# Modeling with Deterministic Functions - Capturing Signal

Zack Treisman

Spring 2021

WESTERN
COLORADO UNIVERSITY
MATHEMATICS & COMPUTER SCIENCE DEPARTMENT

# Philosophy

Data analysis and statistics are tools used in modeling.

- A **model** is a proposed distribution of a variable or variables
- Separate any model into two parts: the **signal** and the **noise**.
- This week we are focused on **signal**.

The most fundamental setting is a pair of variables, $x$ and $y$. We know something about $x$, and would like to leverage this to learn something about $y$, to the extent that this is possible. We call $x$ the **predictor** and $y$ the **response**. Write

$$y = f(x) + \epsilon$$

where the model function $f(x)$ is what we call the **signal** and $\epsilon$ is the **noise**.

"All models are wrong but some are useful" - George Box

The usefulness of a model comes when the signal is not drowned out by the noise. In other words the model is **statistically significant**.

# xkcd

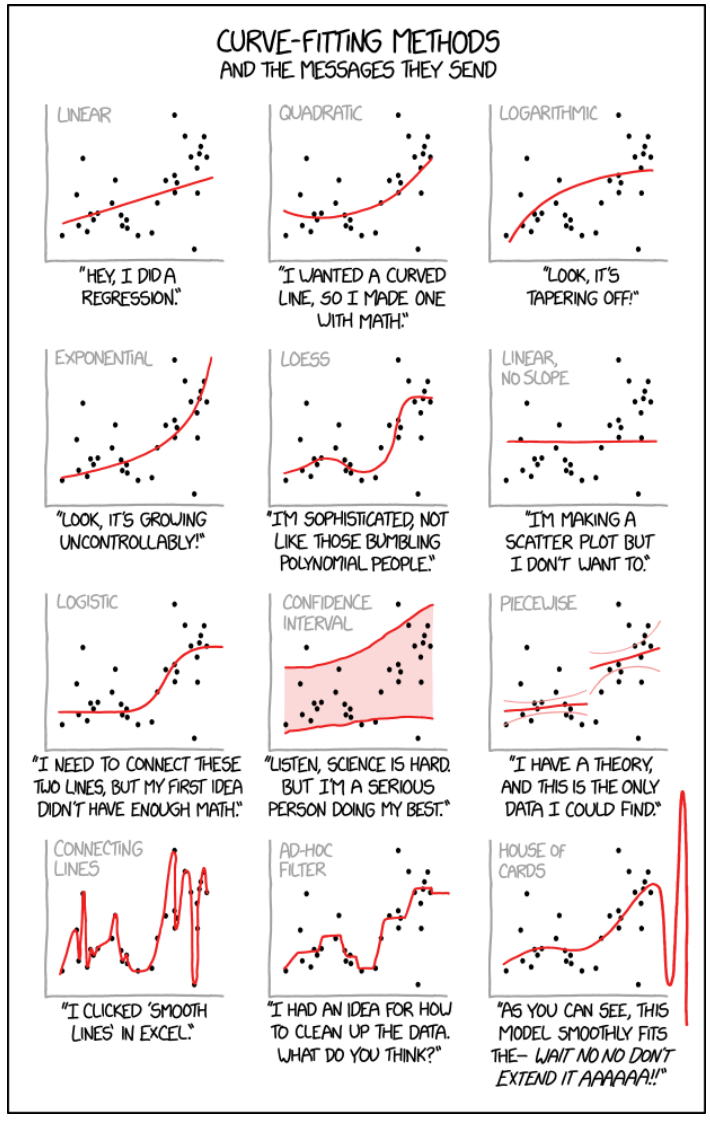



Figure 1: https://xkcd.com/2048

# Model misuse is not a joke

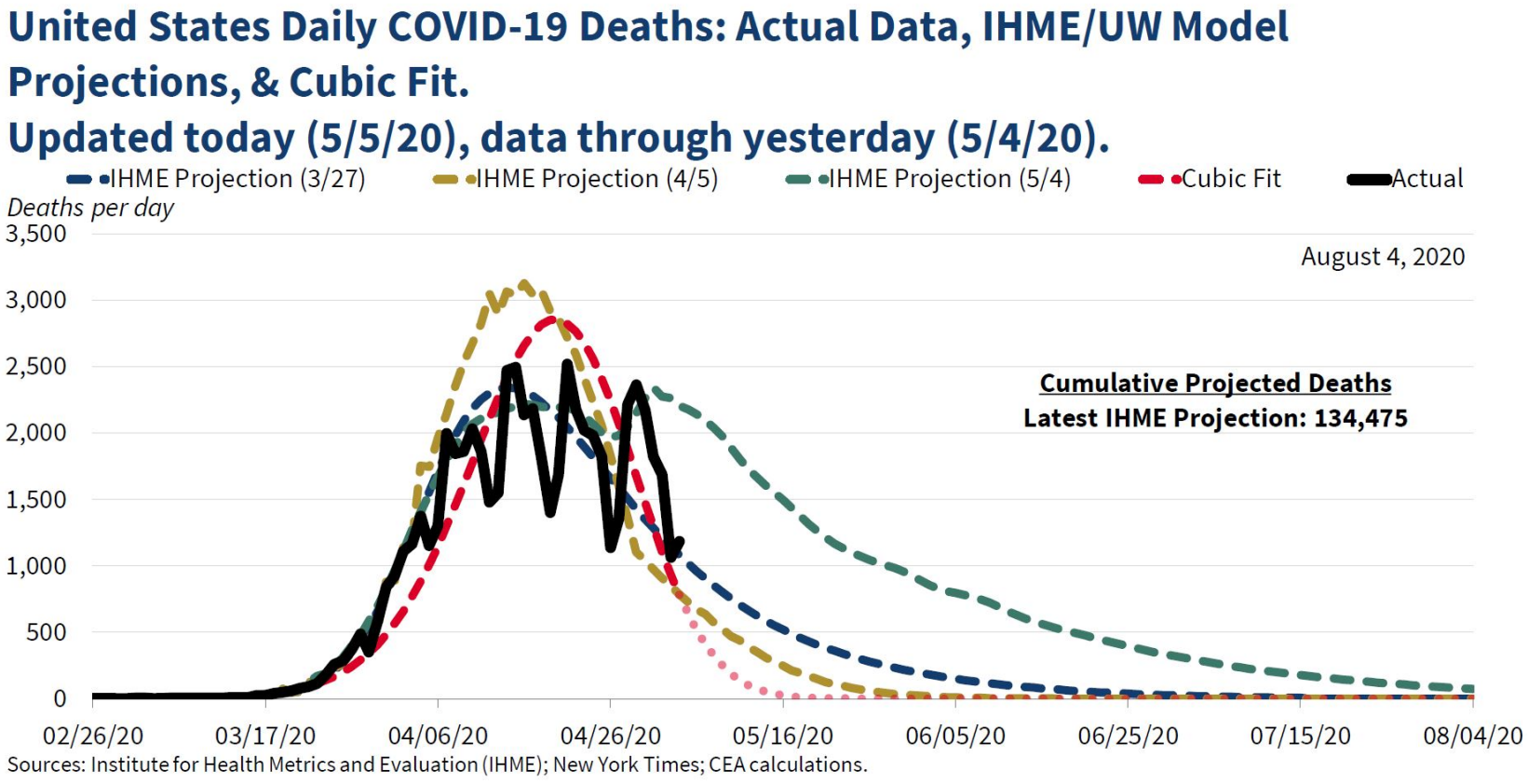



Figure 2:
https://twitter.com/WhiteHouseCEA/status/1257680258364555264

# Reducible and irreducible error

If we had infinite knowledge, we could choose for our model function the expected value, or mean, of all $y$ such that $(x, y)$ is a possible data point. Write $\mu(x)$ for this expected value.

$$y = \mu(x) + \varepsilon$$

We call $\varepsilon$ the **irreducible error** or **intrinsic variance**. It is the uncertainty that exists because of natural variation in the system described.

Any actual model function that we come up with will differ from this optimal function. Suppose we have a model function $f(x)$. We call the difference $f(x) - \mu(x)$ the **reducible error**. With a better $f$ we can reduce the reducible error.

# Bias and Variance

The reducible error can be broken down into two parts.

- The error due to **bias** is that part of the reducible error that comes from a model function's inability to change when it needs to.
- The error due to **variance** is that part of the reducible error that comes from a model function's excessive flexibility to match the particular data that are observed.

A model function with high bias error is said to **underfit** the data, and one with high variance error is an **overfit**. Whenever we are choosing a model, we must consider this **bias-variance tradeoff**.

# Parametric vs Non-parametric models

- A **parametric** model function is one defined in terms of arithmetic and analytic functions, such as logarithms, polynomials, or anything else you might have encountered in a math class like Calculus. The numbers such as coefficients and exponents defining the function are called the **parameters**.
- A **non-parametric** model function is defined in some other way. The first example we will encounter and use is *local regression* or *loess*. Trees and random forests are also non-parametric models.

