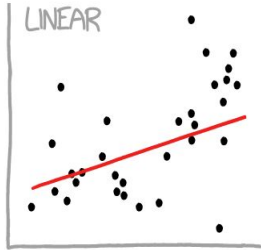


# Goodness of fit

## Badness of fit?

Lydia Brenner

# CURVE-FITTING METHODS AND THE MESSAGES THEY SEND



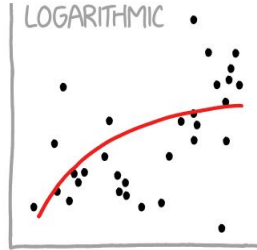
LINEAR

"HEY, I DID A REGRESSION."



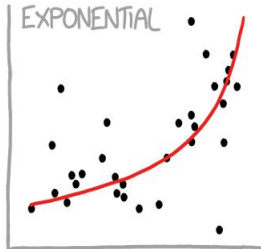
QUADRATIC

"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."



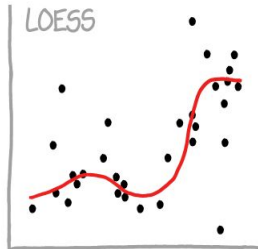
LOGARITHMIC

"LOOK, IT'S TAPERING OFF!"



EXPONENTIAL

"LOOK, IT'S GROWING UNCONTROLLABLY!"



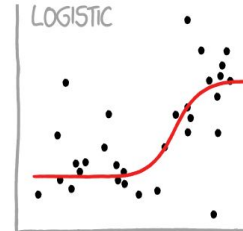
LOESS

"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."



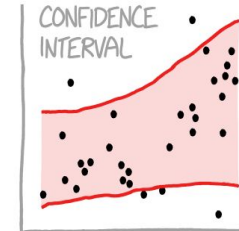
LINEAR,  
NO SLOPE

"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."



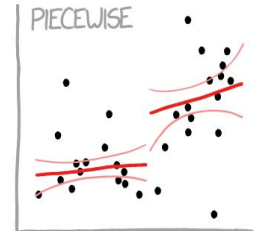
LOGISTIC

"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."



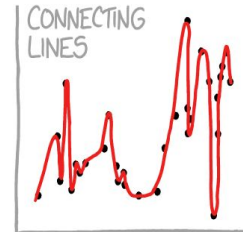
CONFIDENCE INTERVAL

"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."



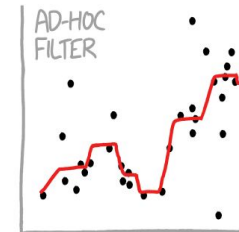
PIECEWISE

"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."



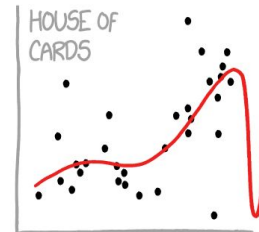
CONNECTING LINES

"I CLICKED 'SMOOTH LINES' IN EXCEL."



AD-HOC FILTER

"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"



HOUSE OF CARDS

"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE- WAIT NO NO DON'T EXTEND IT AAAAAA!!!"

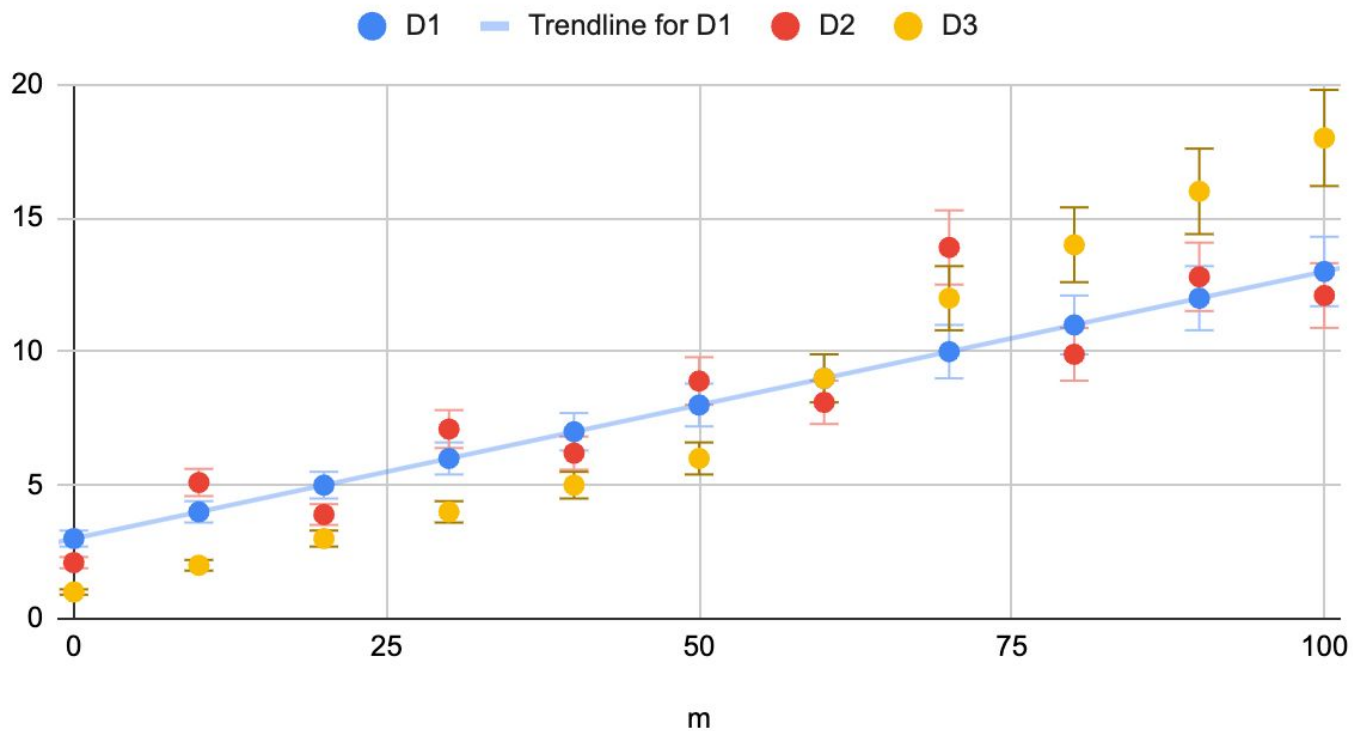
## The question: How well can I fit?

Basic question: how well does my hypothesis describe the data?

