

# Fitting mathematical models to data using Non-linear Least-Squares

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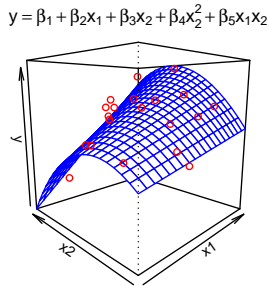
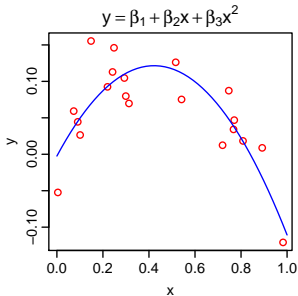
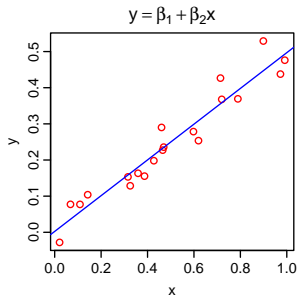


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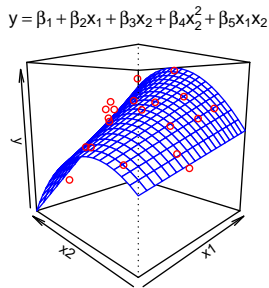
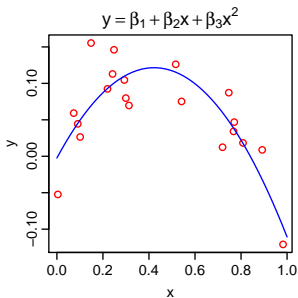
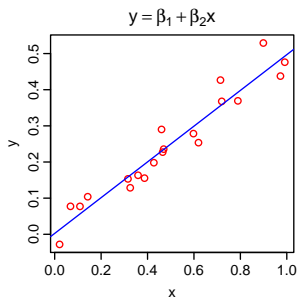
# OUTLINE

- Why Non-Linear Least Squares regression / fitting?
- The NLLS fitting method
- NLLS in R
- Afternoon practicals overview

# LINEAR MODELS ARE GREAT

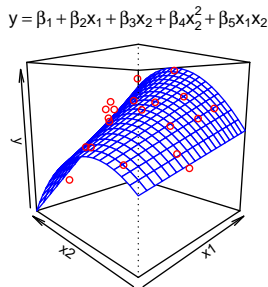
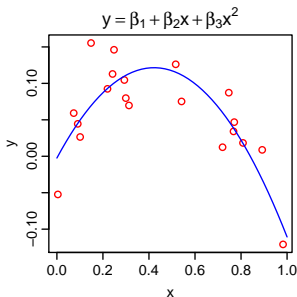
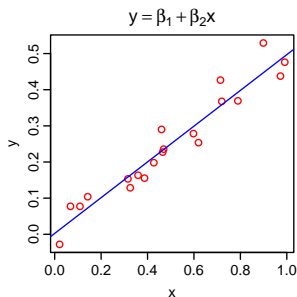


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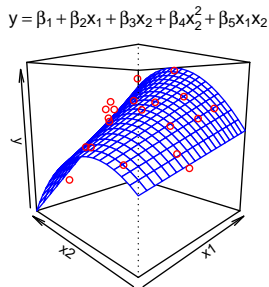
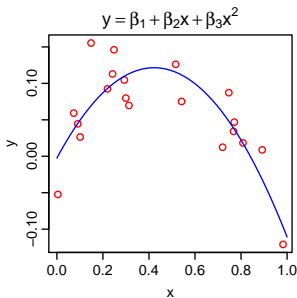
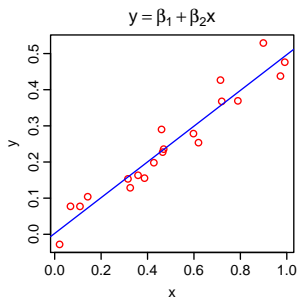
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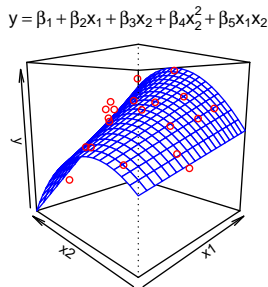
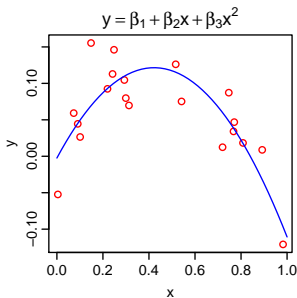
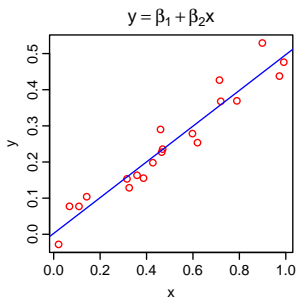
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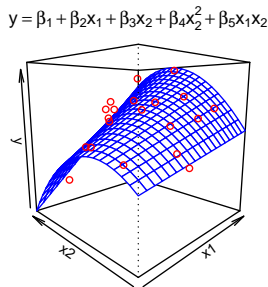
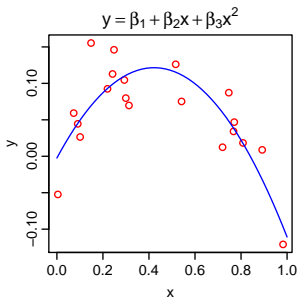
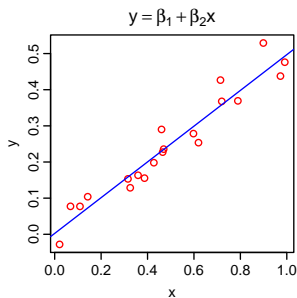
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- Linear models can *include curved responses* (e.g. polynomial regression)
- OK, so then *why Non-Linear Least Squares (NLLS) fitting?*



