Nonlinear models

I don't think we're in Kansas anymore

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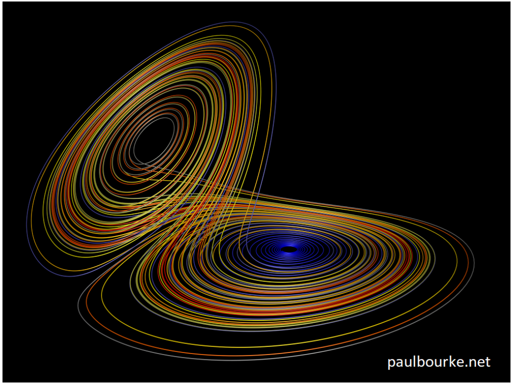
Outline

- What are nonlinear models?
- Mechanistic models
  - Some common models
  - Strategies for fitting
- Empirical models
  - Some common models
  - GAMs



The Lorenz System: a classical 3D nonlinear system

What are nonlinear models?

- **Linear models** take the form:

$$\hat{y} = X\beta = b_0 1 + b_1 x_1 ... + b_i x_i$$
$$y \sim Normal(\hat{y}, \sigma)$$

- **Nonlinear models** are any kind of model that can't be reduced to this linear (matrix) form:

$$\hat{y}_t = \hat{y_{t-1}} r(1 - \frac{\hat{y_{t-1}}}{k})$$
$$y \sim Normal(\hat{y}, \sigma)$$

Two common situations

1. "I have governing equations for this system, and I want to fit them to my data"
   - e.g. Logistic growth equation, Michaelis-Menten kinematrics, Ricker model
2. "I don't know what equations represent my system, but I need some kind of *smooth* process that describes them"
   - e.g. Changes in organism population over growing season, changes in stock prices over time

Part 1: Mechanistic models

Governing equations

Dynamics of some systems can be described by a set of equations, either in *discrete* or *continuous* time

- Exponential growth: *Discrete time*

$$n_t = n_{t-1} r$$

- Predator prey cycles: *Discrete time*

$$\begin{aligned} \text{prey}_t =& \text{prey}_{t-1}(r_1 - a_1 \text{pred}_{t-1}) \\ \text{pred}_t =& \text{pred}_{t-1}(a_2 \text{prey}_{t-1} - d) \end{aligned}$$

- Exponential growth: *Continuous time*

$$\frac{dn}{dt} = nr$$

- Predator prey cycles: *Continuous time*

$$\begin{aligned} \frac{d\text{prey}}{dt} =& r - a_1 \text{pred} \\ \frac{d\text{pred}}{dt} =& a_2 \text{prey} - d \end{aligned}$$

Some other common dynamic models

- Logistic growth

$$n_t = n_{t-1}(1 + r(1 - \frac{n_{t-1}}{k}))$$

- Beverton-Holt model

$$\mathrm{N}_t = \frac{R_0 N_{t-1}}{1 + N_{t-1}/M}$$

- Michaelis-Menten

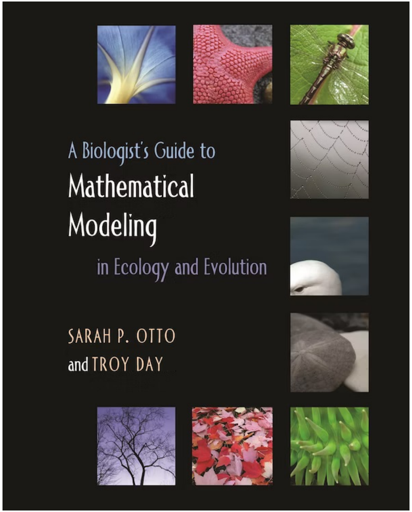
$$\frac{dp}{dt} = \frac{V_{max}\, a}{K_m + a}$$

- Susceptible-Infected-Recovered (SIR) model

$$\frac{dS}{dt} = -\frac{\beta IS}{N}$$
$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

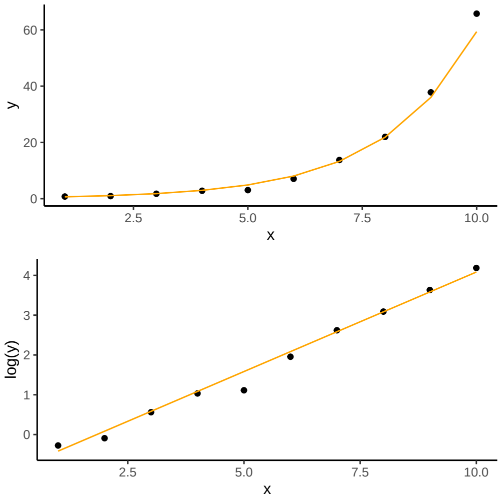
Where do these equations come from?

