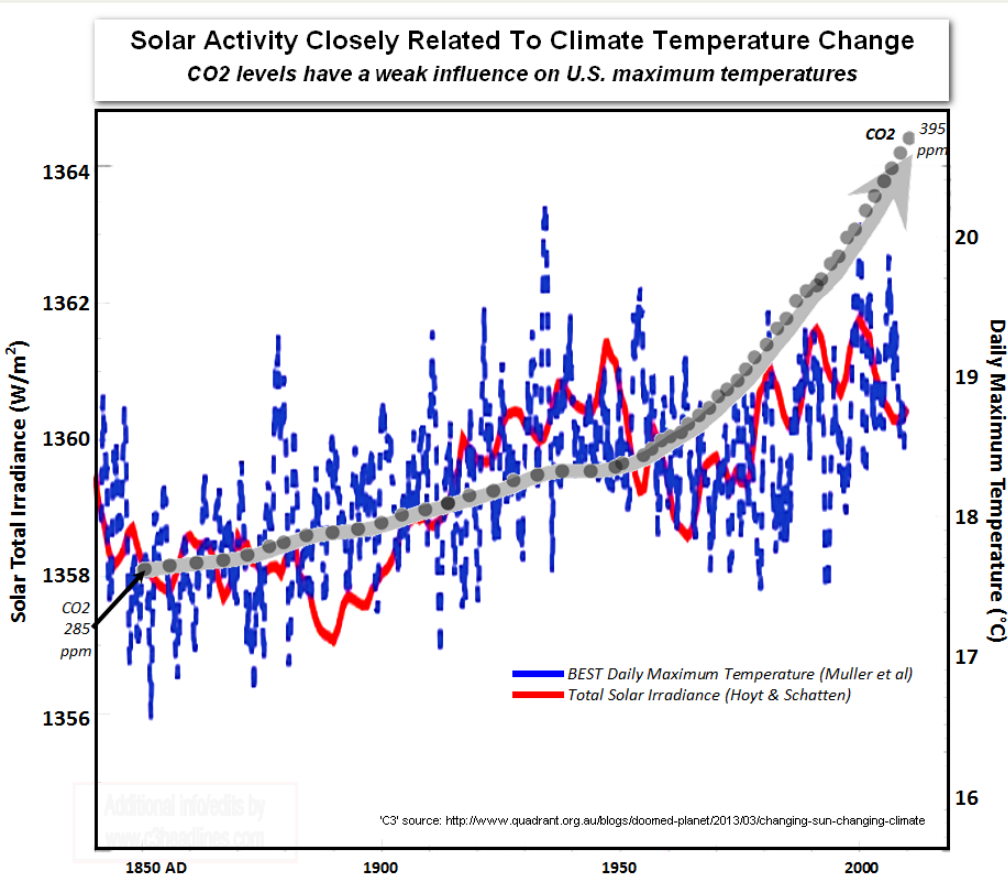


2. to predict

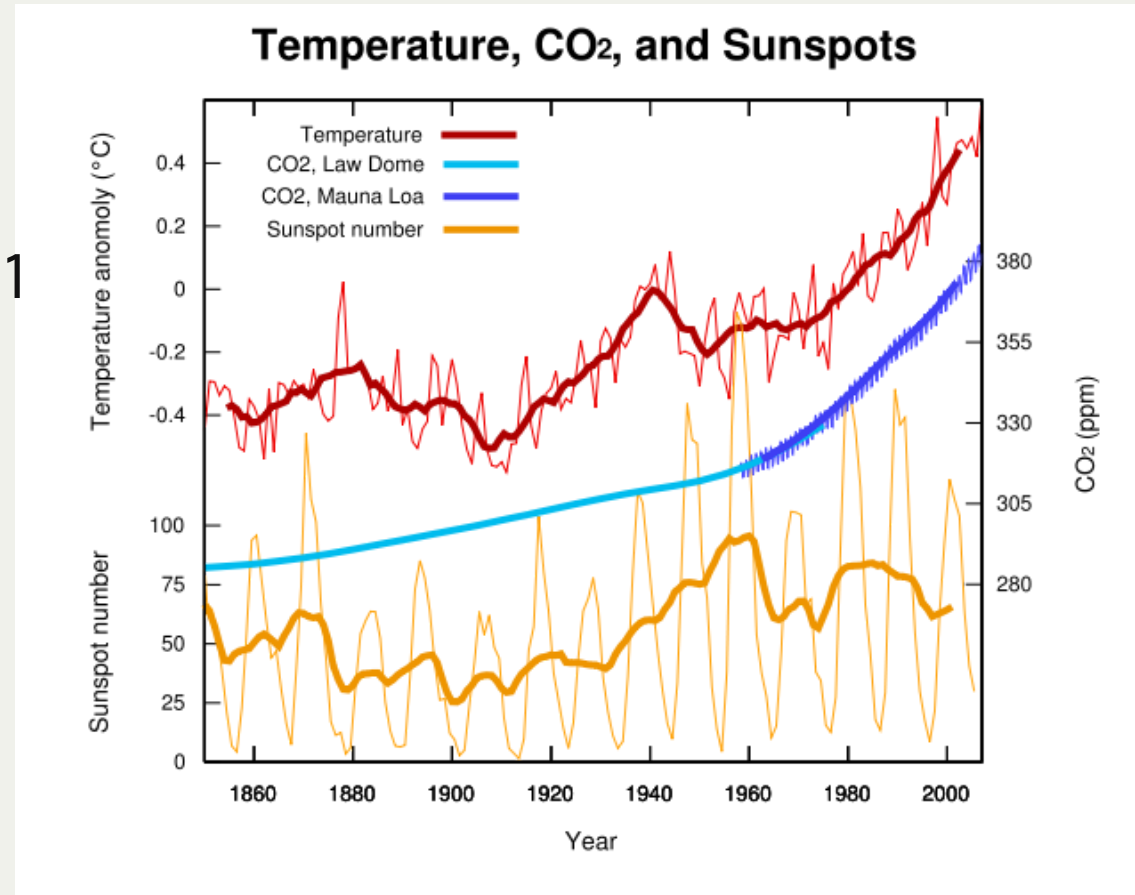
$$r(\nu) = \frac{a(1-e^2)}{1+e \cos(\nu)}$$

what is a model?

why do we model?



1



to understand + predict

what is a model?

the best way to think about it
in the ML context:

a model is a low dimensional
representation of a higher
dimensionality dataset

2

the principle of
parsimony

the princile of parsimony or Ockham's razor

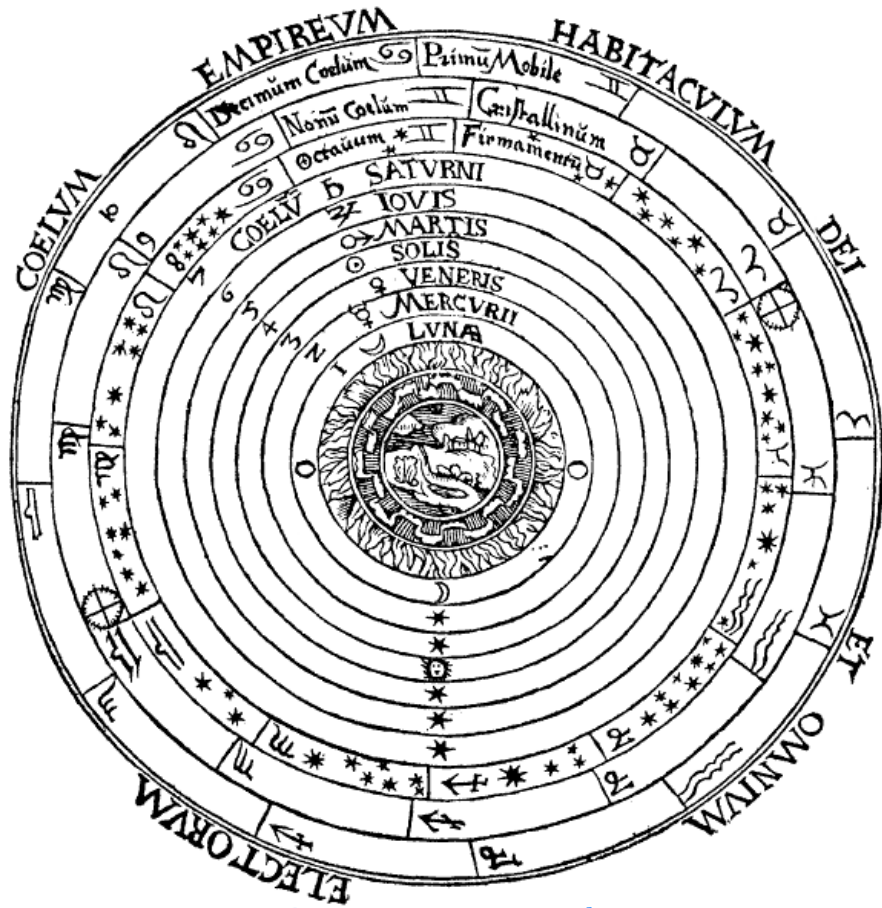
Pluralitas non est ponenda sine neccesitate

William of Ockham (logician and Franciscan friar) 1300ca
but probably to be attributed to [John Duns Scotus](#) (1265–1308)

“Complexity needs not to be postulated without a need for it”

the princile of parsimony

Schema huius præmissæ diuisionis Sphærarum.