- Would like a clearly understandable number
- Would like it to match with visual input
- Would like it to have a meaningful interpretation in terms of the likelihood

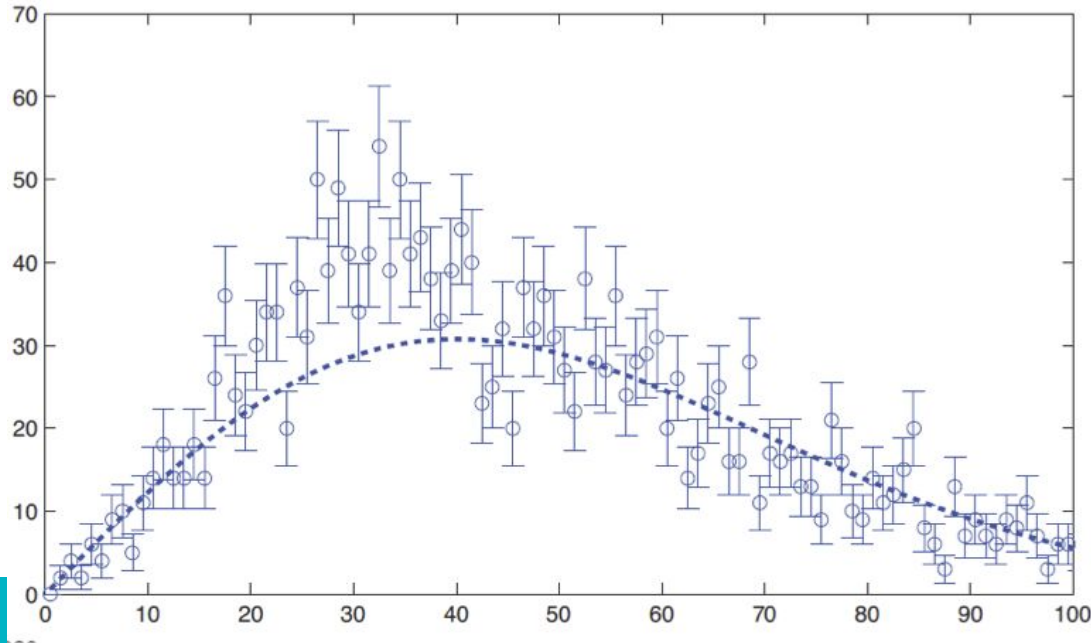
# The question: How well can I fit?

Three datasets



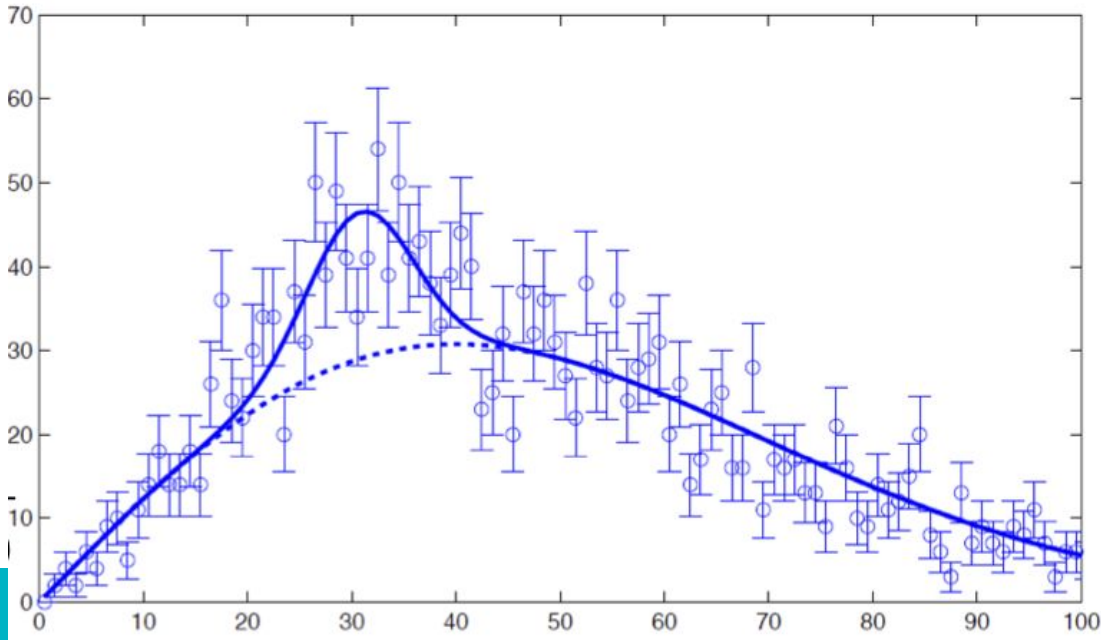
# Is there a signal?

Try to distinguish background fluctuations from signals.



# Is there a signal?

Looks like a signal around  $m=30$  maybe



## Is there a signal?

For GOF tests with binned data:

→ compare observed event numbers  $n_i$  with expectation values  $f_i$

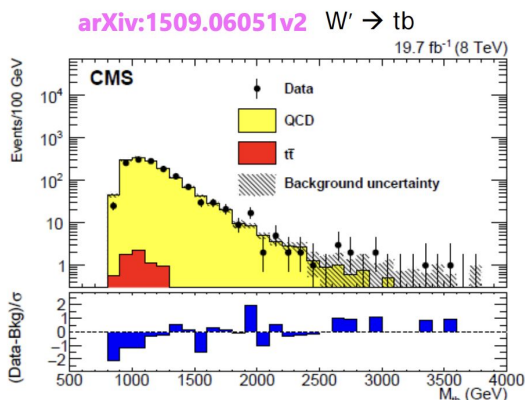
Since no  $H_1$  specified there are many different GOF tests possible

$$\chi^2 = \sum_i (f_i - n_i)^2 / \sigma^2$$

→ Basically does what you do by eye; Minimise distance from hypothesis to the data points

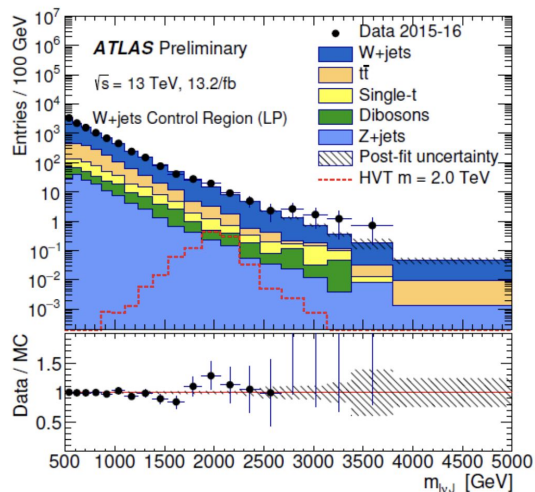
# Do we use by eye?

Yes!