- Mostly from literature, sometimes from your own derivations
- Can be derived from causal models, flow diagrams, organismal life cycles
- Math-heavy topic for another class! If you're interested, I might start with this book:



Fitting nonlinear models: transformations

- Sometimes you can transform your data to approximate nonlinear models
- e.g. $y = b_0 e^{xb1}$ (Exponential growth)
  - Transformation: $ln(y) = ln(b_0 e^{xb1}) = ln(b_0) + ln(e^{xb1}) = ln(b_0) + xb_1$
  - Linear model in R: `lm(log(y)~x)`
- This can cause problems because *distances* don't mean the same thing at all ranges of x-values; in general, it's better to use a NLM if you're able to

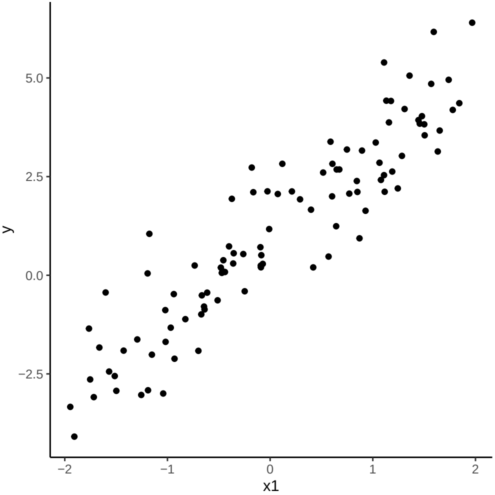


Fitting nonlinear models: simple example

- We have a *pretty good idea* what rules the system is following, and we want to figure out the parameters that it uses
- Simple example: let's start with a simple linear model, where we have *2 parameters* b_0 and b_1 that we're looking for

$$\hat{y} = X\beta = b_0 + b_1 x_1$$

- We're trying to find the parameters of a line that *most closely* fits our data:

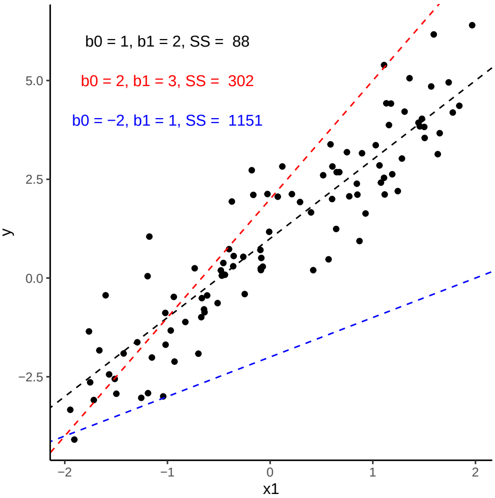


Fitting mechanistic models (cont.)

- How might we define "closest fit" in a mathematical sense?
- One common measure is *sum of squared distances*. This is just the difference between the data and the line:

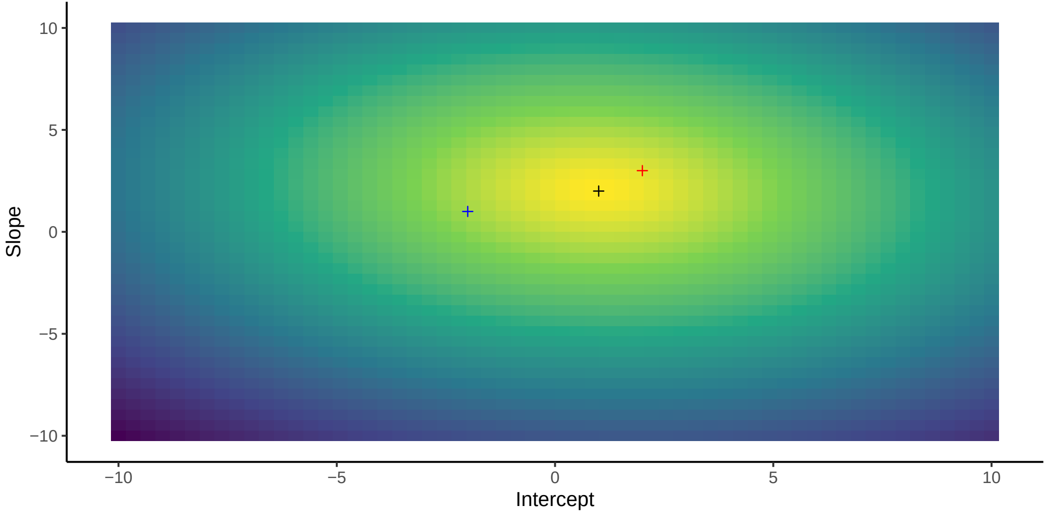
$$S = \sum_{i=1}^{N} (y_i - (b_0 + b_1 x_i))^2$$

- Here are three "guesses" at the slope and intercept, along with their SS scores. Which one looks to be the best?



Map of fitting surface

We can try this for a whole bunch of intercepts and slopes:



Getting R to do this

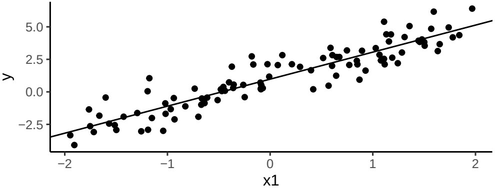
- It's pretty clear where the best intercept and slope is, but how do we get R to do this?
- First, we need a function that returns SS given a set of parameters:

```r
#Function to calculate SS
ssFun <- function(B,xdat,ydat){
  sum((ydat - (B[1] + B[2]*xdat))^2)
}
```

- Next, we use the `optim` function to find the intercept and slope values that return the minimum value of SS. How did it do? (Actual values: b_0:1, b_1:2)

```r
#Starts at 0,0 and "looks around" fr
optim(par = c(0,0) , fn = ssFun)
```

```
## $par
## [1] 0.9769795 2.0779779
##
## $value
## [1] 86.78819
##
## $counts
## function gradient
##       67       NA
##
## $convergence
## [1] 0
##
## $message
## NULL
```