# Linear function models

If $x$ and $y$ are both numeric variables, then the simplest possible relationship between them is a linear relationship.

$$y = \beta_0 + \beta_1 x + \epsilon$$

- $\beta_0$ is the *intercept*, the value we predict for $y$ when $x$ is zero.
- $\beta_1$ is the *slope*, or predicted rate of change in $y$ with respect to $x$. Often written $\frac{\Delta y}{\Delta x}$ or $\frac{dy}{dx}$.

The tremendous advantage of the linear function model over all others is its simplicity. A disadvantage is a tendency towards high bias error.

Note: This model is linear in the variable $x$ **and** in the *parameters* $\beta_i$. The term "linear model" is frequently applied with both meanings, but the latter is more useful. The R command `lm` refers to linearity in the parameters.

# Linear models with multiple predictors

Extending to multiple predictor variables is straightforward.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

- $\beta_i$ is the expected change in $y$ as $x_i$ changes and all else is constant.
- If the $x_i$ are correlated, these models can be unreliable.

# Linear models with categorical predictors

If a predictor variable is categorical, the linear model can still be used.

- One level is set as the **reference** level of the variable.
- For every other level of the variable, an **indicator variable** is defined, taking the value 1 when the variable has that level and 0 otherwise.
- The coefficient $\beta_i$ is the expected effect from observing level $i$ instead of the reference level.

Examples:

- Control/ Treatment: Control is reference, $x_{\text{treat}}$
- Low/ Medium/ High: Low is reference, $x_{\text{med}}, x_{\text{high}}$

# Polynomial functions

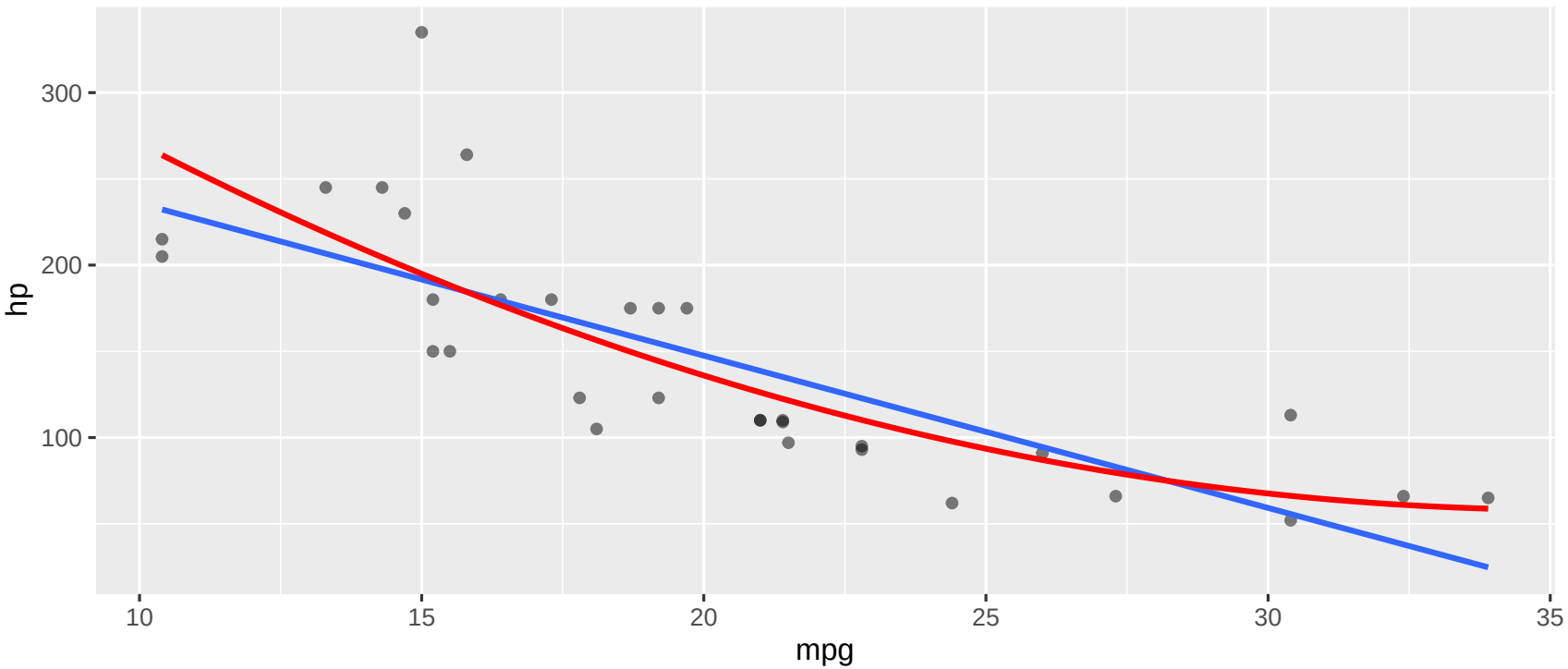
Including powers of $x$ such as $x^2$ or $x^3$ can reduce bias.