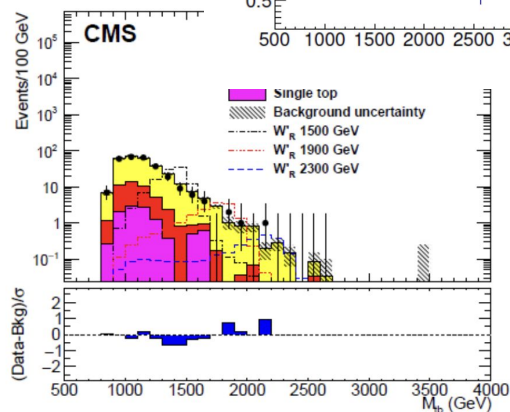


“This test (optical inspection) shows good agreement”

ATLAS-CONF-2016-062 Diboson resonance



“Good agreement is observed (optical inspection of pulls) between the data and the background prediction”



“Good agreement (optical inspection) between data and expectation from SM”



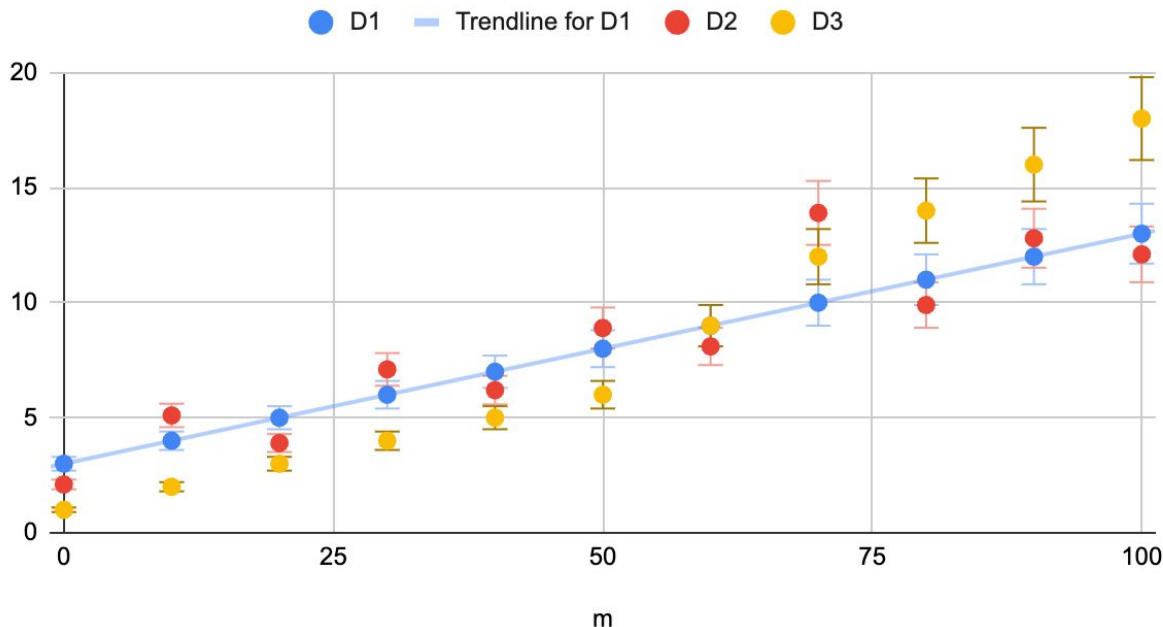
## Three datasets

Is there a signal?

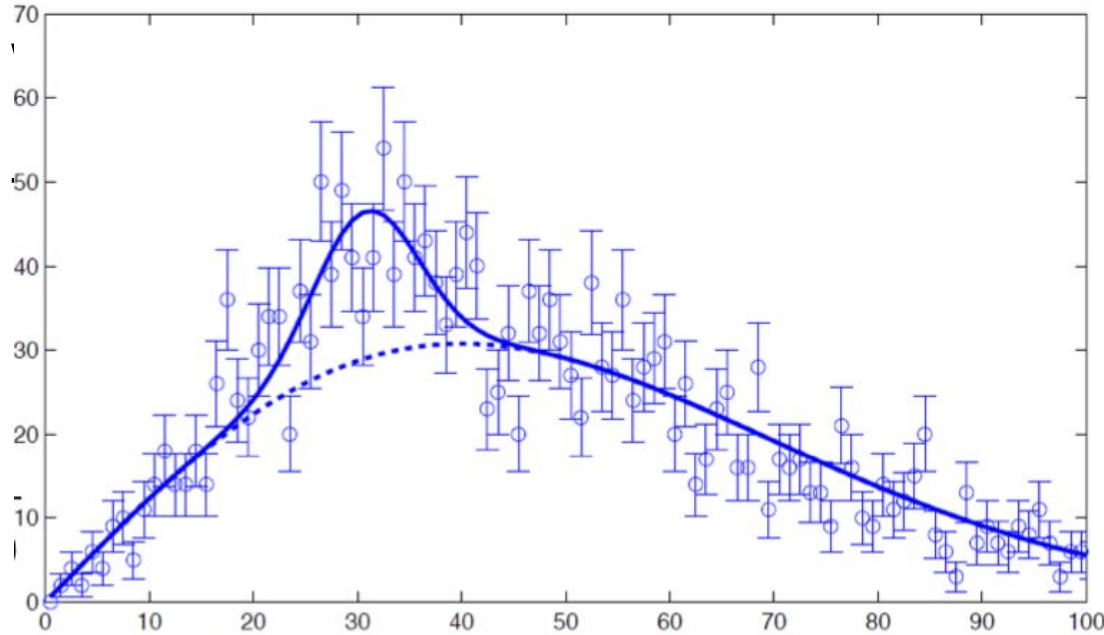
$$\chi^2 = \sum_i (f_i - n_i)^2 / \sigma^2$$

$\chi^2$  throws away all **sign and order info**

- Not very sensitive to correlated shifts in a certain region.
- Apply further GOF tests to check all data/model facets!