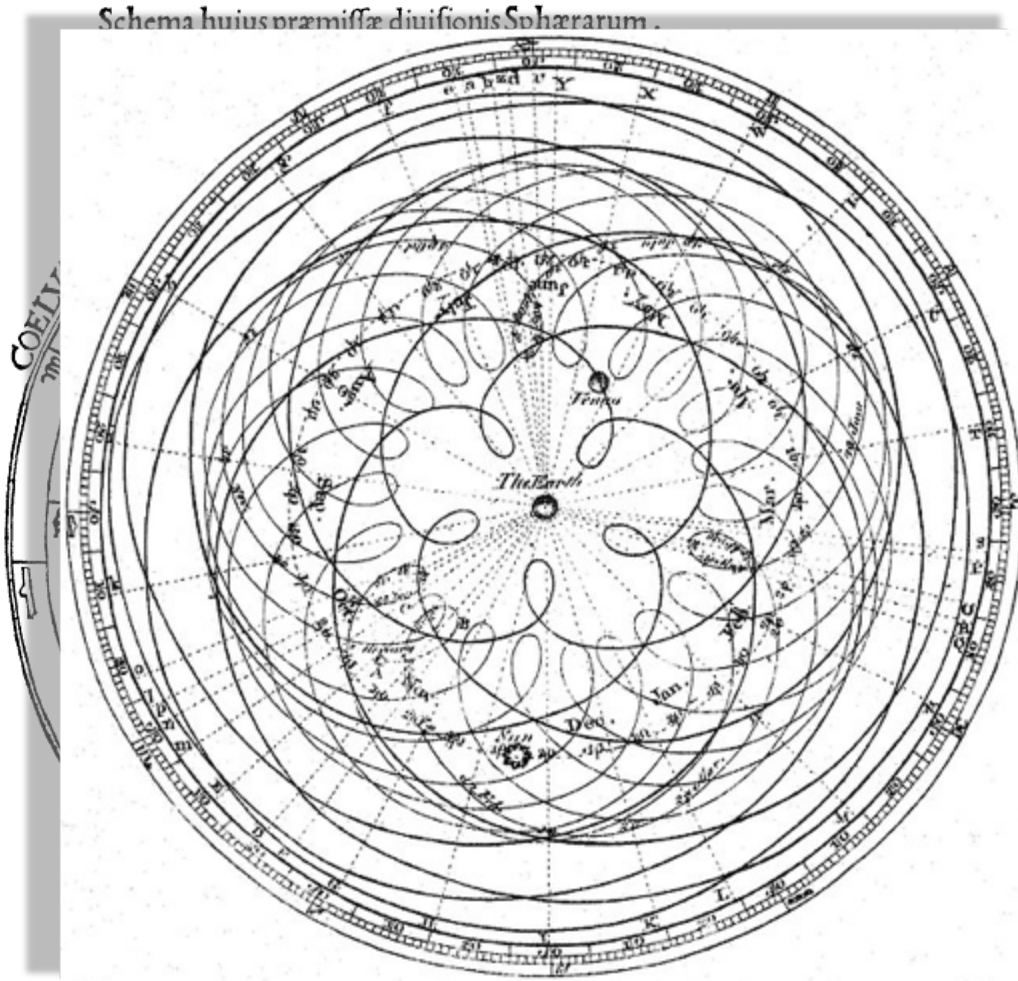
the earth is round,
and it orbits around the sun

Geocentric models are intuitive:
from our perspective we see the Sun
moving, while we stay still

Peter Apian, *Cosmographia*, Antwerp, 1524 from Edward Grant,
"Celestial Orbs in the Latin Middle Ages", *Isis*, Vol. 78, No. 2. (Jun., 1987).

the princple of parsimony

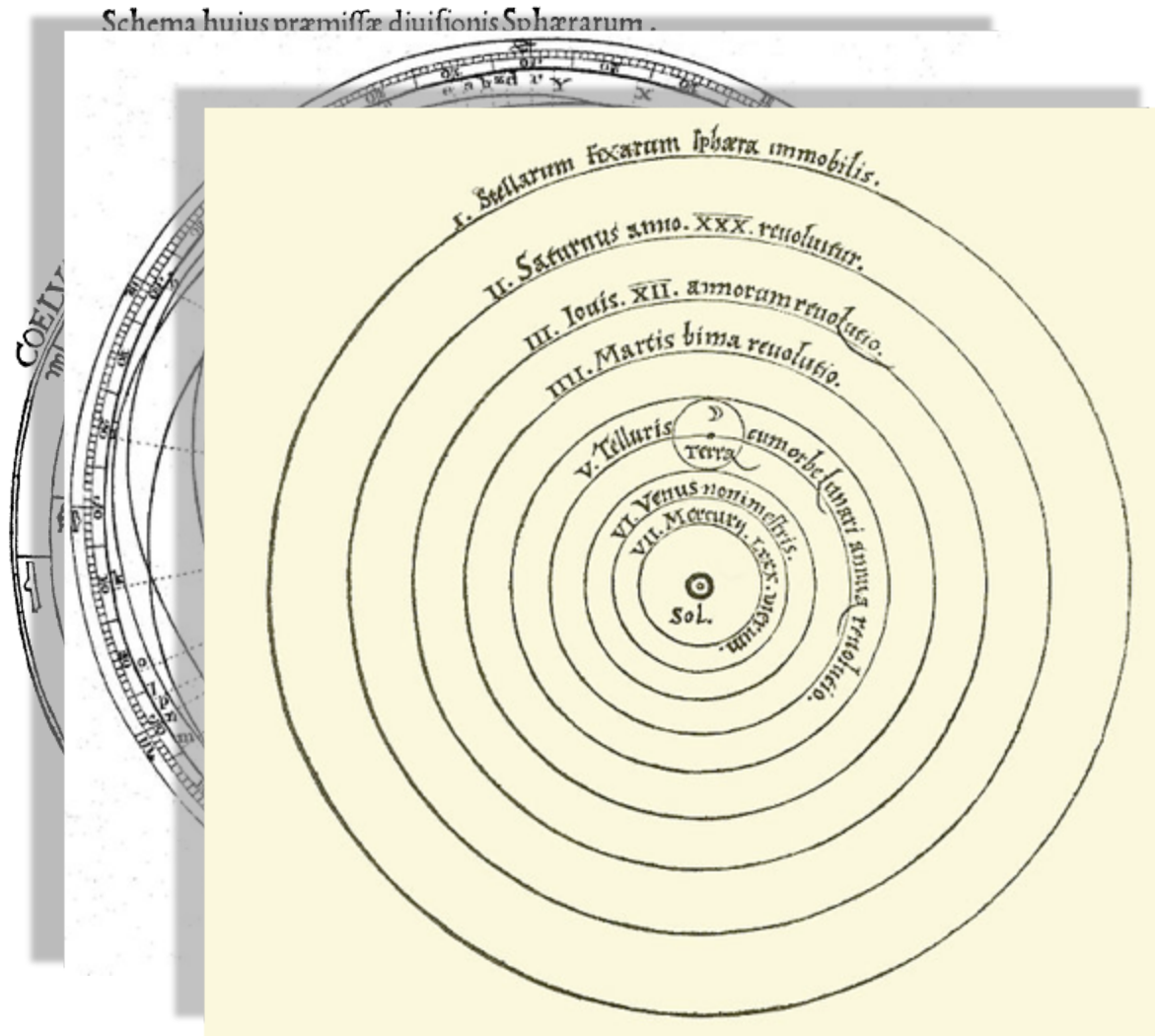
the earth is round,
and it orbits around the sun



As observations improve
this model can no longer fit the data!
not easily anyways...

Encyclopaedia Britannica 1st Edition
Dr Long's copy of Cassini, 1777

the princple of parsimony



the earth is round,
~~and it orbits around the sun~~

A new model that is much simpler fit the
data just as well
(perhaps though only until better data
comes...)

Heliocentric model from Nicolaus Copernicus' *De revolutionibus orbium coelestium*.

the princile of parsimony or Ockham's razor

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"Complexity needs not to be postulated without a need for it"

"Between 2 theories that perform similarly choose the *simpler one*"

the princile of parsimony or Ockham's razor

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"Complexity needs not to be postulated without a need for it"

"Between 2 theories that perform similarly choose the *one with fewer parameters*"

the princile of parsimony

Science and Statistics George E. P. Box (1976)

Journal of the American Statistical Association, Vol. 71, No. 356, pp. 791-799.

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

Since all models are wrong the scientist must be alert to what is importantly wrong.