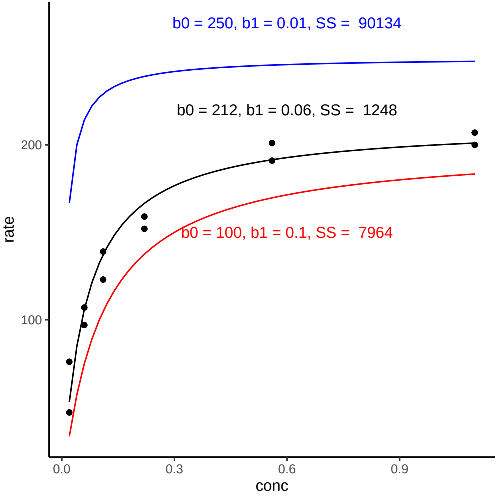


Fitting mechanistic models: nonlinear example

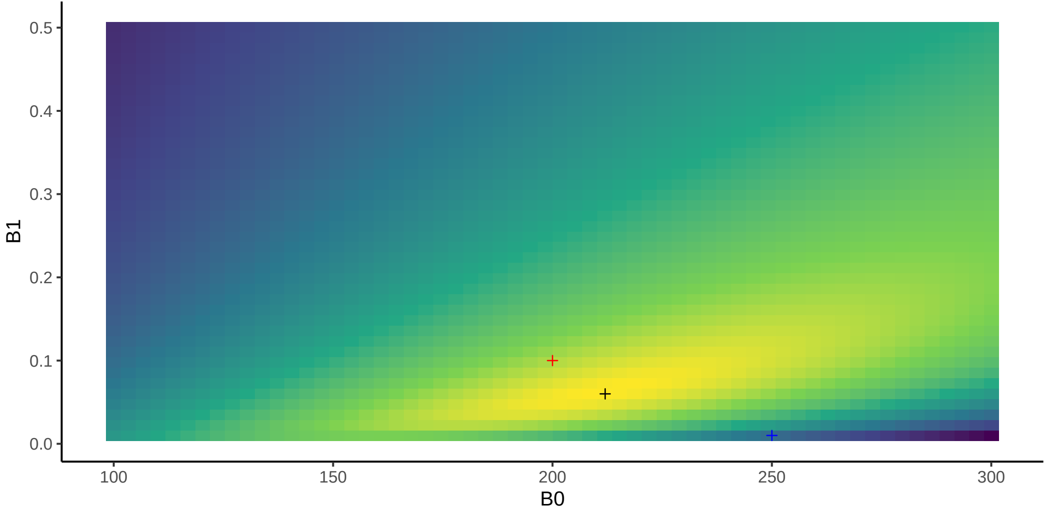
- Let's move on to a nonlinear model (Michaelis-Menten), where we also have *2 parameters* b_0 and b_1 that we're looking for

$$\hat{y} = \frac{b_0 x_1}{b_1 + x_1}$$

- Again, we're trying to find the parameters of a nonlinear curve that *most closely* fits our data:



Nonlinear example (cont.)



Get R to do it

Mind your starting parameters!

Better to start with more “realistic” values

General framework

Here are some simple rules for fitting models:

1. Think about how your system works. What rules do you think your system follows?
2. Write down these rules as equations, with **parameters** that control the system at time `t`
   - Some differential ($\frac{dx}{dt}$) equations can sometimes be solved by hand
   - Otherwise you need to use an ODE solver (`fme` in R)
3. Come up with an *objective function* that describes the differences between predictions and actual data
4. Get R to find parameters that *minimize* the objective function
5. See how well your model predicted your data:
   - Are all of your parameters *identifiable* from your data?
   - Do you need to go back to step 1?

First challenge

- Broken stick model

First challenge results

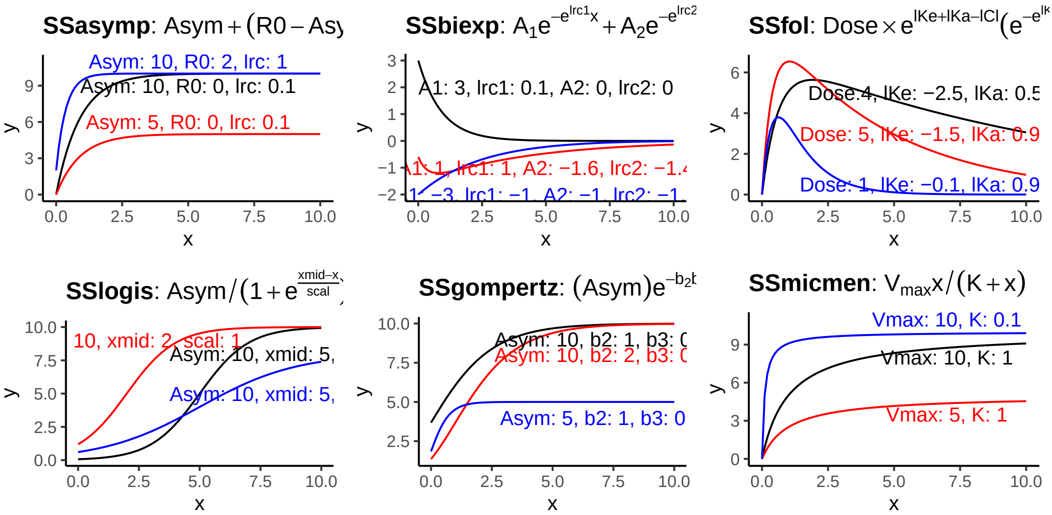
- Broken stick model

How do you get SEs on parameters?

- Easy way: bootstrapping
- Medium way: MCMC sampling (Bayesian estimation)
- Hard way: calculate Hessian of the objective function (serious math)

“There’s got to be a better way!”