## Is there a signal?

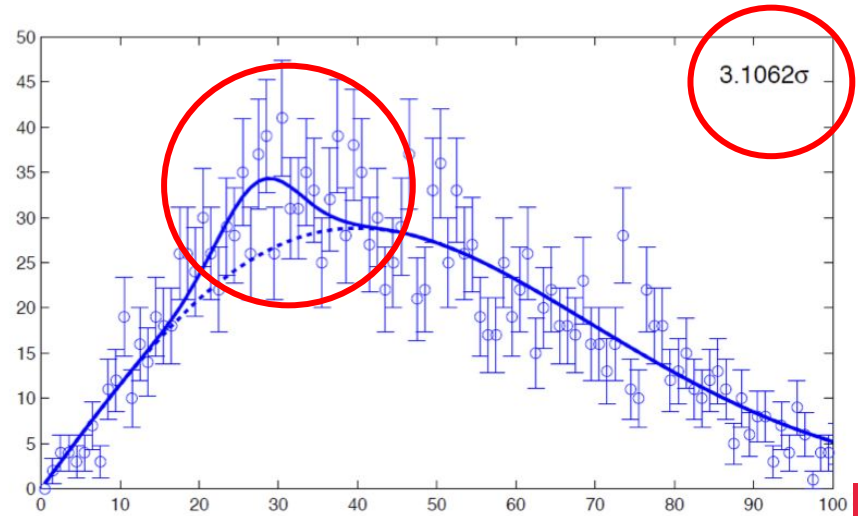


$$q_{fix,obs} = -2 \ln \frac{L(b)}{L(\hat{\mu}s(m=30) + b)}$$

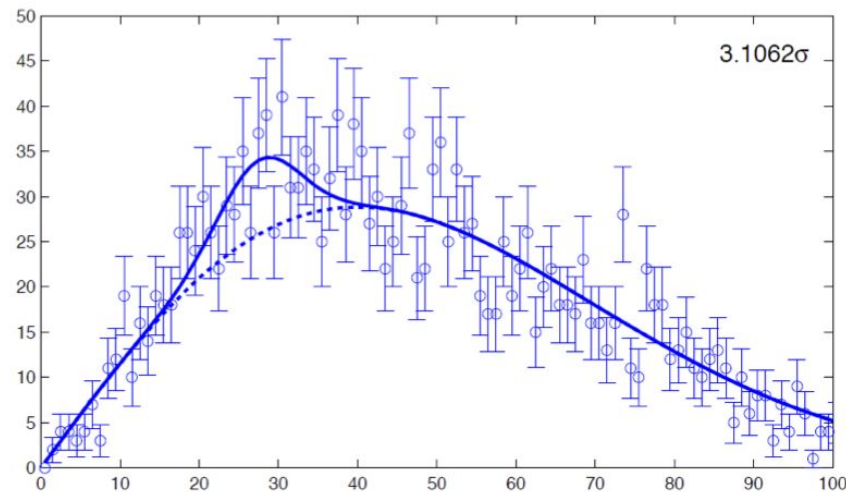
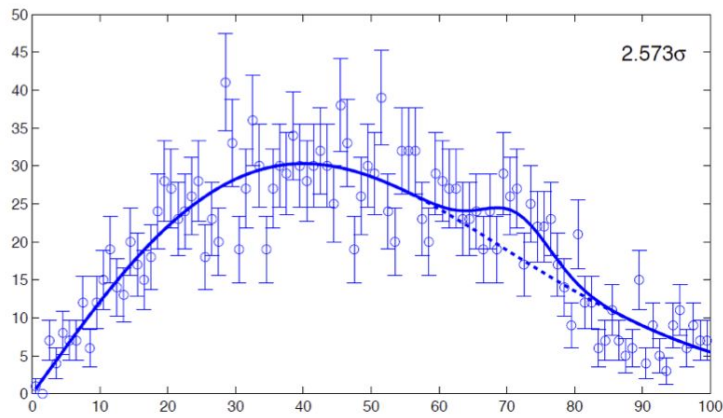
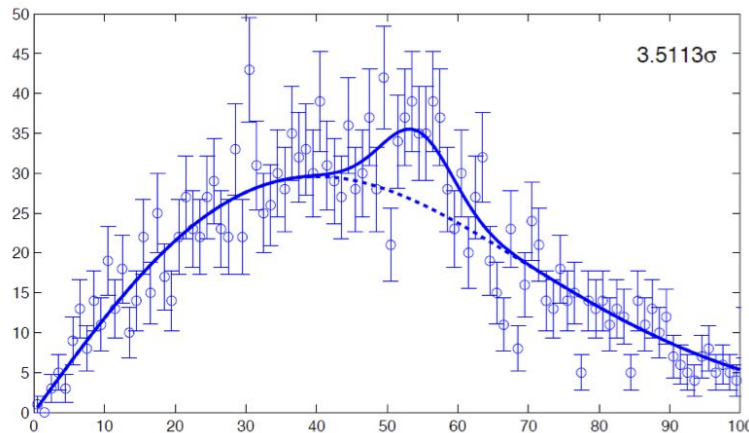
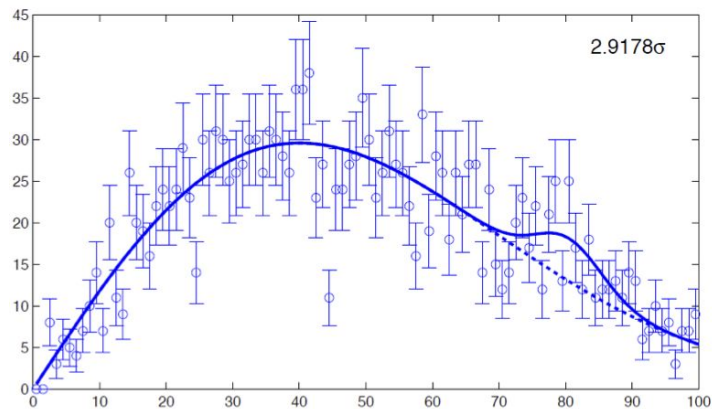
# What about these signals?