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NO!

# SO WHAT — WHY IS INTRINSIC NON-LINEARITY A PROBLEM?

**Recall what the Least Squares method does:**

- Consider a predictor  $x$ , data  $y$ ,  $n$  observations, and a model that we want to fit to the data:

$$f(x_i, \beta) + \varepsilon_i$$

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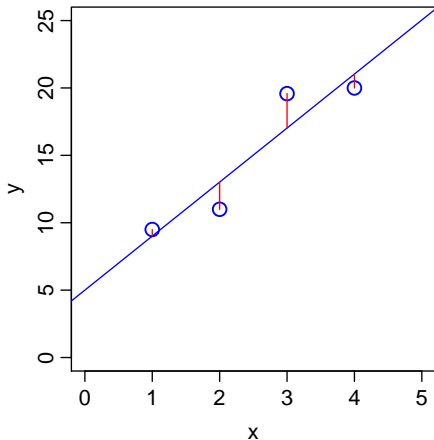
- The objective is to find estimates of values of the  $k$  parameters ( $\hat{\beta}_j$ ) that minimize the sum ( $S$ ) of squared residuals ( $r_i$ ) (AKA RSS):

$$S = \sum_{i=1}^n [y_i - f(x_i, \beta)]^2 = \sum_{i=1}^n r_i^2$$

# THE LEAST-SQUARES SOLUTION

OLS minimizes the *sum* of the *squared* residuals

# IF THE MODEL IS LINEAR, THE SOLUTION IS EASY USING ALGEBRA



$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

$$9.50 = 5 + 4 \times 1 + 0.50$$

$$11.00 = 5 + 4 \times 2 - 2.00$$

$$19.58 = 5 + 4 \times 3 + 2.58$$

$$20.00 = 5 + 4 \times 4 - 1.00$$

$$\beta_0 = 5; \beta_1 = 4$$

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- So the nice trick of solving  $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$  is impossible *mathematically*



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- Whether a refinement has taken place in any step of the iteration is determined by re-calculating the residuals at that step
- Eventually, if it all goes well, we find a combination of  $\beta_j$ 's that is *very close* to the desired solution  $\frac{\partial S}{\partial \beta_j} = 0, j = 0, 1, 2, \dots, k$



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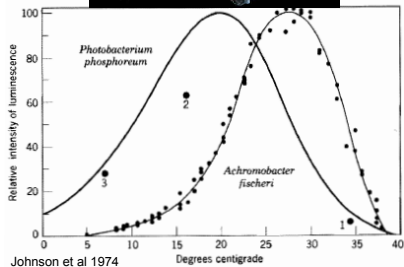
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- *Can you think of some examples?*

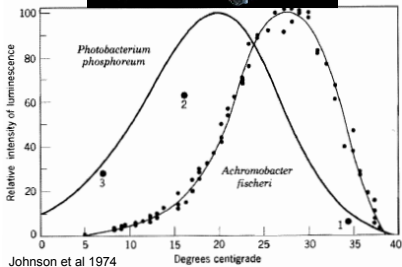


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$k$  = Boltzmann constant ( $\text{eV K}^{-1}$ )