Good news: someone already did the scary math for you!



Second challenge

- Try fitting Michaelis-Menten model using:
  - Your own custom function
  - `SSmicmen`

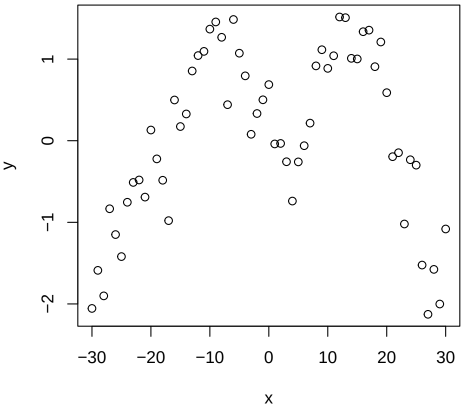
Second challenge results

- Second challenge

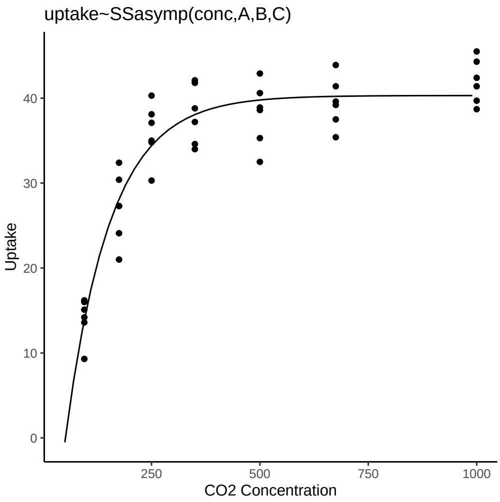
Part 2: Empirical models

Empirical smoothing

- Sometimes we don't know the specific rules that govern your system, but we want to know the *general shape*
  - e.g. population changes across time or space, temperature across seasons
- We want something that can give us *general predictions* across the range of your data without actually dealing with the underlying process
- Solution: "empirical" smoothing



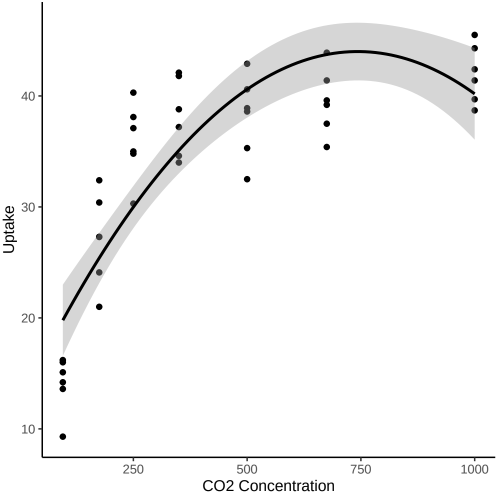
“Guess the family”

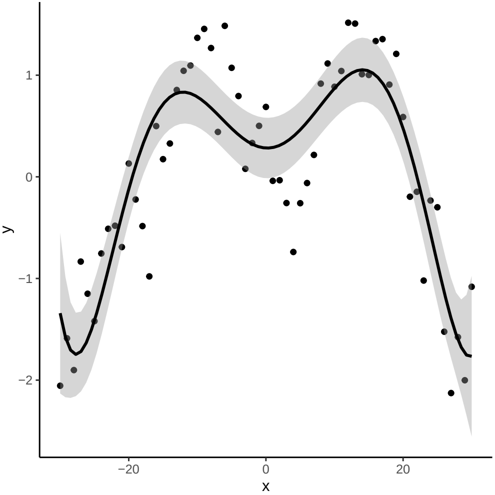


- Sometimes you can use a preset nonlinear family that looks “similar enough” to your data
- e.g. `SSlogis`, `SSweibull`
- See also: “Transformations” slide from first section