3

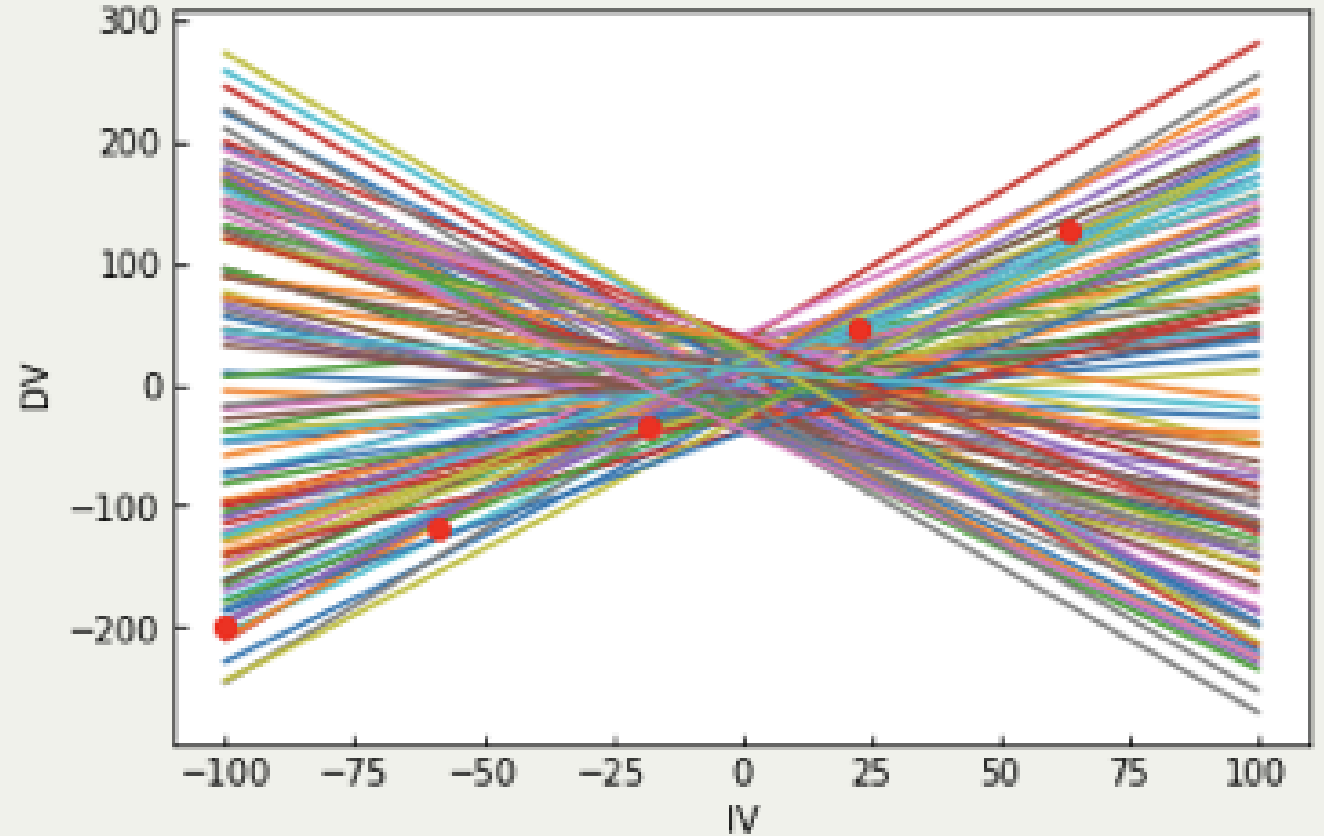
fitting a simple
model to data

Many packages do it in python!

- numpy (e.g. `np.polyfit`)
- scipy (e.g. `sp.optimize.curve_fit`)
- sklearn.linear_model.LinearRegression()

but what are
they doing??

line model: $ax+b$

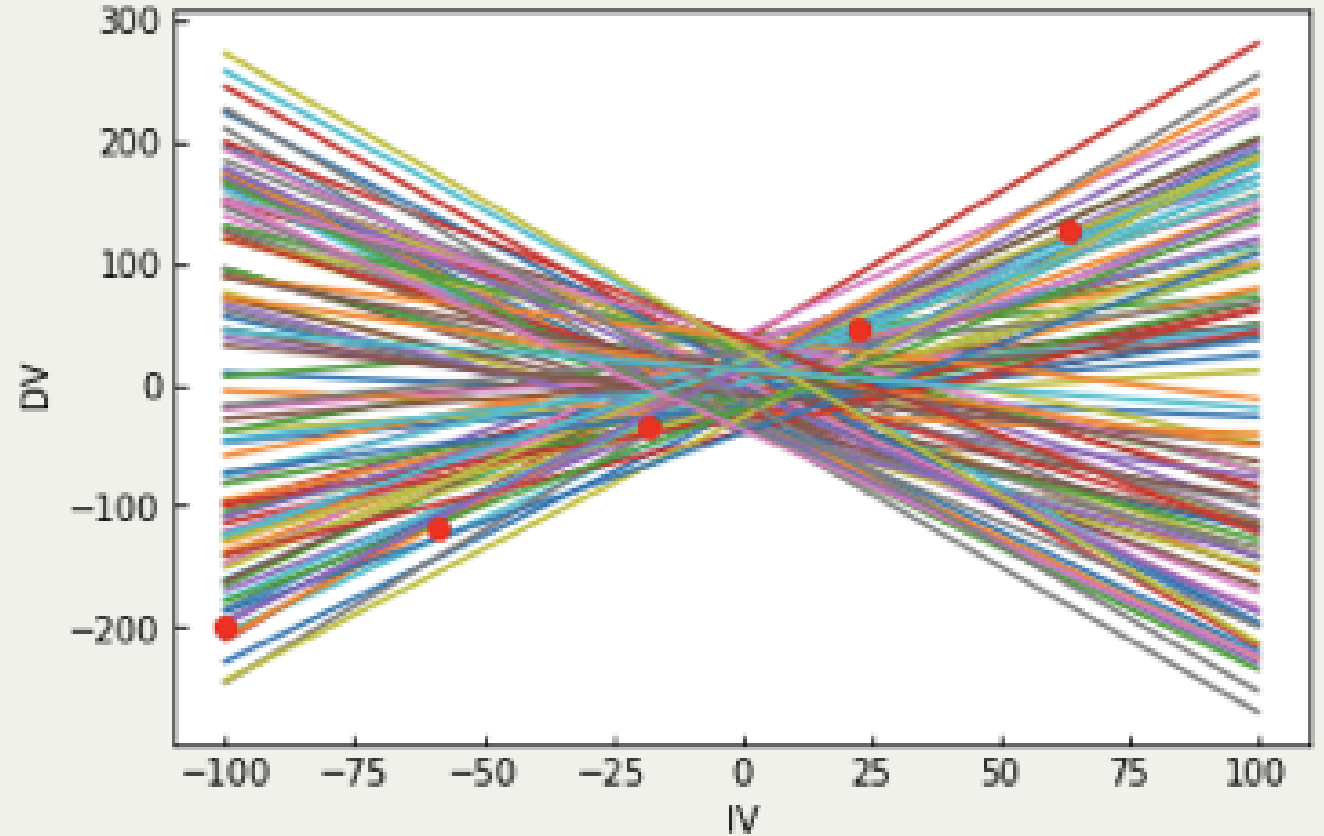


1

choose your model :

choose a mathematical formula to represent
the behavior you see/expect in the data

line model: $ax+b$



2

choose an objective function :

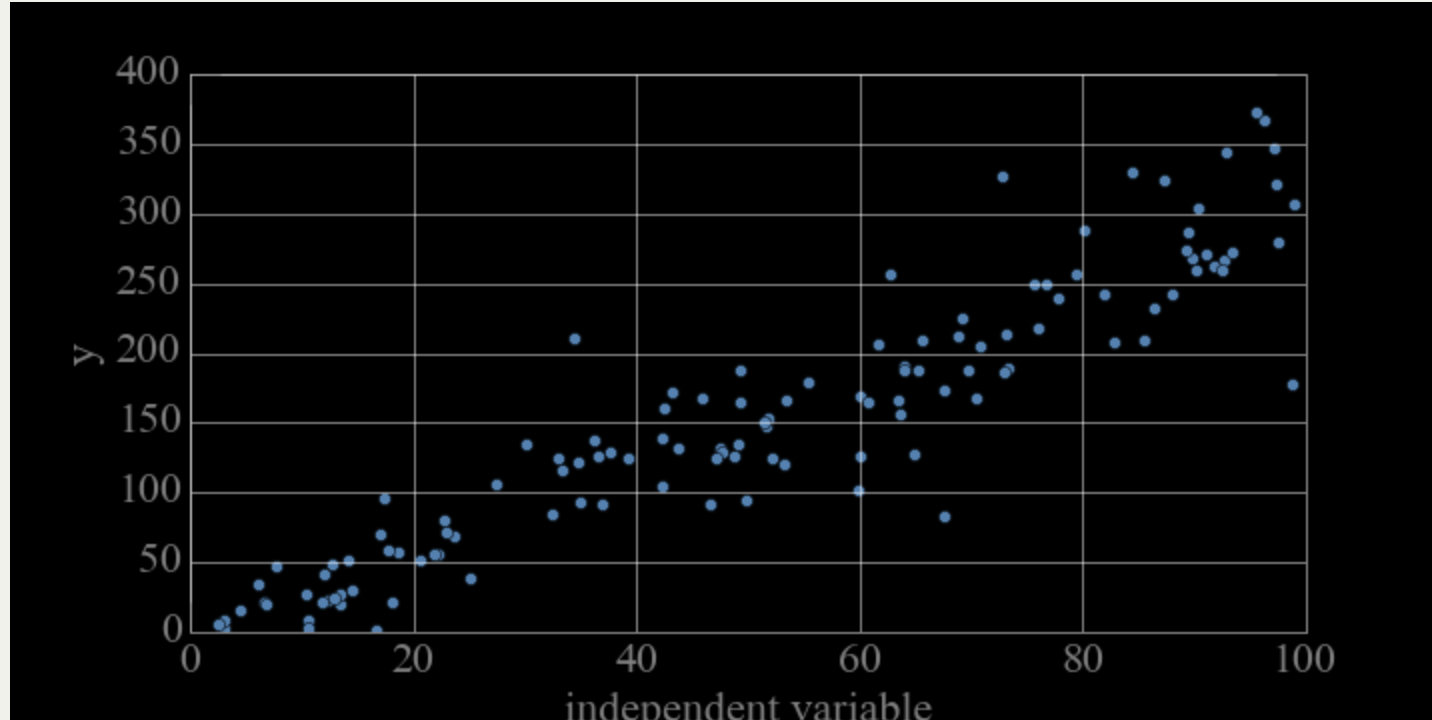
you need a plan to choose the parameters of
the model: to "optimize" the model.
You need to choose something to be
MINIMIZED or MAXIMIZED

objective function:

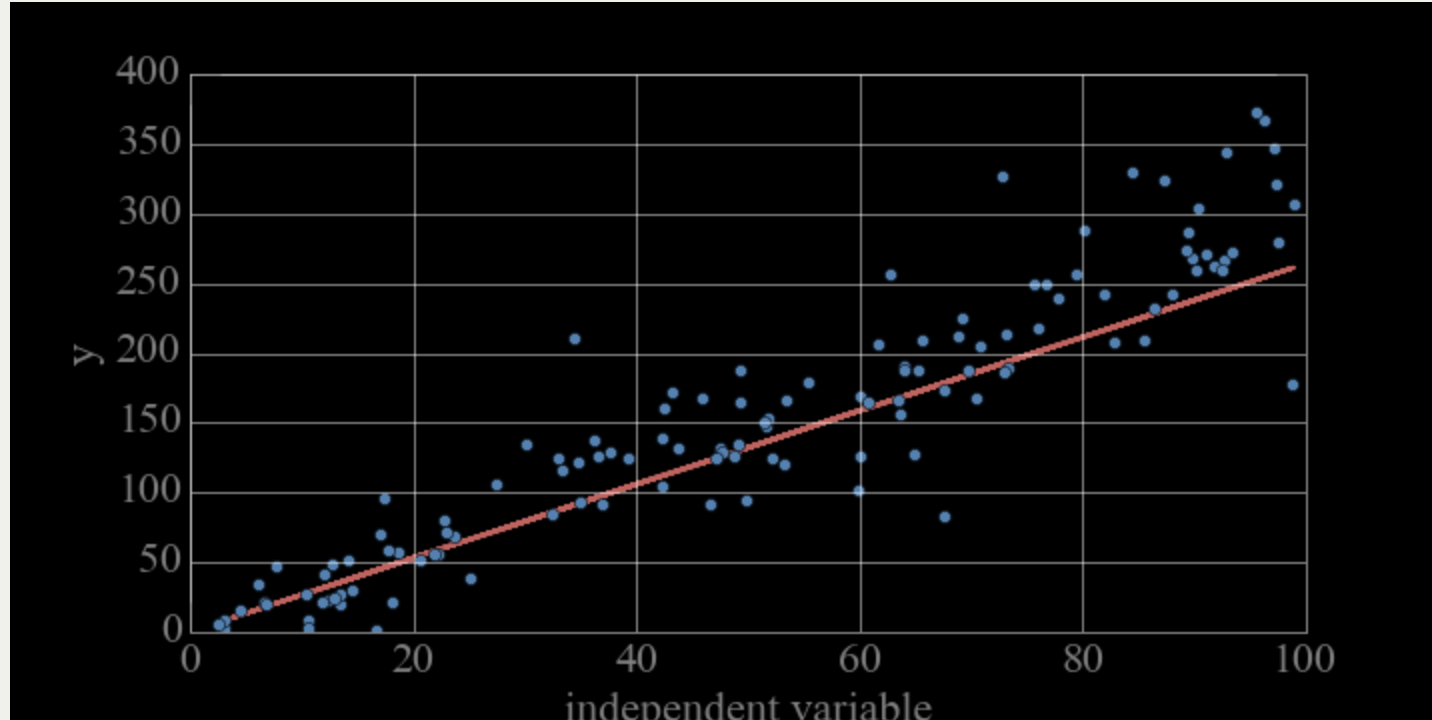
what you want to optimize for

In principle, there are many choices for objective function. But the only procedure that is truly justified—in the sense that it leads to interpretable probabilistic inference, is to make a generative model for the data.

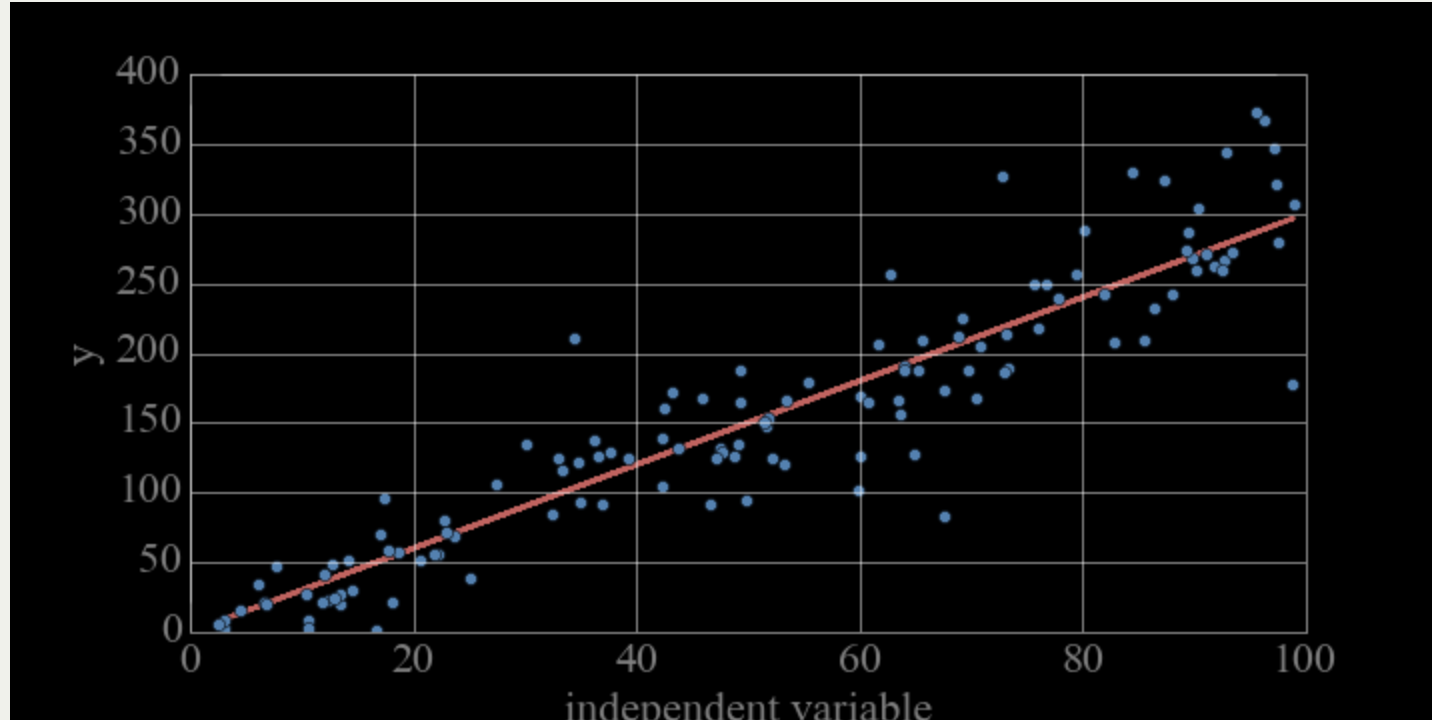
objective function:



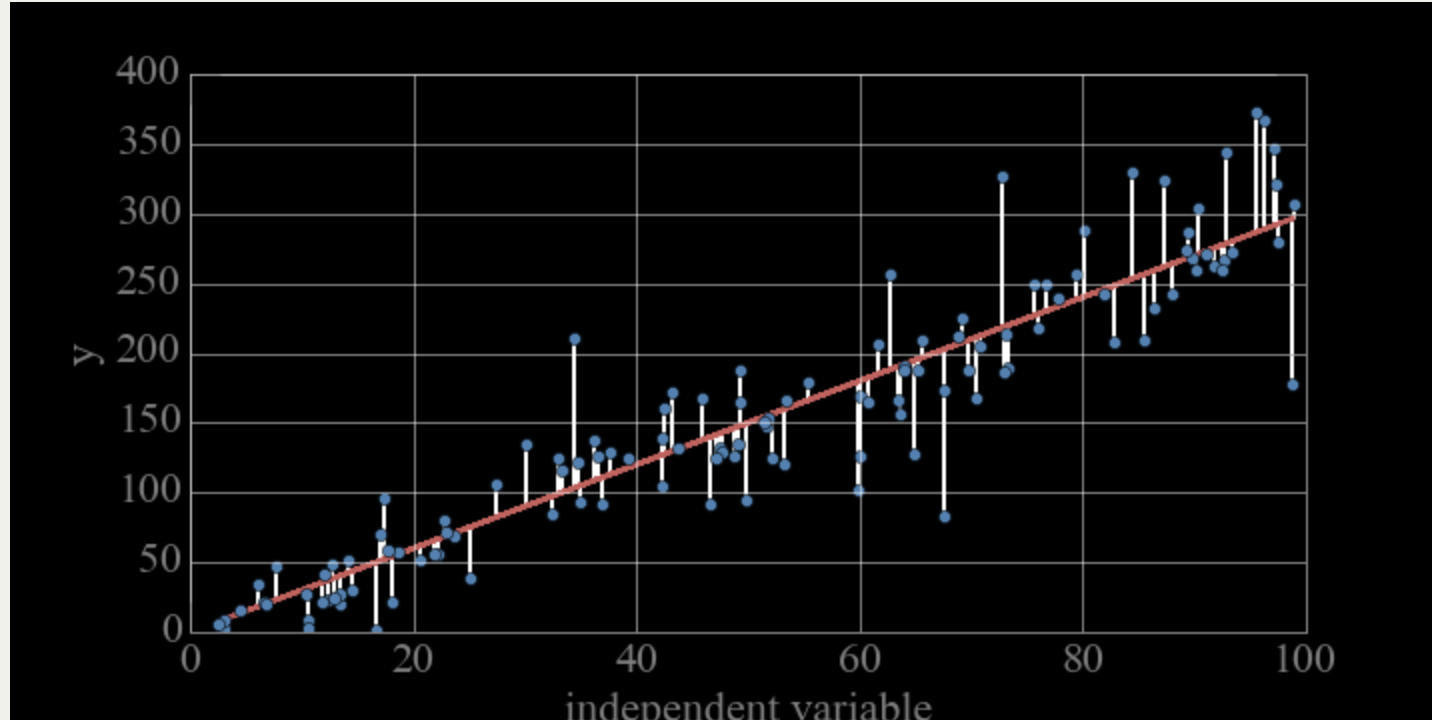
objective function:



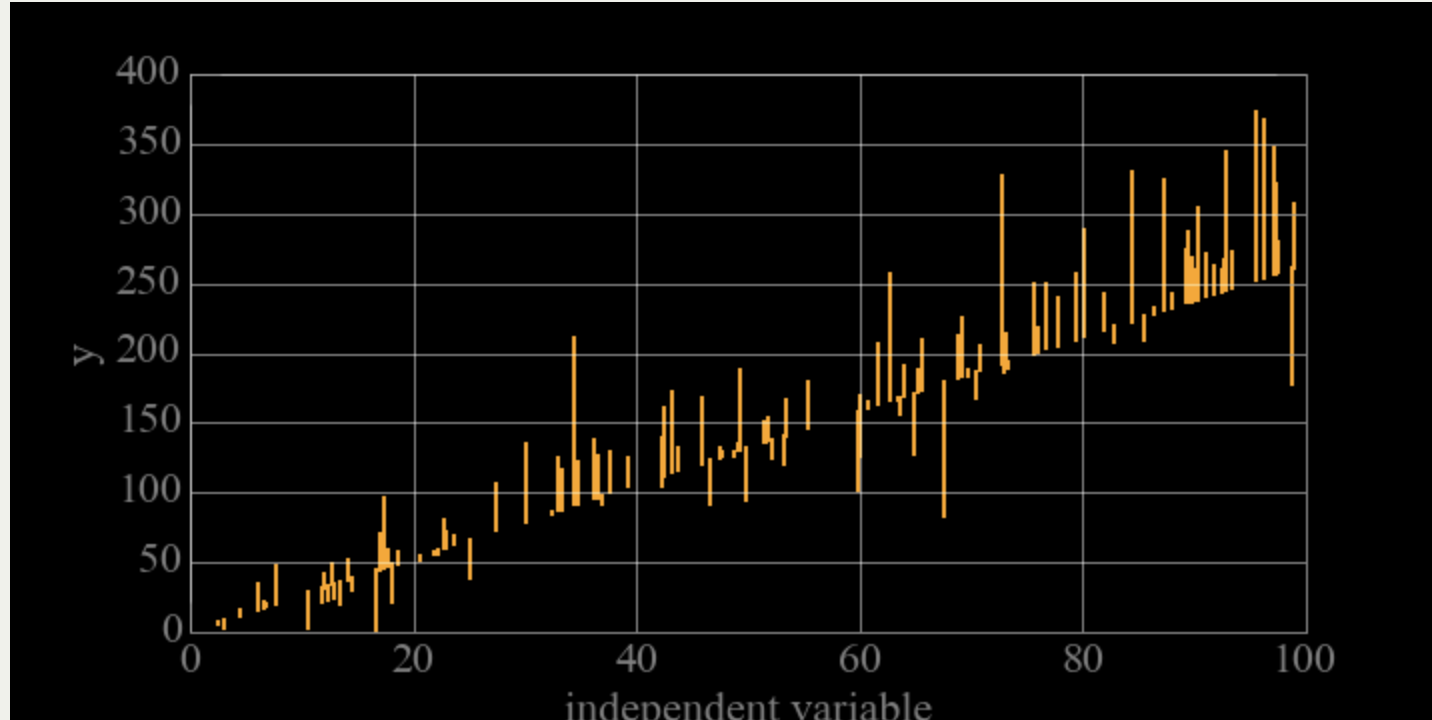
objective function:



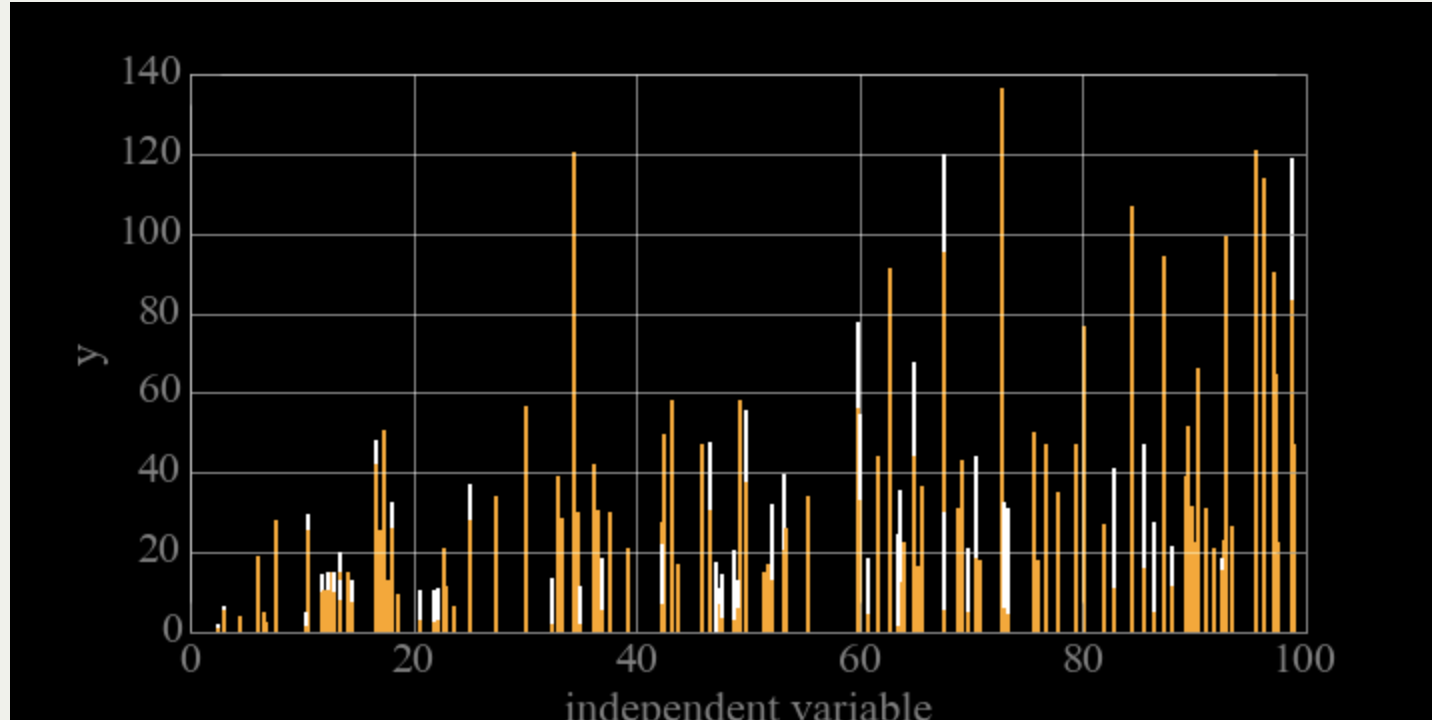
objective function:



objective function:



objective function:



$$R^2 = 1 - \frac{\sum_i (y_i - f_i)^2}{\sum_i (y_i - \bar{y})^2}$$

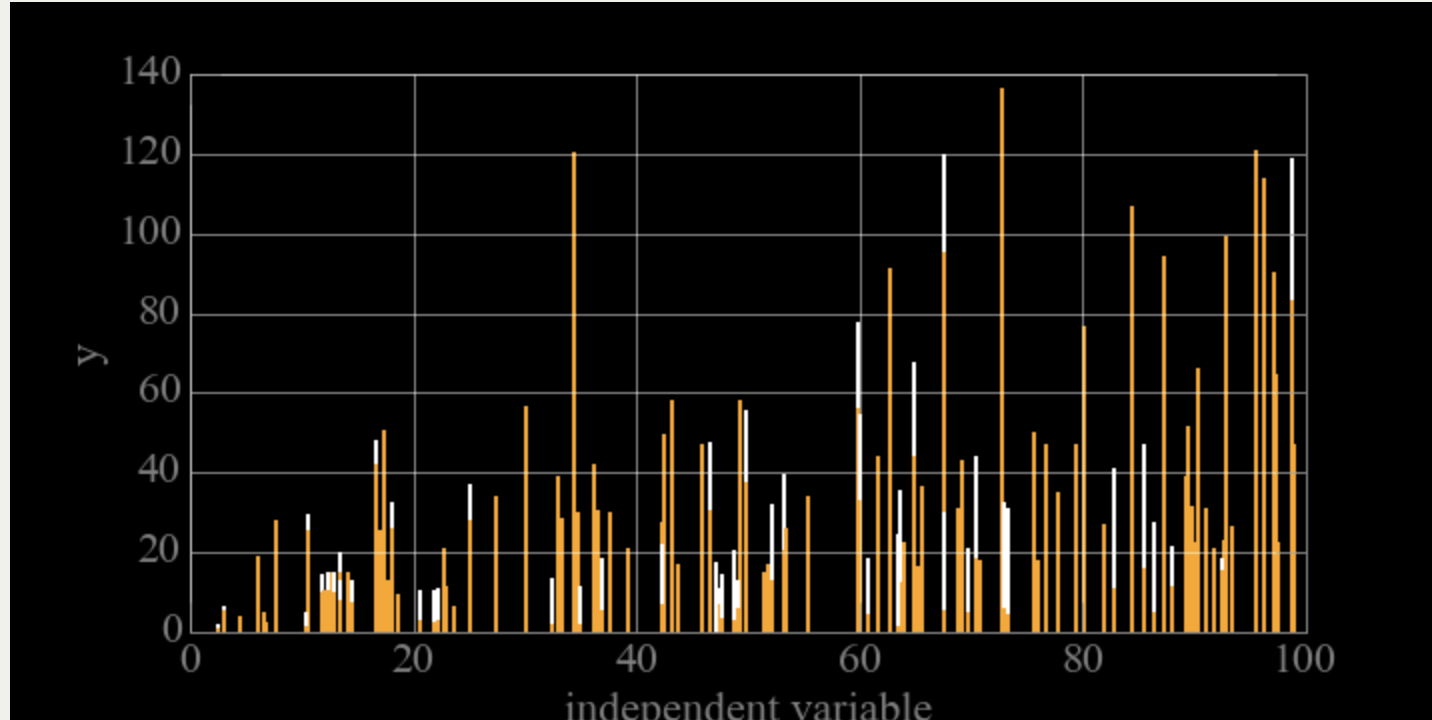
y_i : i-th observation

x_i : i-th measurement "location"