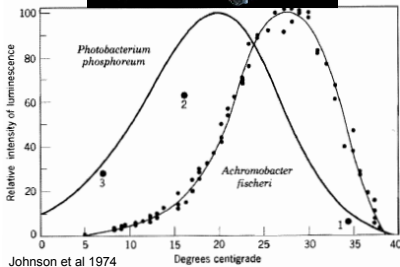
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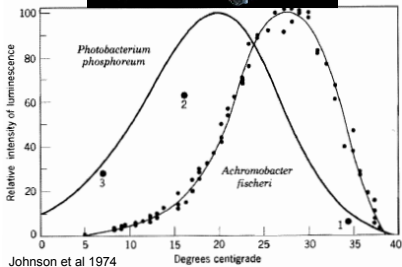
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- *What about alternative models?*

# EXAMPLE: FUNCTIONAL RESPONSES

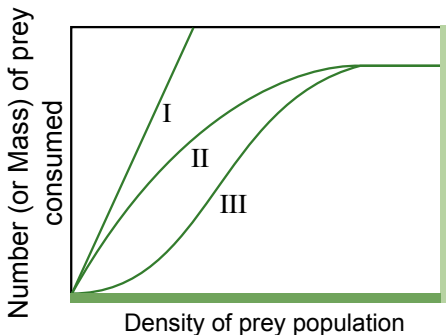
$$f(x_R) = \frac{ax_R^{q+1}}{1+hax_R^{q+1}} \text{ (Holling, 1959)}$$

$x_R$  = Resource density (Mass / Area or Volume)

$a$  = Search rate (Area or Volume / Time )

$h$  = Handling time

$q$  = Shape parameter (dimensionless)



Note that:

- NLLS fitting can yield  $h < 0$ ,  $q < 0$ , or both
- $h < 0$  is biologically impossible but indicates an upward curving response
- $q < 0$  is biologically unlikely as it indicates a decline in search rate with resource density (but is useful as a measure of deviation away from a type III response)

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- ➎ Adjust the parameters again so that the curve comes even closer to the points (rss decreases)
- ➏ Repeat 4–5
- ➐ Stop simulations when the adjustments make virtually no difference to the rss

# NLLS FITTING

The *tricky part* — *adjust parameters to make curve come closer to the data points* (step 4) has two main algorithms that you can choose between:

- The Gauss-Newton algorithm is the default in the `nls` package (part of the `stats` base package) — good in many cases, but doesn't work very well if the model is mathematically weird (the optimization landscape is difficult) and the starting values for parameters are far-off-optimal

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- The Gauss-Newton algorithm is the default in the `nls` package (part of the `stats` base package) — good in many cases, but doesn't work very well if the model is mathematically weird (the optimization landscape is difficult) and the starting values for parameters are far-off-optimal
- The Levenberg-Marquardt (LM) switches between Gauss-Newton and “gradient descent” and is more robust against starting values that are far-off-optimal — available in R through the `minpack.lm` package

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- The command is `nlsLM`



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- What if the errors are not normal? — use Maximum Likelihood or Bayesian methods instead.

## MORE NLLS TIPS

- You can use mixed-effects modelling with NLLS in R; the package is `nlme` <https://stat.ethz.ch/R-manual/R-devel/library/nlme/html/nlme.html> (You are probably stuck with the Gauss-Newton algorithm with `nlme` though)

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- You can also use Python — look up `lmfit` <https://lmfit.github.io/lmfit-py/index.html>. python seems to have a better Levenberg-Marquardt implementation than R



# READINGS AND RESOURCES

- Motulsky, Harvey, and Arthur Christopoulos. Fitting models to biological data using linear and nonlinear regression: a practical guide to curve fitting. OUP USA, 2004.
- Johnson, J. B. & Omland, K. S. 2004 Model selection in ecology and evolution. Trends Ecol. Evol. 19, 101–108.

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- Or,  $2 \sum_{i=1}^n r_i \frac{\partial r_i}{\partial \beta_j} = 0$

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- Then we want to solve
$$\frac{\partial S}{\partial \beta_0} = \sum_{i=1}^n \frac{\partial [y_i - (\beta_0 + \beta_1 x_i)]^2}{\partial \beta_0} = 0$$
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just boils down to solving two simultaneous equations because  $\frac{\partial r_i}{\partial \beta_j}$  is simple *because* the model is intrinsically linear:

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- That is, we need to solve  $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$  (*this is what R solves when you use `lm()`*)