By eye; does not really look like a signal **but: >3 sigma!**

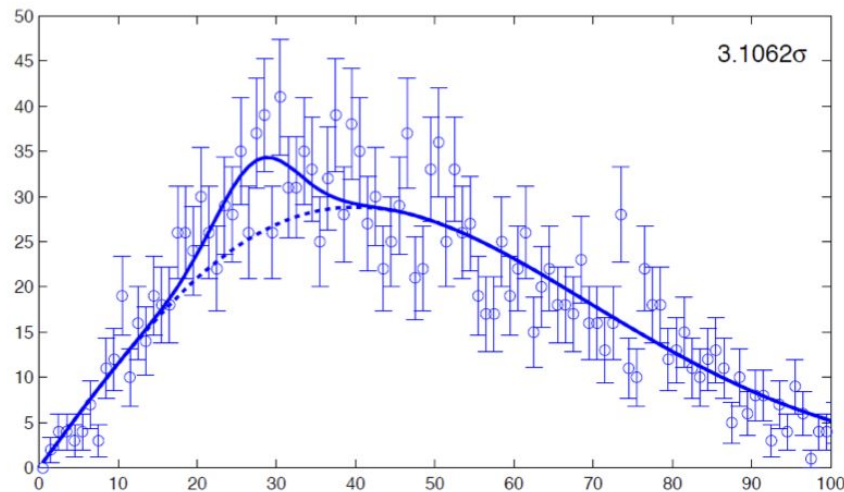
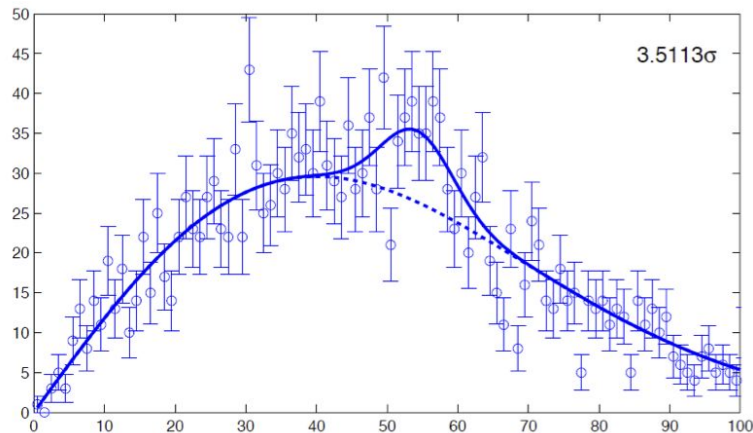
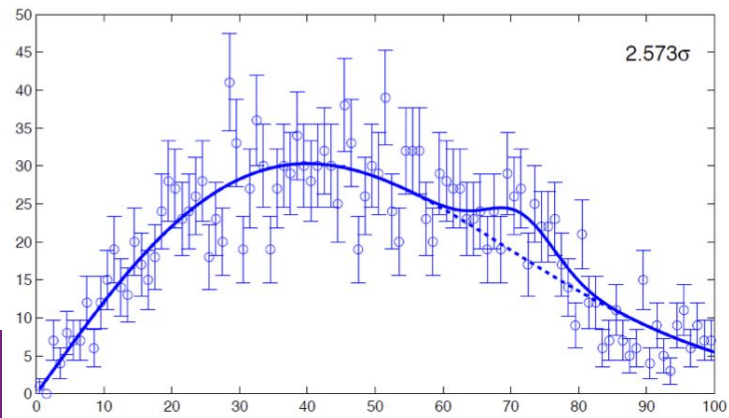
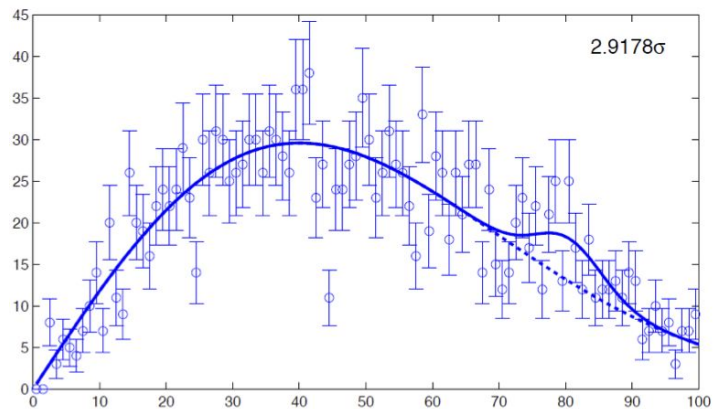
$$q_{fix,obs} = -2 \ln \frac{L(b)}{L(\hat{\mu}s(m=30) + b)}$$



# What about these signals?



Answer: All background fluctuations:

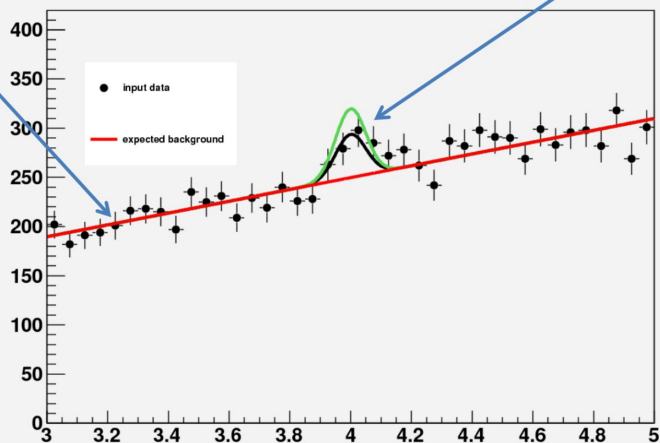


# How many parameters do I need?

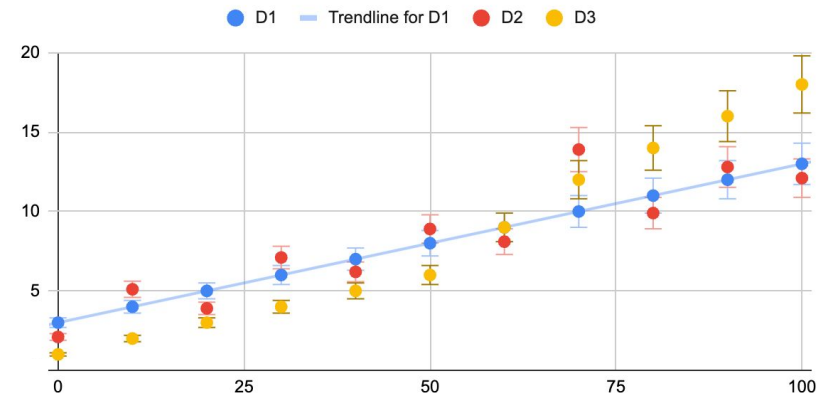
$$\chi^2 = \sum_i (f_i - n_i)^2 / \sigma^2$$