s_i : i-th uncertainty

Fit model parameters \iff minimize the Sum of residuals squared

objective function:



$$R^2 = 1 - \frac{\sum_i (y_i - f_i)^2}{\sum_i (y_i - \bar{y})^2}$$

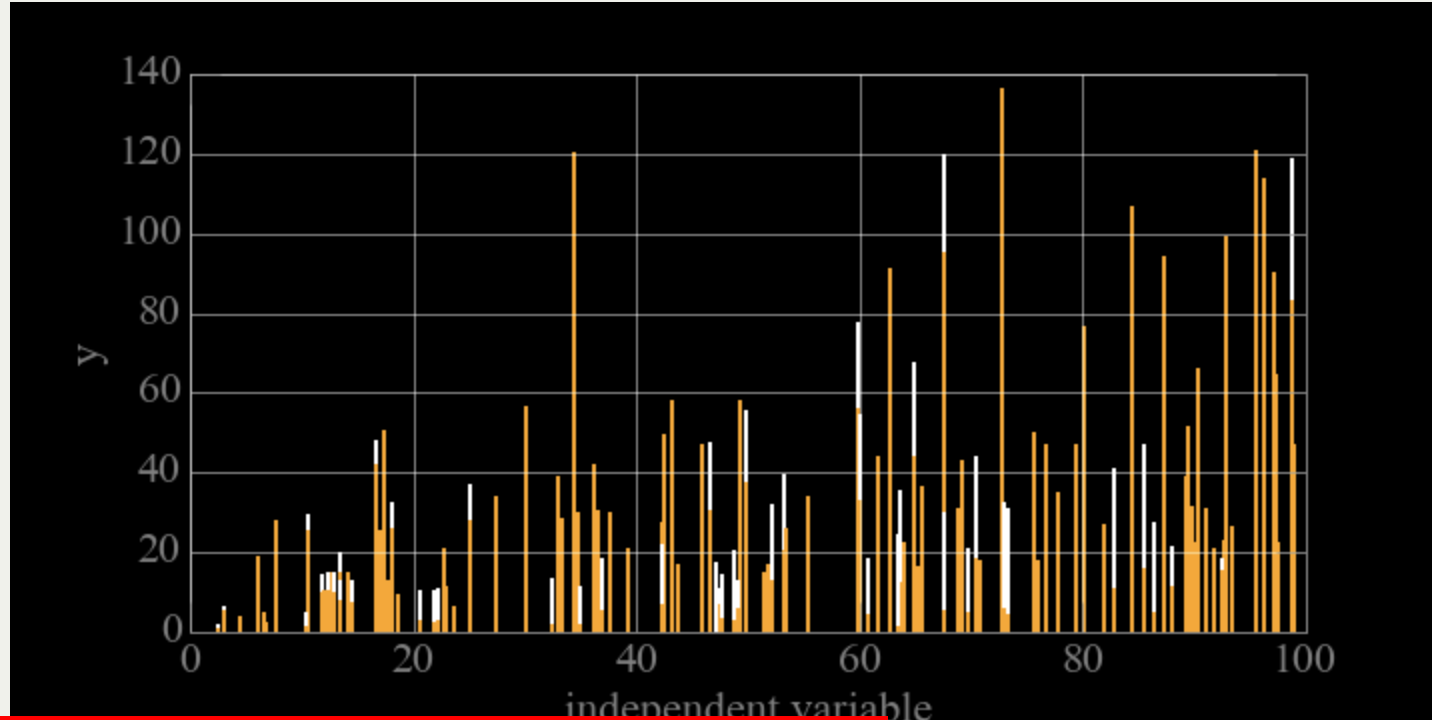
y_i : i-th observation

f_i : i-th prediction

s_i : i-th uncertainty

Fit model parameters \iff minimize the Sum of residuals squared

objective function:



if you have
uncertainties

(almost always in
observational and
experimental
physics)

$$\chi^2 = \sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}$$

y_i : i-th observation

x_i : i-th measurement "location"

σ_i : i-th uncertainty

Fit model parameters \Leftrightarrow minimize the Sum of residuals squared

objective function:

what you want to optimize for

homoscedastic :

the uncertainty is the same for all data points

heteroscedastic :

the uncertainty different for each datapoint

(almost always the case in physics!)

$$\chi^2 = \sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}$$

yi: i-th observation

xi: i-th measurement "location"

sigma_i: i-th uncertainty

Fit model parameters \iff minimize the Sum of residuals squared

objective function:

what you want to optimize for

homoscedastic :

the uncertainty is the same for all data points

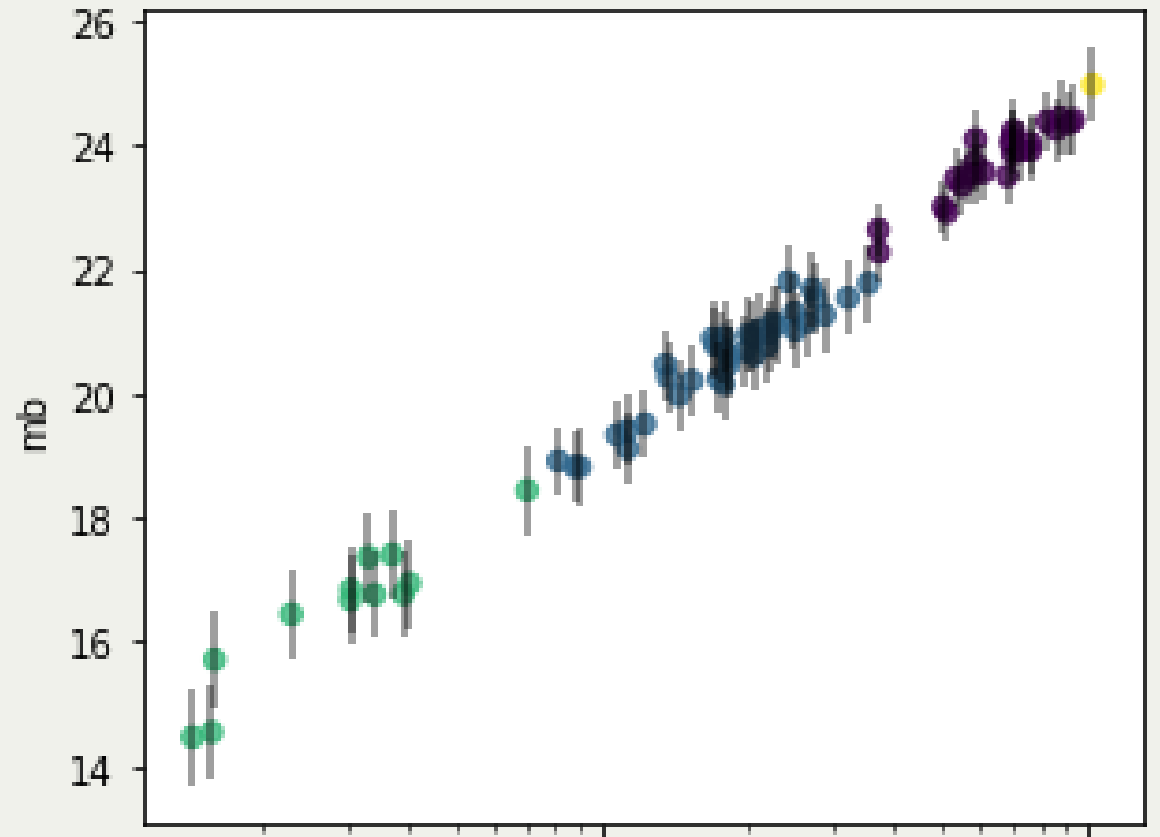
heteroscedastic :

the uncertainty different for each datapoint

(almost always the case in physics!)

datapoints have different uncertainty

(almost always in physics)



objective function:

what you want to optimize for

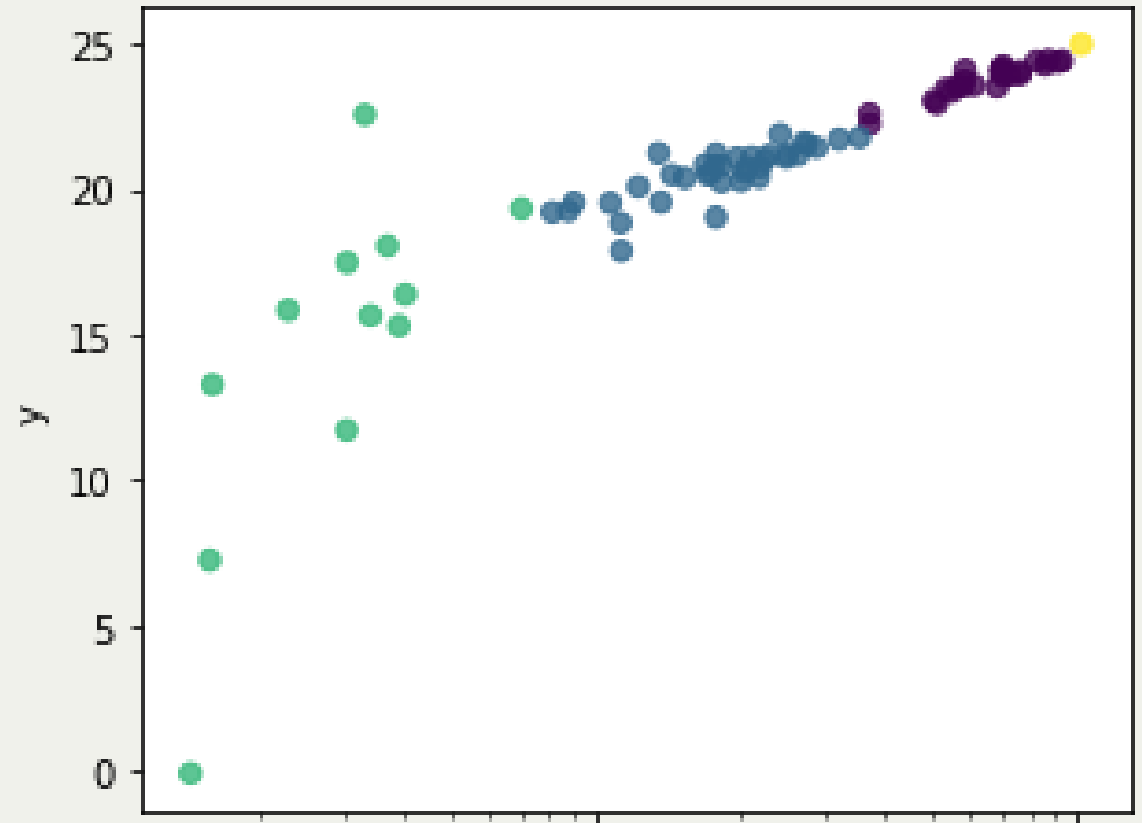
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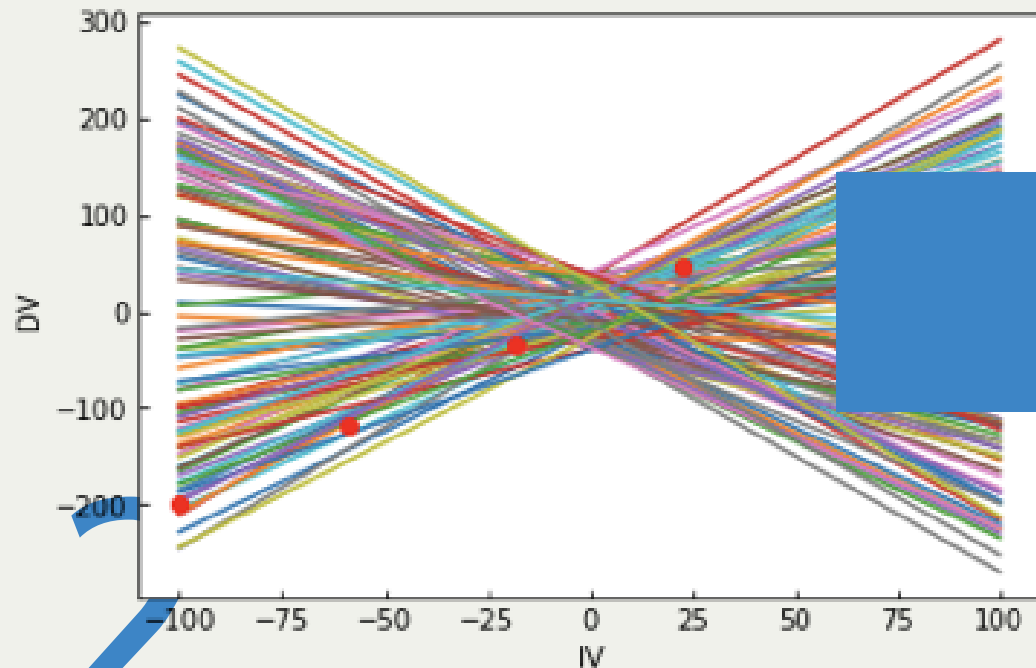
heteroscedastic:

the uncertainty different for each datapoint
(almost always the case in physics!)

scatter **dependent on exogenous variable**
(very difficult problem not well studied in
statistics - very common in physics!)

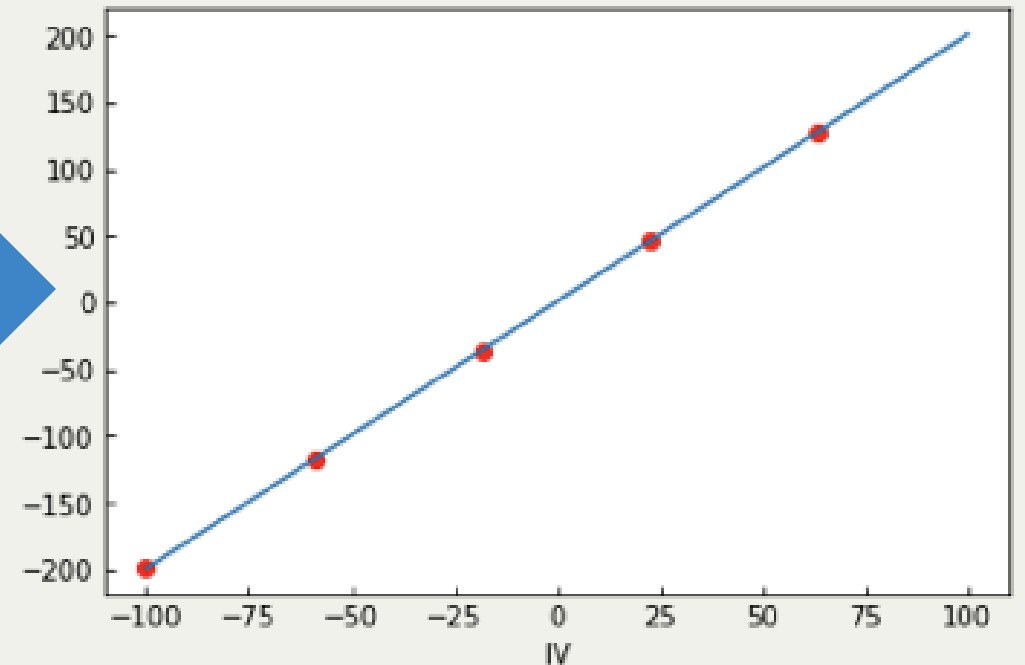


a line is a family of models



line model: $ax+b$

a line with set parameters is a models



choose an objective function :

you need a plan to choose the parameters of
the model: to "optimize" the model.
You need to choose something to be
MINIMIZED or MAXIMIZED

line model: $ax+b$

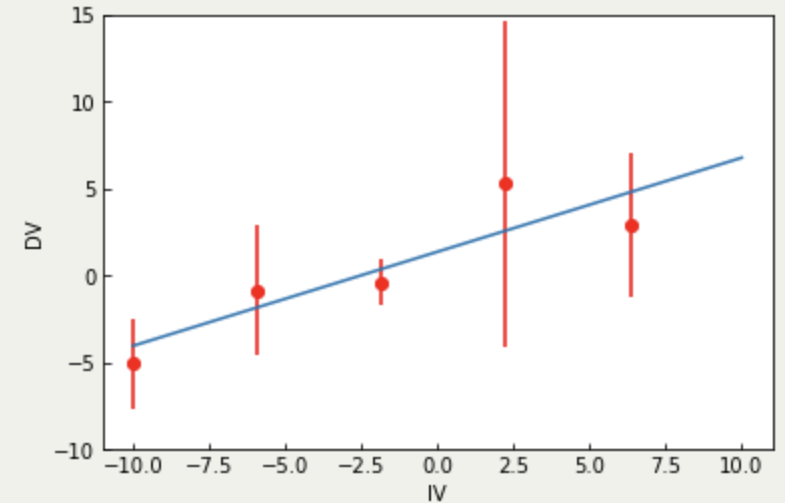
$$\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2} \sim \chi^2(dof = DOF)$$

i.e. the χ^2 (the quantity above)

follows a χ^2 distribution with degrees of freedom equal to the number of degrees of freedom in the problem (generally $N_{\text{datapoints}} - N_{\text{parameters}}$)

3

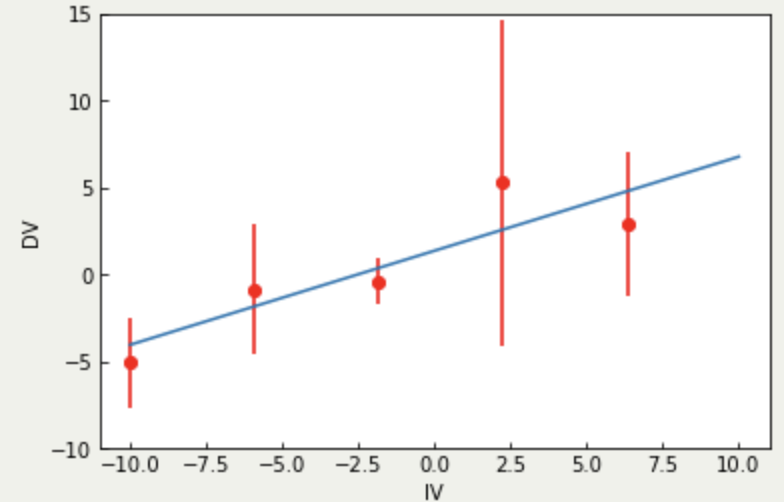
evaluate the quality of your model
again: many options!



line model: $ax+b$

$$\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2} \sim \chi^2(dof = DOF)$$

$$\frac{\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}}{DOF} \sim \chi^2(dof = 1)$$



i.e. the "reduced χ^2 " (χ^2/DOF) follows a χ^2 distribution with 1 degree of freedom

The expectation value (mean) of such a distribution is 1

evaluate the quality of your model
again: many options!

