Fitting models to data using Non-linear Least-Squares

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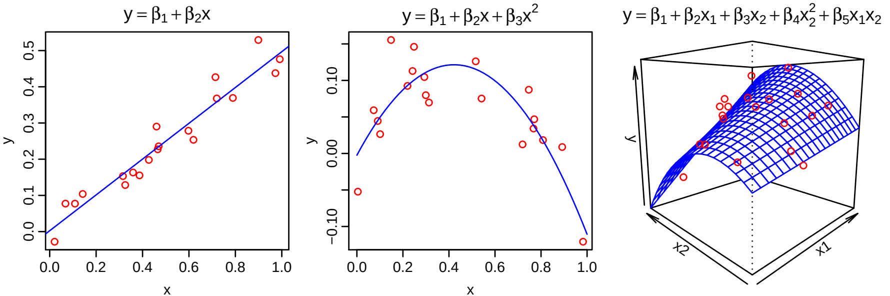
OUTLINE

- Why Non-Linear Least Squares regression / fitting?
- The NLLS fitting method
- NLLS in `R`
- Afternoon practicals overview (two examples)


$y = \beta_1 + \beta_2 x$
y
x
0.0
0.1
0.2
0.3
0.4
0.5
0.0
0.2
0.4
0.6
0.8
1.0
$y = \beta_1 + \beta_2 x + \beta_3 x^2$
y
x
−0.10
0.00
0.10
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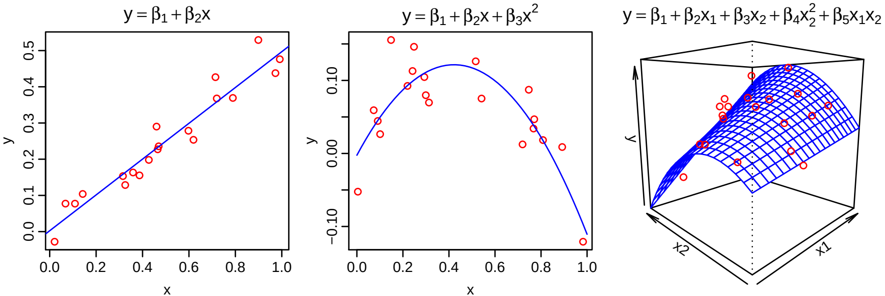
$y = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_2^2 + \beta_5 x_1 x_2$
y
x2
x1



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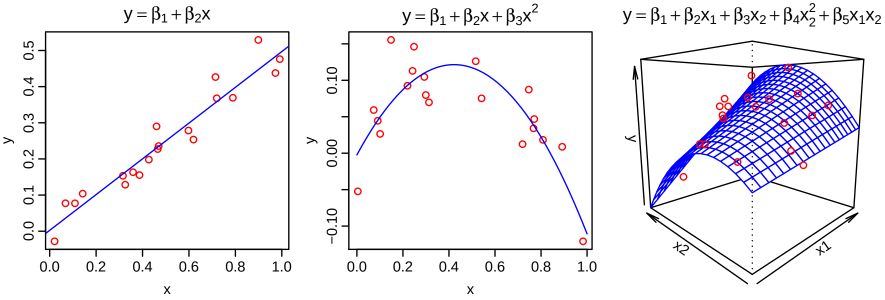
LINEAR MODELS ARE GREAT



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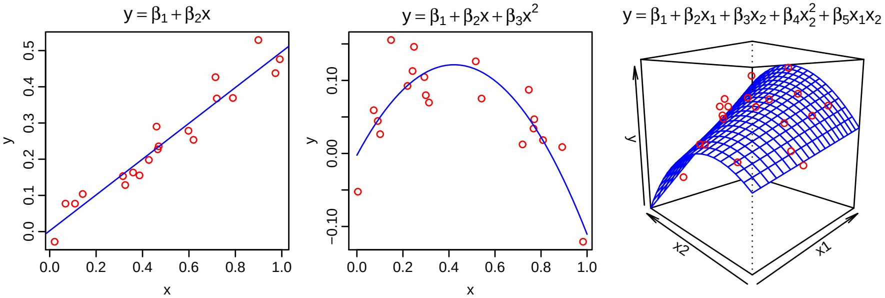

