Introduction to Modeling

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Modeling with rates

Big picture: how to do modeling for real problems

Using modeling results

Why models?

What does it mean to make good decisions using models?

What is a model?

A model is a mathematical relationship that comes with a story. Stokey and Zeckhauser (1978) give a definition:

> *"A model is a simplified representation of some aspect of the real world, sometimes of an object, sometimes of a situation or a process"*

A good model reduces a complex situation to a set of essential mechanisms, or dynamics, that an analyst needs in order to make a good decision.

A bad model mischaracterizes the mechanism of interest, is too simple to capture important dynamics, or is too complicated to be calibrated or understood.

Examples

- Optimizing the HIV care pipeline
- Counting drug users and other risk groups
- Deciding whom to vaccinate against disease
- Stopping infectious disease outbreaks
- Optimizing hospital staffing

Modeling and scientific hypotheses

Models formalize scientific hypotheses about the mechanism that produces a phenomenon of interest.

When data agree with our model, then we may accumulate evidence that the model is correct, or at least that the data do not falsify the model.

When we observe data that do not agree with the predictions of our model, then this might be evidence that our hypotheses are wrong.

Model fit to empirical data

Observing that a model fits data well is not a sufficient condition to imply that the model is correct.

What do we mean "correct"? We mean mechanistic or causal. This goes beyond fitting data well. We mean that a model captures the mechanistic features of the data-generating process that are important for the decisions we want to make.

All models are wrong, but some are useful. – George Box

Why are mechanistic models useful?

A few explanations:

- Intuitive: they formalize hypotheses
- Statistical: limit free parameters
- Curse of dimensionality
- Interpretability
- Causal interpretation of counterfactual comparisons

Why are mechanistic models sometimes dangerous?

- Limit hypotheses to models that are easy to specify
- Inflexible structure limits fitting
- Sometimes you don't know when they are wrong, even when they fit data well
- More complicated reasons related to causal inference

Statistical vs mechanistic models

If you have taken a statistics class, you have seen statistical approaches to explaining variation. For example, consider the "statistical regression model"

$$y = \alpha + \beta x + \epsilon$$

If we regard x as a treatment and y as a health outcome for a given patient, then we would like to think of β as the "effect" of the treatment.

This model posits a linear relationship between treatment and outcome. Given a one-unit change in x, we expect the outcome y to change by an increment of β.

My philosophy

I think there is *no difference* between "statistical" and "mechanistic" models, except for the stories we tell about their structure and coefficients. This suggests:

- We should strive to interpret statistical models in a mechanistic way, and reject them if they are deemed unrealistic in their structure.
- We should treat mechanistic models as statistical models and fit them to data, whenever possible. When not possible, we should ask what new data we ought to collect.

Prescriptive versus descriptive models

?

The importance of prediction in public health decision-making

Principles of mechanistic thinking

flow, mass action, density/frequency dependence

The role of causal inference: if I change this input, the effect will be thus

Agent-based models

networks spatial models

Shapes of functions

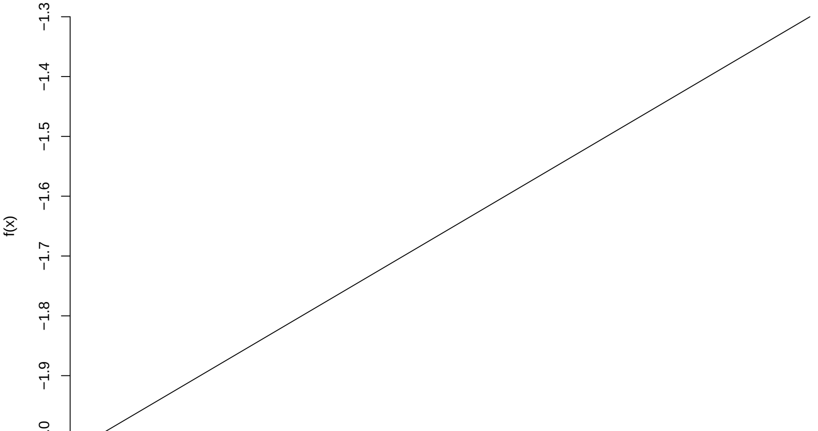
As we begin to construct models, let's think about the building blocks of mathematical relationships: functions and their shapes.

As a brief review, we will go over the basic function types we will see in this course.

