

# Curve fitting

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February 7, 2013



- ▶ Random variables
- ▶ Probability functions
  - ▶ Discrete PMF
  - ▶ CDF

$$F_X(x) = \text{Prob}\{X \leq x\} \quad (1)$$

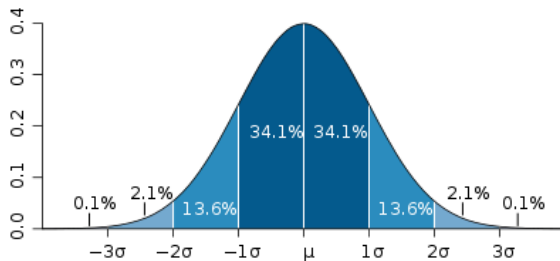
- ▶ PDF

$$f_X(x) = F'(x) \quad (2)$$

# Moments

- ▶ Central moment —  $\langle (x - \mu)^m \rangle = \langle (x - \langle x \rangle)^m \rangle$ 
  - ▶ Zeroth and First — 1 and 0
  - ▶ Second — Variance  $\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$
  - ▶ Third and Fourth — Skewness and Kurtosis
- ▶ Non-central moment —  $\langle X^m \rangle$

# Gaussian (Normal)



$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left\{ -\frac{(x - \mu)^2}{2\sigma^2} \right\} \quad (3)$$

$$Q = \sum_{i=1}^k X_i^2 \quad (4)$$

$$f_Q(x; k) = \begin{cases} \frac{1}{2^{k/2}\Gamma(k/2)} x^{k/2-1} e^{-x/2} & ; x \geq 0 \\ 0 & ; x < 0 \end{cases} \quad (5)$$

where  $X_i$ 's are normally distributed random variables with 0 mean and variance 1.

# Chi-square CDF

After integration, we get the Chi-square CDF in terms of an lower incomplete  $\gamma$  function defined as

$$\gamma(s, x) = \int_0^x t^{s-1} e^{-t} dt \quad (6)$$

Then the Chi-square CDF equals

$$\frac{\gamma(\frac{k}{2}, \frac{\chi^2}{2})}{\Gamma(\frac{k}{2})} \quad (7)$$

# What does curve fitting mean?

- ▶ Fitting data to a model with adjustable parameters
- ▶ Design figure-of-merit function
- ▶ Obtain best fit parameters by adjusting parameters to achieve min in merit function
- ▶ More details to take care of
  - ▶ Assess appropriateness of model; goodness-of-fit
  - ▶ Accuracy of parameter determination
  - ▶ Merit function may not be unimodal



# Least squares fitting

Maximizing the product

$$P \propto \prod_{i=1}^N \exp \left[ -\frac{1}{2} \left( \frac{y_i - y_{i(t)}}{\sigma} \right)^2 \right] \Delta y \quad (8)$$

ie. Minimizing its negative logarithm

$$\left[ \sum_{i=1}^N \frac{[y_i - y_{i(t)}]^2}{2\sigma^2} \right] - N \log \Delta y \quad (9)$$

Minimizing this sum over  $a_1, a_2, ..a_M$ , we get the final form:

$$\sum_{i=1}^N [y_i - y_{i(t)}]^2 \quad (10)$$

# Chi-square fitting

Modifying equation ?? to replace the  $\sigma$  by  $\sigma_i$  and going through the same process, we get

$$\chi^2 = \sum_{i=1}^N \left( \frac{y_i - y_{i(t)}}{\sigma_i} \right)^2 \quad (11)$$

where

$$y_{i(t)} = f(a_1, a_2, ..a_M) \quad (12)$$

For models that are linear in the a's, however, it turns out that the probability distribution for different values of chi-square at its minimum can nevertheless be derived analytically, and is the chi-square distribution for  $N-M$  degrees of freedom.

```
gnuplot> fit f(x) 'foo.data' u 1:2:3:4 via a, b
```

- ▶ Uses WSSR: Weighted Sum of Squared Residuals
- ▶ Marquardt-Levenberg algorithm to find parameters to use in next iteration
- ▶ After fitting, gnuplot reports *stdfit*, the standard deviation of the fit

- ▶ Numerical Receipies in C
- ▶ The gnuplot manual
- ▶ Miscellaneous books on elementary probability
- ▶ Presentation created using  $\text{\LaTeX}$  and Beamer

Presentation source code available on [github.com/artagnon/curve-fitting](https://github.com/artagnon/curve-fitting)