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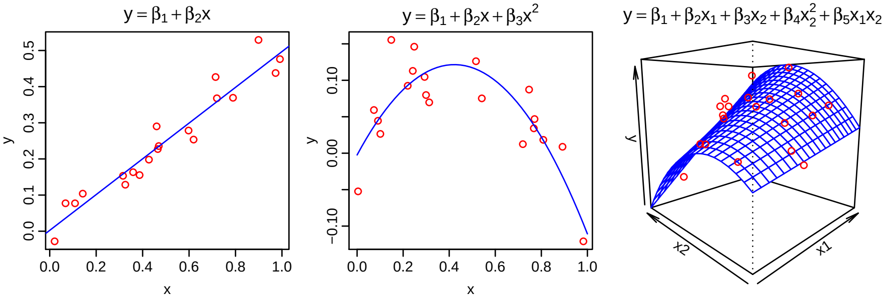

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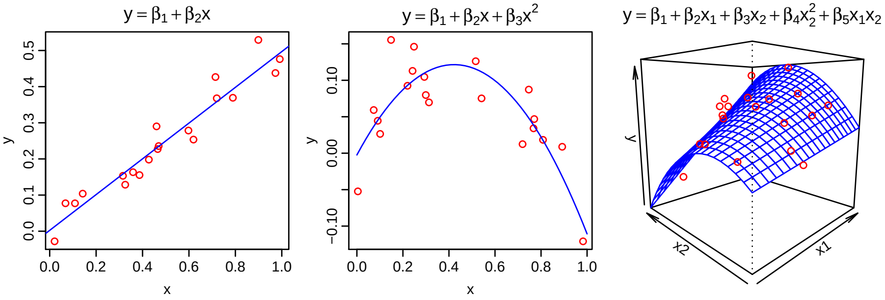

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- *OK, so then why Non-Linear Least Squares (NLLS) fitting?*

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

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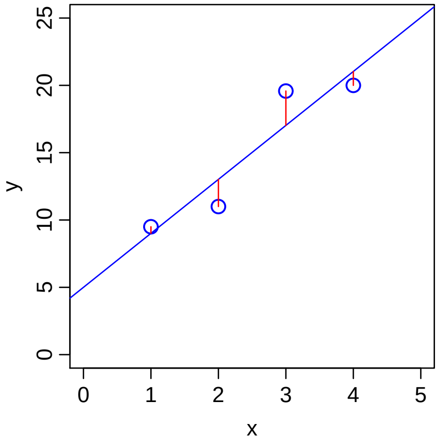

$$y_1 = \beta_0 + \beta_1 x_1 + \varepsilon_i$$

$$9.50 = 5 + 4 \times 1 + 0.50$$
$$11.00 = 5 + 4 \times 2 - 2.00$$
$$19.58 = 5 + 4 \times 3 + 2.58$$
$$20.00 = 5 + 4 \times 4 - 1.00$$

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

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

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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 β_j's that is *very close* to the desired solution $\frac{\partial S}{\partial \beta_j} = 0, j = 0, 1, 2, \ldots, k$

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  - *Can you think of some examples?*

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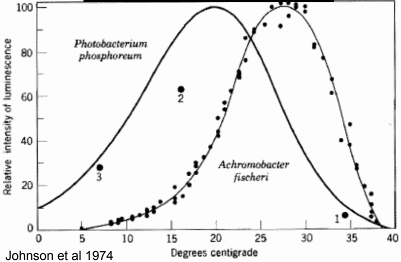
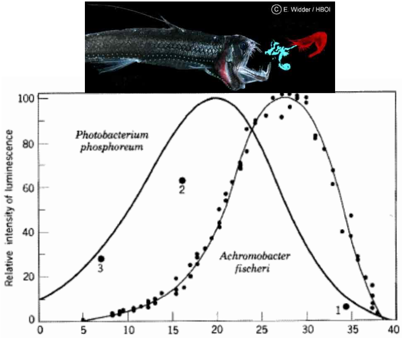


Johnson et al 1974



$$B = B_0 \boxed{e^{-\frac{E}{kT}}} f(T, T_{pk}, E_D)$$

T = temperature (K)
k = Boltzmann constant (eV K^{-1})
E = Activation energy (eV)
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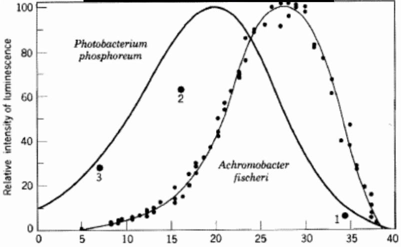

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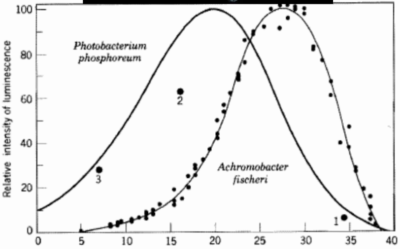