Example:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

This is still a linear model even though it includes the $x^2$ term.

```
ggplot(mtcars, aes(mpg, hp)) + geom_point(alpha=0.5) +
  geom_smooth(method = lm, formula = y~x, se=F) +
  geom_smooth(method = lm, formula = y~poly(x,2), se=F, color="red")
```



# Power functions

A power function model is of the form

$$y = ax^k + \epsilon$$

Note that $k$ can be any number, not just a positive integer. This is *not* a linear model because of the parameter $k$.

- Power models can have explanatory meaning if $x$ and $y$ have relevant dimensionality, like mass or area.

Power function models can be fit using linear model techniques by taking logarithms. Ignoring the error term for a moment:

$$\hat{y} = ax^k \qquad \Longleftrightarrow \qquad \log(\hat{y}) = \log(a) + k\log(x)$$

# Back-transforms and error

Models fit on log-transformed variables can be exponentiated back to the original variables. How the error transforms can cause issues.

- Exponentiating the predicted mean of a log-transformed variable does **not** predict the untransformed mean.
  - When back-transforming, add half the variance in the residuals before exponentiating to recover the mean.
  - Diagnostics such as $R^2$ and p values apply to the transformed variables, not after back-transformation.
- Linear regression assumes that the error is additive. Exponentiation changes this addition into multiplication.

Suppose we fit a model:

$$\log(y) \sim N\left(\hat{\beta}_0 + \hat{\beta}_1 \log(x), \sigma^2\right).$$

Then the prediction for the mean of $y$ is

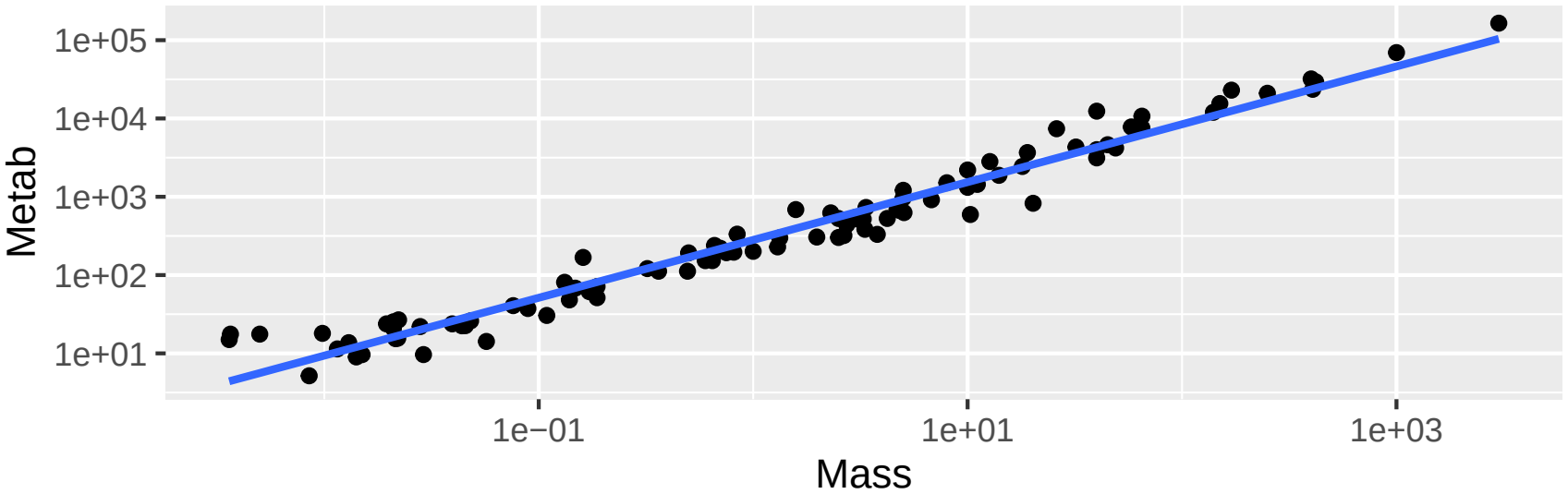
$$e^{\hat{\beta}_0 + \hat{\beta}_1 \log(x) + \sigma^2/2} = e^{\hat{\beta}_0 + \sigma^2/2} x^{\hat{\beta}_1}$$

and the variance is dependent on $x$.