Straight lines

$$f(x) = ax + b$$

```
xs = seq(0,1,by=0.01)
plot(xs, -2 + 0.7*xs, type="l", xlab="x", ylab="f(x)", bty=
```



Polynomials

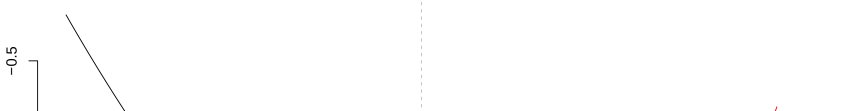
A quadratic equation

$$f(x) = ax^2 + bx + c$$

A cubic equation

$$f(x) = ax^3 + bx^2 + cx + d$$

```
xs = seq(-1,1,by=0.01)
plot(xs, -2 - 0.7*xs + xs^2, type="l", xlab="x", ylab="f(x
lines(xs, -2 - 0.7*xs + xs^2 + xs^3, col="red")
abline(v=0, lty="dashed", col="gray")
abline(h=0, lty="dashed", col="gray")
```



Exponential function

The exponential function is the unique function $f(x)$ such that $f'(x) = f(x)$ for all x. When we write e, it means the "natural number" $e \approx 2.71\ldots$.

$$f(x) = ae^{bx}$$

This may also be written as

$$f(x) = a\exp(bx)$$

when a and b are positive, $f(x) = a\exp(bx)$ grows quickly. Exponential growth happens when a quantity increases at a rate proportional to how big it already is. More on this later.

```
xs = seq(-1,1,by=0.01)
plot(xs, exp(xs), xlab="x", type="l", ylab="f(x)", bty="n")
lines(xs, exp(-xs), col="red")
abline(h=0, lty="dashed", col="gray")
abline(v=0, lty="dashed", col="gray")
```

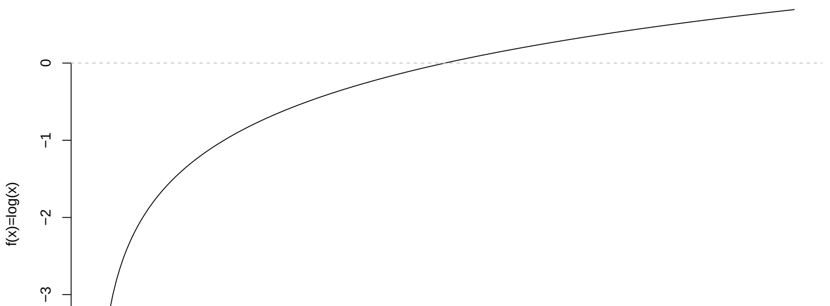
Logarithmic function

The inverse function of exp() is the natural logarithm

$$f(x) = \log(x)$$

That is, if x is any real number and $y = \exp(x)$, then $x = \log(y)$

```
xs = seq(0.01,2,by=0.01)
plot(xs, log(xs), xlab="x", type="l", ylab="f(x)=log(x)", b
abline(h=0, lty="dashed", col="gray")
```



Logistic function

Logistic growth happens when initially a quantity grows quickly (as in exponential growth), but then saturates, or plateaus as its argument gets large.

$$f(x) = \frac{e^{ax}}{1 + e^{ax}}$$

An equivalent way to write this is

$$f(x) = \frac{1}{1 + e^{-ax}}$$

The logistic transform is an easy way to take a quantity x that can be positive or negative, and rescale it so that it is always between 0 and 1.

```
xs = seq(-3,3,by=0.01)
plot(xs, 1/(1+exp(-xs)), xlab="x", type="l", ylab="f(x)", b
abline(h=0, lty="dashed", col="gray")
```

Sinusoidal functions

A useful class of sinusoidal functions is

$$f(x) = a + b\sin(c(x - d))$$

where a is the offset, b is the amplitude, c is the rate or frequency, d is the phase shift.

In this course, the argument to all sinusoidal functions will be in radians.

```
xs = seq(0,4*pi,by=0.01)
plot(xs, sin(xs), xlab="x", type="l", ylab="f(x)=sin(x)", b
abline(h=0, lty="dashed", col="gray")
```