Polynomial smoothing

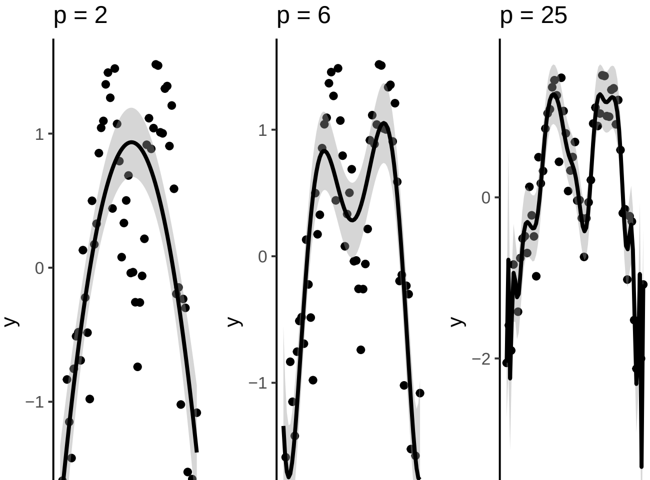
If the pattern is "wiggly", you can use polynomials:





Problems with polynomials

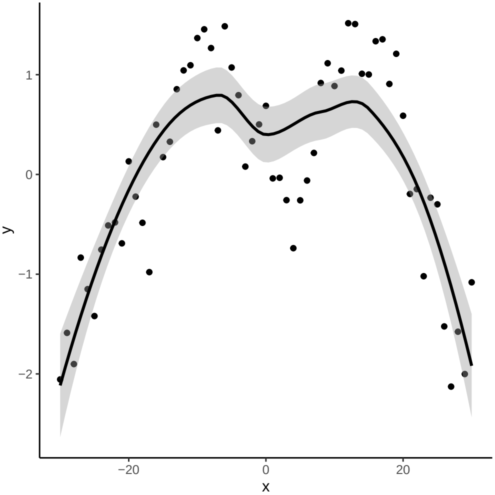
- How many orders of polynomials do you use? Limited to discrete values
- Polynomial models don't do well outside of the range of prediction, especially at the edges of your data



LOESS smoothers

- LOESS (LOcal regrESSion) fits mini-polynomial models for various "chunks" of your data
- Makes sure that the line at the "knots" (divisions between data chunks) is smooth

```
## `geom_smooth()` using formula = 'y ~ x'
```



LOESS problems

- Require a fair bit of data to get good predictions, sensitive to outliers
- Doesn't really work with extra terms: hard to test for differences in LOESS curves
- Similar to polynomials, doesn't do well outside the range of the data

GAM: Generalized Additive Models

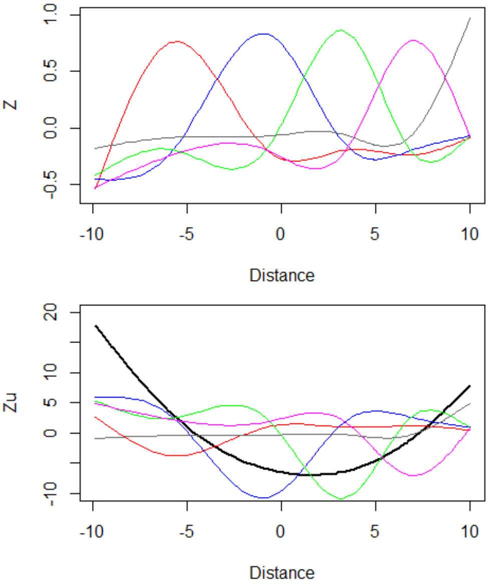
- Additive models are a hybrid linear model that use *basis functions* to approximate "wiggly" data
- Uses random effects to penalize curves in order to avoid overfitting (i.e. "just wiggly enough")
- The `mgcv` package can deal with a large range of additive models, from a large range of distributions (count data, presence/absence, survival, categorical, and more)
- This package is useful for a wide variety of things, and it's definitely worth learning

How do GAMs work?

GAMs take the form:

$$\text{Prediction} = \text{Fixed Effect} + \text{Random Effect}$$
$$\mu = X\beta + Zu$$
$$\text{Yield} \sim Normal(\mu, \sigma)$$
$$u \sim Normal(0, \lambda S)$$

- Creates *basis functions* across the range of data stored in columns of Z
- Finds values u
- λS penalty term: selects for optimal "wiggliness"



GAM example

Let's see how this works on a dataset:

More GAM things

- More tips and tricks about GAMs

2-column slide

a

b