1)  $H_1$ : add more background pars

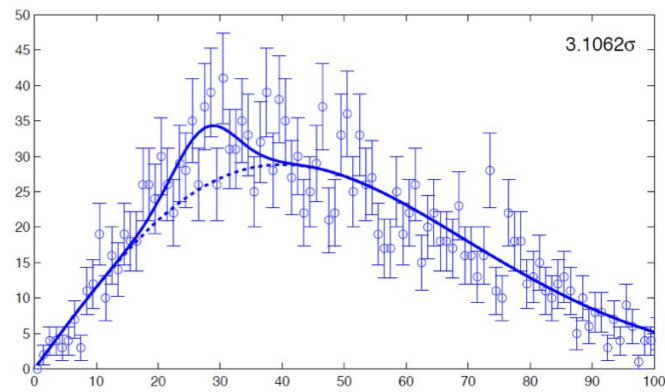
2)  $H_1$ : there is a signal



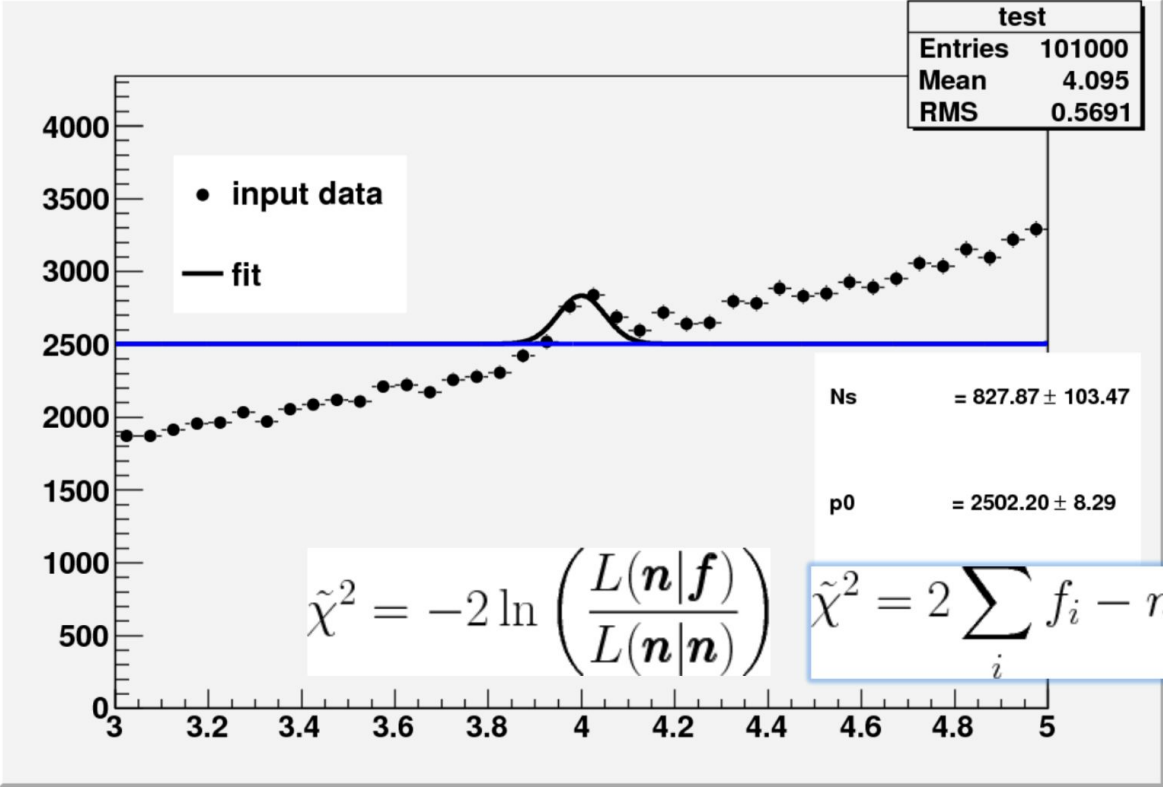
Three datasets



$$q_{fix,obs} = -2 \ln \frac{L(b)}{L(\hat{\mu}s(m=30) + b)}$$



# How many parameters do I need? – Example

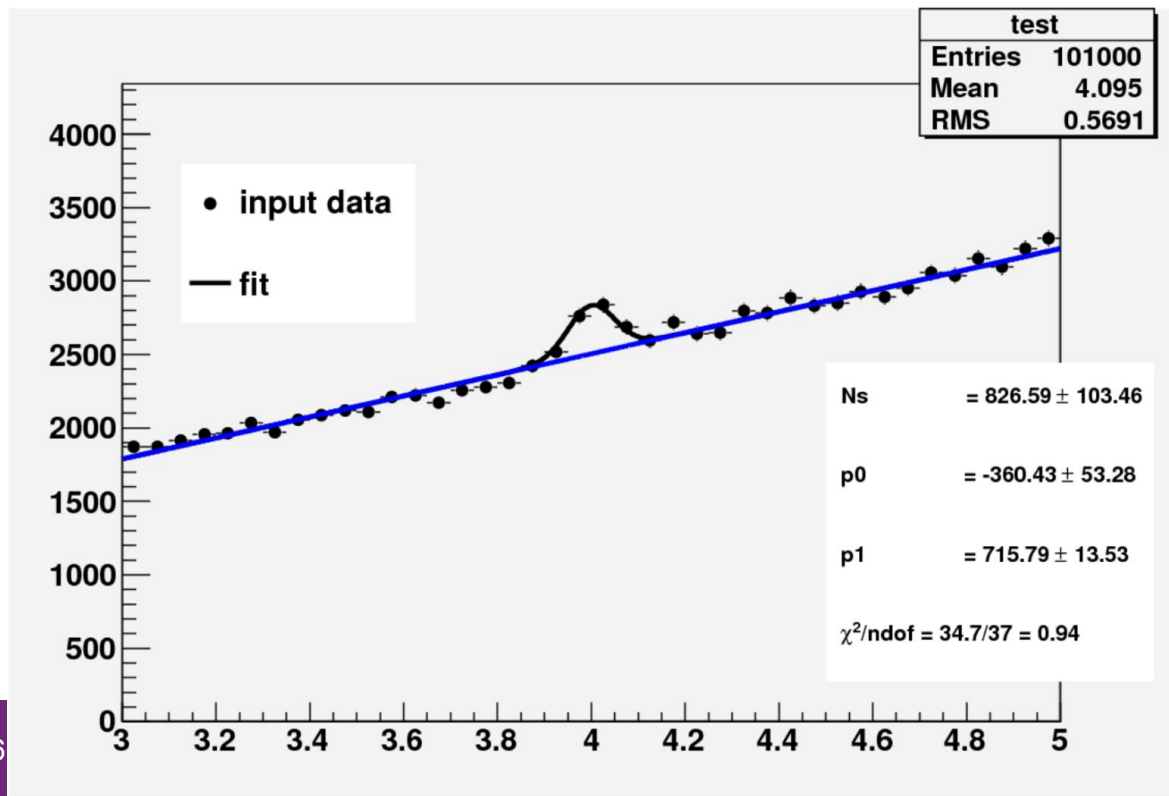


Fit function:  
gauss+p0

$$\chi^2 = \sum_i (f_i - n_i)^2 / \sigma^2$$