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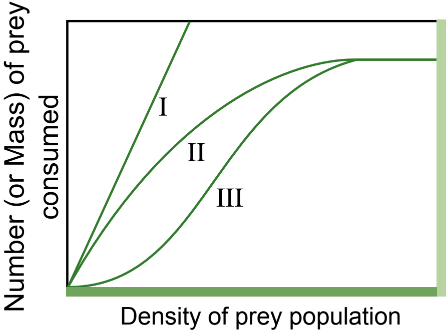
- *What about alternative models?*

EXAMPLE 2: 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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7. Stop simulations when the adjustments make virtually no difference to the rss

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The *tricky part — adjust parameters to make curve come closer to the data points* (step 4) has at least two algorithms:

- 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 command is `nlsLM`

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- The measurement/observation error distribution is Gaussian — for example, what would the error distribution of this non-linear model be: $y_i = \beta_0 e^{\beta_2 x_i} + \varepsilon_i$
- What if the errors are not normal? — use maximum likelihood instead! (e.g., using `nlm` for optimizing/fitting)

COMPARING MODELS

- It's all about the "Likelihood" of a model:
- That is, the likelihood of a set of parameter values (of a model), θ, given outcomes x, equals the probability of those observed outcomes given those parameter values, that is,

$$\mathcal{L}(\theta|x) = P(x|\theta)$$

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This is how you can calculate these (using `R` syntax):

- residuals = Observations - Predictions
- `rss = sum(residuals ^ 2)`
- Then, AIC is `n * log((2 * pi) / n) + n + 2 + n * log(rss) + 2 * k`
  (*what is* `n` *and* `k`*?*)
- And BIC is `n + n * log(2 * pi) + n * log(rss / n) + (log(n)) * (k + 1)`
- For both AIC and BIC, If model **A** has AIC lower by 2-3 or more than model **B**, its better — Differences of less than 2-3 don't really matter

COMPARING MODELS

The easiest thing to do for you is to use information theory (including AIC and BIC) to compare models.
Both use estimated likelihood of a model
This is how you can calculate these (using `R` syntax):

- residuals = Observations - Predictions
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- Then, AIC is `n * log((2 * pi) / n) + n + 2 + n * log(rss) + 2 * k`
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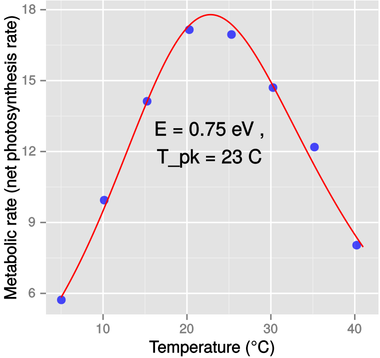
Also note that:

- R^2 = 1 - (rss/tss), where tss is total sum of squares:
  `tss = sum((Observations - mean(Predictions)) ^ 2)`

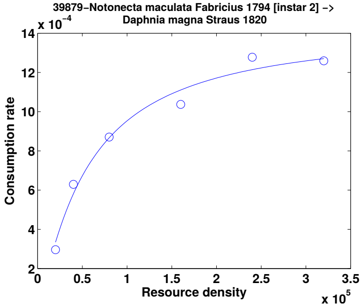
PRACTICALS: INSTRUCTIONS

- We shall start off with some simple examples (`NLSFitEx1.R`, `NLSFitEx2.R`, etc.)
- You can then choose either Practical 1 or 2, or do both!
- In each, make sure you have a good look at the data first by plotting them up in a loop
- Keep workflow organized in `Code`, `Results`, `Data` !
- You may also find your own model to fit some data related to your interests or project
- Your demonstrators and I will help you get started in any case

- Use `nls` (or `nlsLM`) to fit the `ThermRespData.csv` dataset to the model: $B = B_0 \boxed{e^{-\frac{E}{kT}}} f(T, T_{pk}, E_D)$
- Plot the data and output coefficient estimates and fit stats to a file
- Here's an example of how a fitted curve looks (only two fitted parameters are shown):



- Use `nls` (or `nlsLM`) to fit `CRat.csv` dataset to the model:
  $f(x_R) = c = \frac{a x_R^{q+1}}{1 + h a x_R^{q+1}}$
  (c is consumption rate)
- Plot the data and output coefficient estimates and fit stats to a file
- Here's an example of how a fitted curve looks :



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- 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...

READINGS

- 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.