Types of model constructions

Ways of specifying relationships

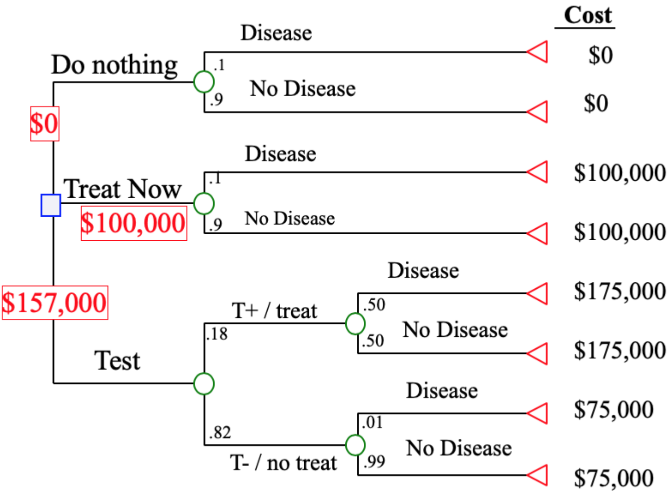
- flow-based
- decision trees
- stochastic and deterministic
- agent-based

Conceptual flow-based

compartmental diagrams

Decision trees

spend some time on this! computing marginal and conditional probabilities on decision trees.



stochastic and deterministic models

Agent-based models

Modeling with rates

Why characterize a process by its rates of change?

It is often easier to think about the dynamics of a process in terms of its rates of change. It is very common that the solution to a system of differential equations is impossible to write down analytically, but very easy to characterize in terms of its rates of change.

So, from a practical perspective, we can often just write the system in terms of its rates of change, and then use a computer to find the "solution" for the dynamics of the system.

In general, the study of analytic solutions of ODEs is a domain of mathematics. We are going to largely avoid analytical solutions and treat these systems as descriptions that can be solved using a computer. We will see several examples next.

Example: A linear model for a treatment effect

Let y be an indicator of 5-year survival in a clinical trial for a new cancer therapy. Let $x \in \{0, 1\}$ the treatment, where $x = 1$ indicates receipt of a new chemotherapy, and $x = 0$ standard of care. We might model the survival outcome as a linear function of x:

$$y = \alpha + \beta x + \epsilon$$

where ϵ is a random number that is zero on average. This is a common statistical model, and people sometimes interpret β as the *causal effect of treatment*.

Example: multiplication of bacteria

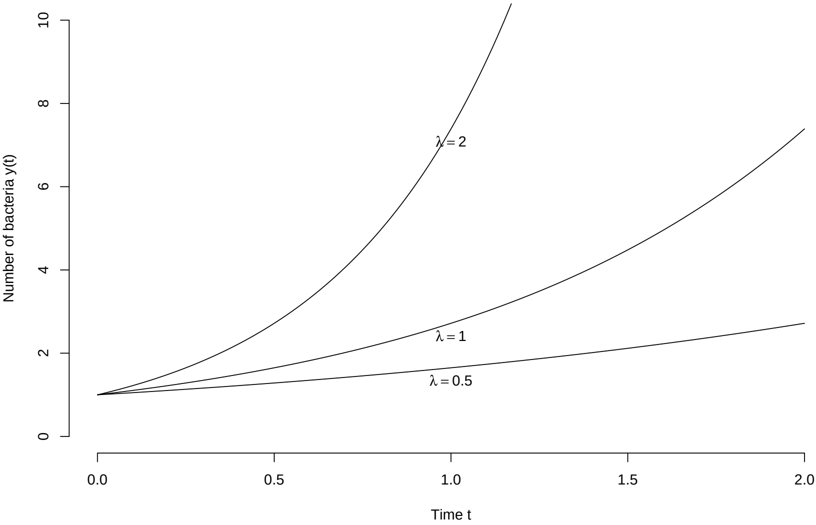
Let $y(t)$ be the number of bacteria in a dish at time t. Suppose at time $t = 0$, there are $y(0) = y_0$ bacterium. Each bacterium is immortal, and divides into two with rate $\lambda > 0$. The number of bacteria at time t is governed by the differential equation

$$\frac{dy}{dt} = \lambda y(t)$$

with initial condition $y(0) = y_0$. The solution is

$$y(t) = y_0 e^{\lambda t}$$

You can verify this by computing dy/dt. The dynamics of this system obey "exponential growth". The speed of this growth is governed by λ.



λ = 2
λ = 1
λ = 0.5
0
2
4
6
8
10
Number of bacteria y(t)
0.0
0.5
1.0
1.5
2.0
Time t

Modeling with compartmental diagrams

Example: HIV care pipeline

Initiation of ART -> viral suppression

Example: spread of an infectious disease

Given $S(0)$ and $N = S(t) + I(t)$, the number of infections at time t is governed by

$$\frac{dI}{dt} = \beta S(t) I(t)$$

Big picture: how to do modeling for real problems

Using modeling results

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References