$$\tilde{\chi}^2 = 2880$$

# How many parameters do I need? – Example



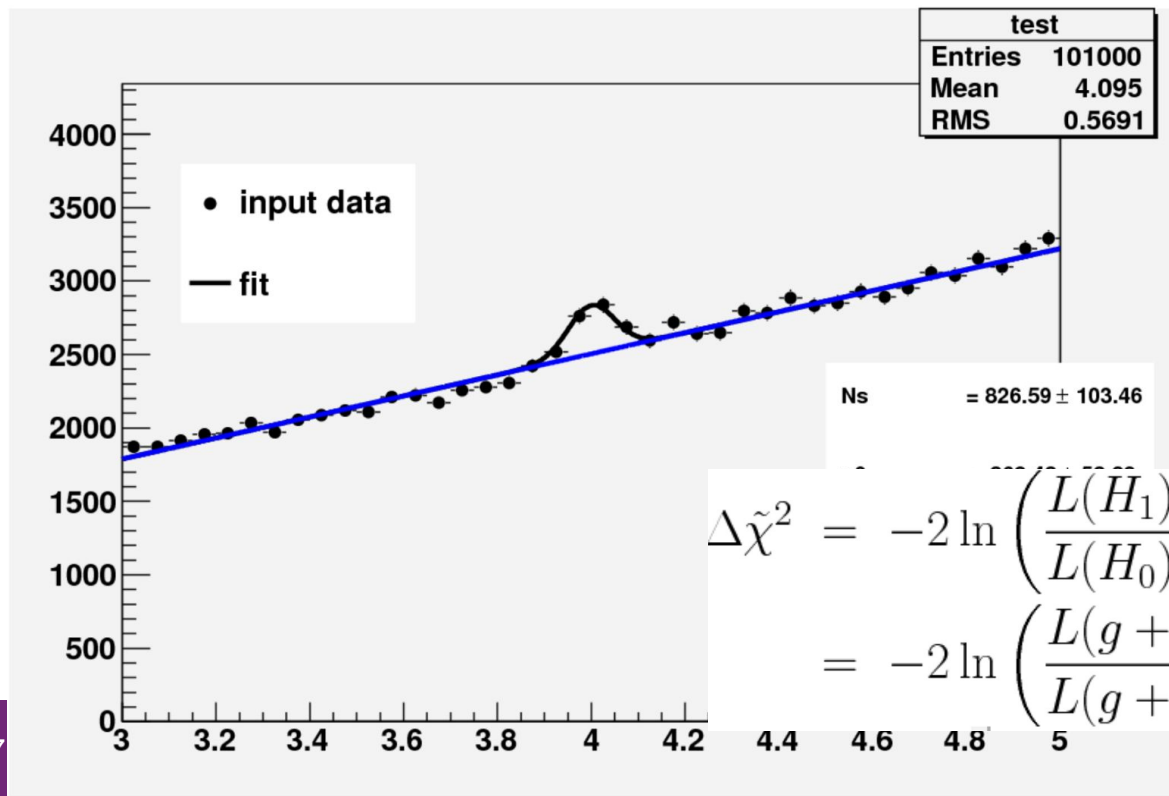
Fit function:  
gauss+p1

$$\tilde{\chi}^2 = 34.7$$

Should we stop here?



# How many parameters do I need? – Example

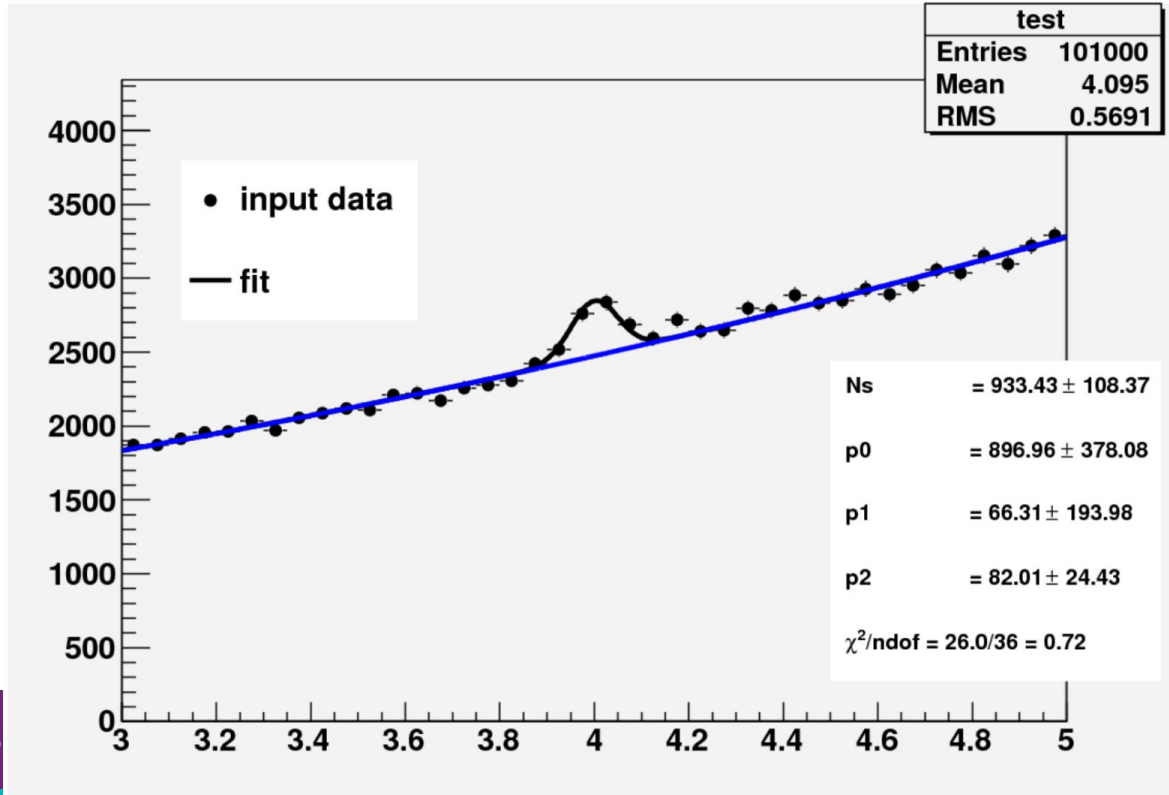


Fit function:  
gauss+p1

$$\tilde{\chi}^2 = 34.7$$

Should we stop here?