If my model is good I should find

$$\chi^2 \sim 1$$

$$\chi_{reduced}^2 = \frac{\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}}{DOF} \sim 1$$

line model: $ax+b$

$$\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2} \sim \chi^2(dof = DOF)$$

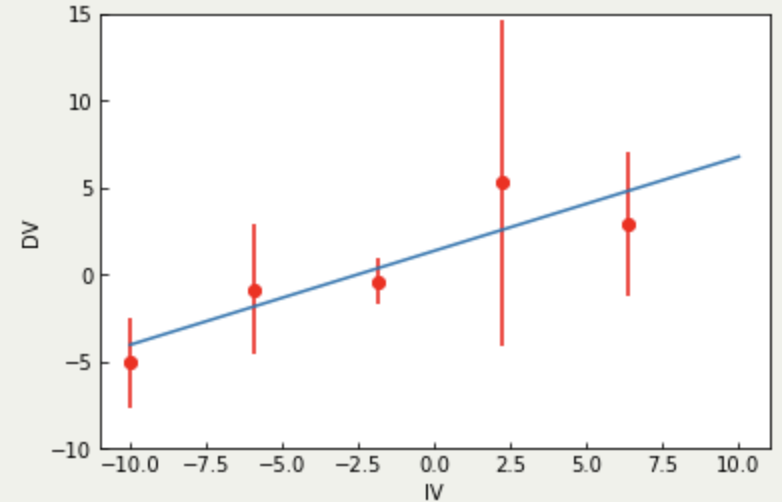
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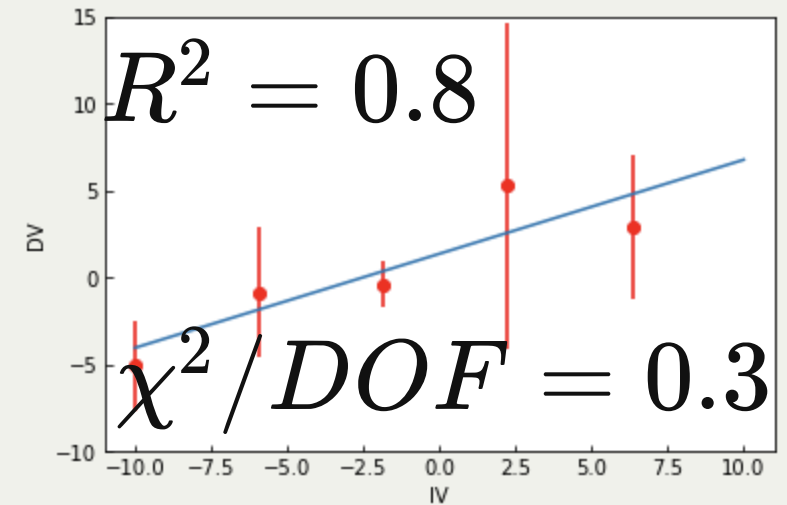
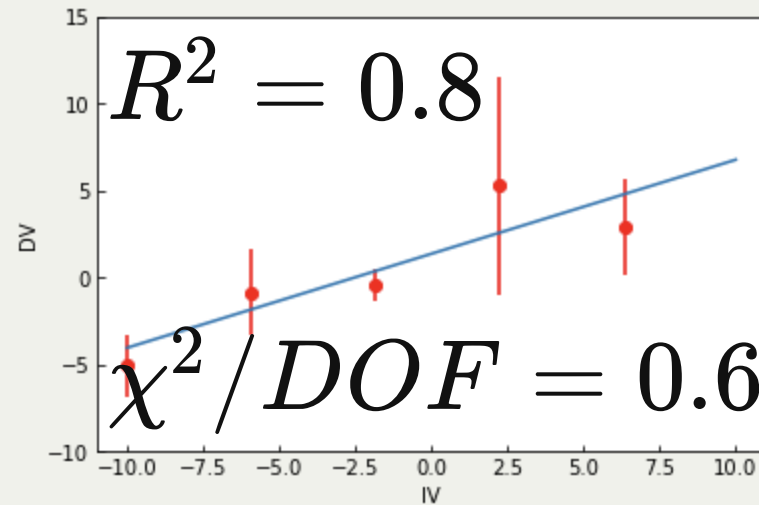
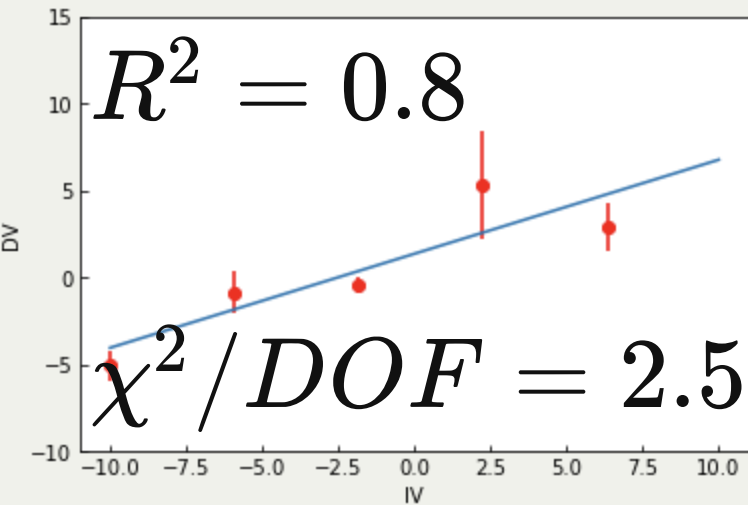


If my model is good I should find

$$\chi^2 \sim 1$$

$$\chi_{reduced}^2 = \frac{\sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}}{DOF} \sim 1$$

line model: $ax+b$



3

evaluate the quality of your model
again: many options!

the χ^2 tells you how well your model fits the data given how confident you are in the data (how much you believe they are correct)

The R^2 just tells you about how well the model fits the data

Data analysis recipes: Fitting a model to data*

David W. Hogg

Center for Cosmology and Particle Physics, Department of Physics, New York University
Max-Planck-Institut für Astronomie, Heidelberg

Jo Bovy

Center for Cosmology and Particle Physics, Department of Physics, New York University

Dustin Lang

Department of Computer Science, University of Toronto
Princeton University Observatory

In the case of the straight line fit in the presence of known, Gaussian uncertainties in one dimension, one can create this generative model as follows: Imagine that the data *really do* come from a line of the form $y = f(x) = m x + b$, and that the only reason that any data point deviates from this perfect, narrow, straight line is that to each of the true y values a small y -direction offset has been added, where that offset was drawn from a Gaussian distribution of zero mean and known variance σ_y^2 . In this model, given an independent position x_i , an uncertainty σ_{yi} , a slope m , and an intercept b , the frequency distribution $p(y_i|x_i, \sigma_{yi}, m, b)$ for y_i is

$$p(y_i|x_i, \sigma_{yi}, m, b) = \frac{1}{\sqrt{2\pi\sigma_{yi}^2}} \exp\left(-\frac{[y_i - m x_i - b]^2}{2\sigma_{yi}^2}\right) \quad , \quad (9)$$

where this gives the expected frequency (in a hypothetical set of repeated experiments¹³) of getting a value in the infinitesimal range $[y_i, y_i + dy]$ per unit dy .

The generative model provides us with a natural, justified, scalar objective: We seek the line (parameters m and b) that maximize the probability of the observed data given the model or (in standard parlance) the *likelihood of the parameters*.¹⁴ In our generative model the data points are independently drawn (implicitly), so the likelihood \mathcal{L} is the product of conditional probabilities

$$\mathcal{L} = \prod_{i=1}^N p(y_i|x_i, \sigma_{yi}, m, b) \quad . \quad (10)$$

likelihood, probability, and objective functions

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, m, b)$$

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, \sigma_i, m, b)$$

$$p(y_i) = \frac{1}{\sigma_i \sqrt{2\pi}} \exp - \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}$$

$$\log a \cdot b = \log a + \log b$$

$$\ln L(m, b|\vec{y}) = \ln \prod_i^N \frac{1}{\sigma_i \sqrt{2\pi}} \exp - \frac{y_i - (mx_i + b)}{2\sigma_i^2}$$

likelihood, probability, and objective functions

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, m, b)$$

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, \sigma_i, m, b)$$

$$p(y_i) = \frac{1}{\sigma_i \sqrt{2\pi}} \exp - \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}$$

$$x^a \cdot x^b = x^{(a+b)}$$

$$\ln L(m, b|\vec{y}) = \ln \prod \frac{1}{\sigma_i \sqrt{2\pi}} + \ln \left(\prod_i^N e^{-\frac{y_i - (mx_i + b)}{2\sigma_i^2}} \right)$$

likelihood, probability, and objective functions

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, m, b)$$

$$L(m, b|\vec{y}) = \prod_i^N p_i(y_i|x_i, \sigma_i, m, b)$$

$$p(y_i) = \frac{1}{\sigma_i \sqrt{2\pi}} \exp - \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2}$$

$$\ln L(m, b|\vec{y}) = \ln \prod \frac{1}{\sigma_i \sqrt{2\pi}} + \ln \left(e^{-\sum_i^N \frac{y_i - (mx_i + b)}{2\sigma_i^2}} \right)$$

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σ_i not part of the model

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$$\ln L(m, b|\vec{y}) = K - \sum \frac{(y_i - (mx_i + b))^2}{2\sigma_i^2} = K - \frac{1}{2} \chi^2$$

Science and Statistics

GEORGE E. P. BOX*

its long,
but you have 2 weeks!

Aspects of scientific method are discussed: In particular, its representation as a motivated iteration in which, in succession, practice confronts theory, and theory, practice. Rapid progress requires sufficient flexibility to profit from such confrontations, and the ability to devise parsimonious but effective models, to worry selectively about model inadequacies and to employ mathematics skillfully but appropriately. The development of statistical methods at Rothamsted Experimental Station by Sir Ronald Fisher is used to illustrate these themes.

1. INTRODUCTION

In 1952, when presenting R.A. Fisher for the Honorary degree of Doctor of Science at the University of Chicago, W. Allen Wallis described him in these words.

He has made contributions to many areas of science; among them are agronomy, anthropology, astronomy, bacteriology, botany, economics, forestry, meteorology, psychology, public health, and—above all—genetics, in which he is recognized as one of the leaders. Out of this varied scientific research and his skill in mathematics, he has evolved systematic principles for

on the one hand, nor by the undirected accumulation of practical facts on the other, but rather by a motivated *iteration* between theory and practice such as is illustrated in Figure A(1).

A. The Advancement of Learning

A(1) An Iteration Between Theory and Practice

A(2) A Feedback Loop