# How many parameters do I need? – Example



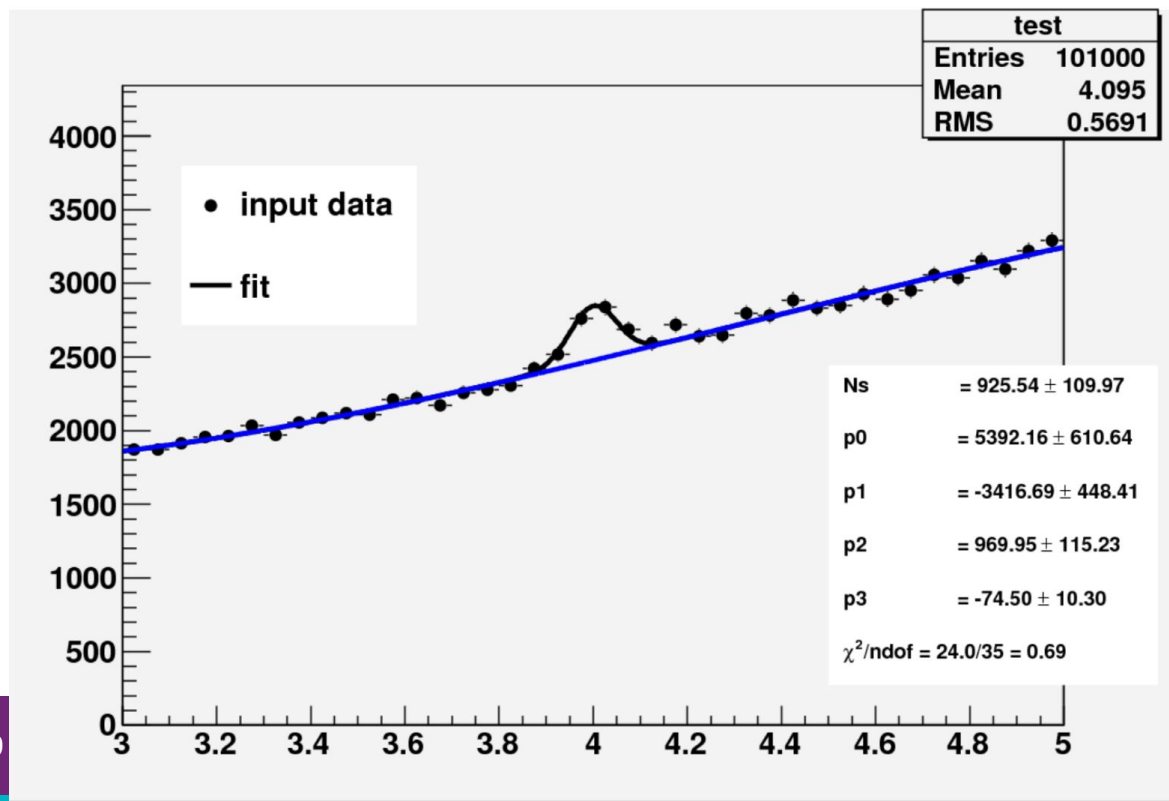
Fit function:  
gauss+p2

$$\tilde{\chi}^2 = 26.0$$

$$\Delta\tilde{\chi}^2 = -8.7$$

Should we stop here?

# How many parameters do I need? – Example



Fit function:  
gauss+p3

$$\tilde{\chi}^2 = 24.0$$

$$\Delta\tilde{\chi}^2 = -2.0$$

Please stop!

## How many parameters do I need? – Example

If H0 correct then according to **Wilks' theorem**:  $-\Delta\chi^2$  should follow a  $\chi^2$  function with ndf=1 (in asymptotic regime of large n)

g+p0

$$\tilde{\chi}^2 = 2880$$

Note: p-values for  $\chi^2$ : TMath::Prob( $\chi^2$  obs,ndf)

g+p1

$$\tilde{\chi}^2 = 34.7 \quad \Delta\tilde{\chi}^2 = -2845.3$$

g+p2

$$\tilde{\chi}^2 = 26.0 \quad \Delta\tilde{\chi}^2 = -8.7$$

P value = 0.003

Favoured over g+p1

g+p3

$$\tilde{\chi}^2 = 24.0 \quad \Delta\tilde{\chi}^2 = -2.0$$

P value = 0.15

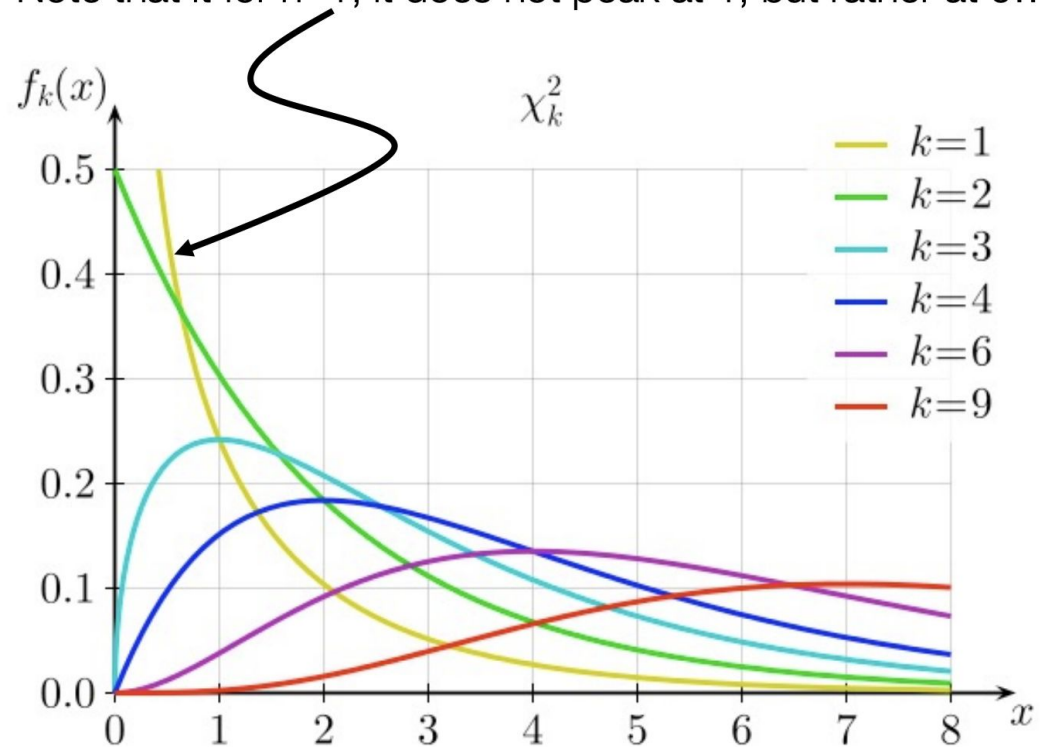
Not favoured over g+p2

## What does a $\chi^2$ distribution look like for $n=1$ ?

$\chi^2$

Remember:

- Note that for  $n=1$ , it does not peak at 1, but rather at 0...





## Wilks theorem

- $H_0$ : Additional parameters (as predicted by  $H_1$ ) not needed
- If  $H_0$  correct then according to Wilks' theorem:  
 $-\Delta\chi^2 = -2\ln[L(H_1)/L(H_0)]$  should follow for  $n \rightarrow \infty$   $\chi^2$  function with  
ndf = #added parameters

Wilks' theorem only applies for nested hypotheses:

$H_0$ : 1st order polynomial    $H_1$ : 2nd order polynomial   ✓

$H_0$ : 1st order polynomial    $H_1$ :  $a \cdot \exp(bx + cx^2)$    ✗

## Improving on $\chi^2$

Likelihood ratio is an improved  $\chi^2$  – S. Baker & R.D. Cousins, NIM 221 (1984) 437

- Still a single number
- “Optimal estimator” e.g. parameter estimation
- Requires a second hypothesis
- Allows taking uncertainties into account systematically!!
  - ◆ What if there’s a correlation?
  - ◆ What if there’s a systematic uncertainty

See Wouter’s slides from yesterday

# Alternatives to Likelihoods and $\chi^2$

## Kolmogorov-Smirnov test

$F_c$ : Cumulative distribution function

$F_e$ : Empirical distribution function

$$q_{GoF,KS} = \sup |F_c(x) - F_e(x)|$$

## Anderson-Darling test

$$q_{GoF,AD} = n \cdot \int dF_e(x) \frac{(F_c(x) - F_e(x))^2}{F_e(x) \cdot (1 - F_e(x))}$$



## Three datasets

# Summary

Not too bad...



"LISTEN, SCIENCE IS HARD.  
BUT I'M A SERIOUS  
PERSON DOING MY BEST."