# Kleiber's law

Mass and metabolic rate of mammals relate via a power law.

```
ggplot(ex0826, aes(Mass, Metab)) + geom_point() + # data in Sleuth3
  scale_x_log10() + scale_y_log10() + geom_smooth(method = lm, se=F)
```




```
lm1 <- lm(log(Metab)~log(Mass), data = ex0826)
lm1$coefficients; var(lm1$residuals)
```

```
## (Intercept)   log(Mass)
##   5.6383307   0.7387436
```

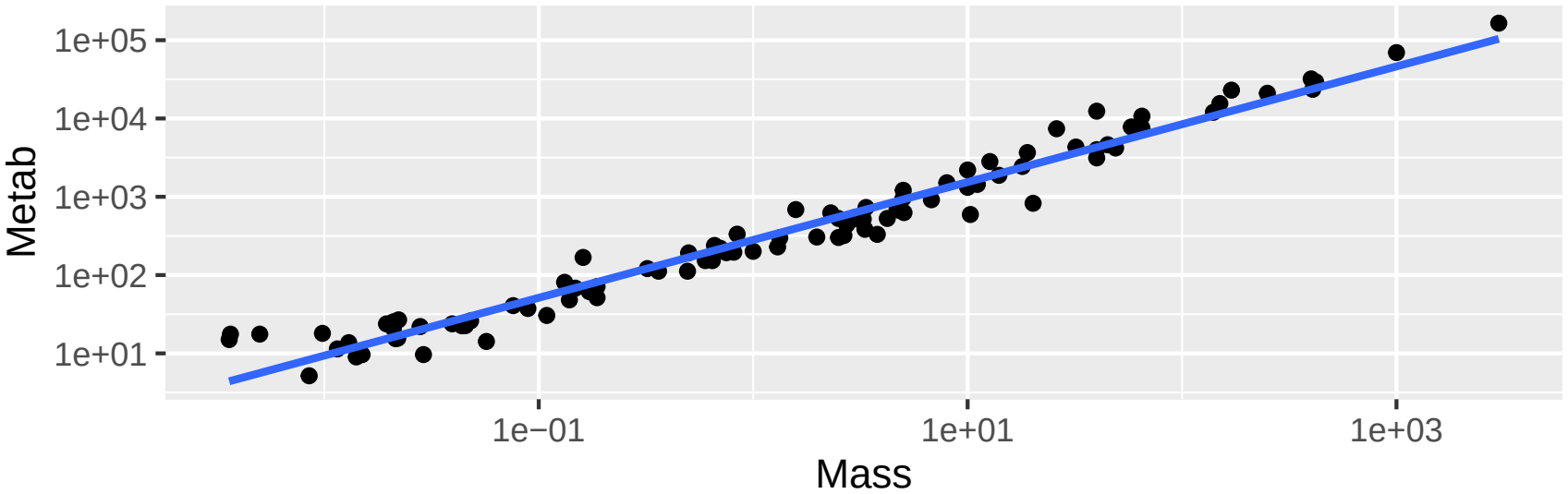
```
## [1] 0.2068395
```

$$\text{Metab} = e^{5.64+0.21/2} \times (\text{Mass})^{0.74} \times \epsilon$$

# Kleiber's law

Mass and metabolic rate of mammals relate via a power law.

```
ggplot(ex0826, aes(Mass, Metab)) + geom_point() + # data in Sleuth3
  scale_x_log10() + scale_y_log10() + geom_smooth(method = lm, se=F)
```




```
lm1 <- lm(log(Metab)~log(Mass), data = ex0826)
lm1$coefficients; var(lm1$residuals)
```

```
## (Intercept)   log(Mass)
##   5.6383307   0.7387436
```

```
## [1] 0.2068395
```

$$\text{Metab} = e^{5.64+0.21/2} \times (\text{Mass})^{0.74} \times \epsilon$$

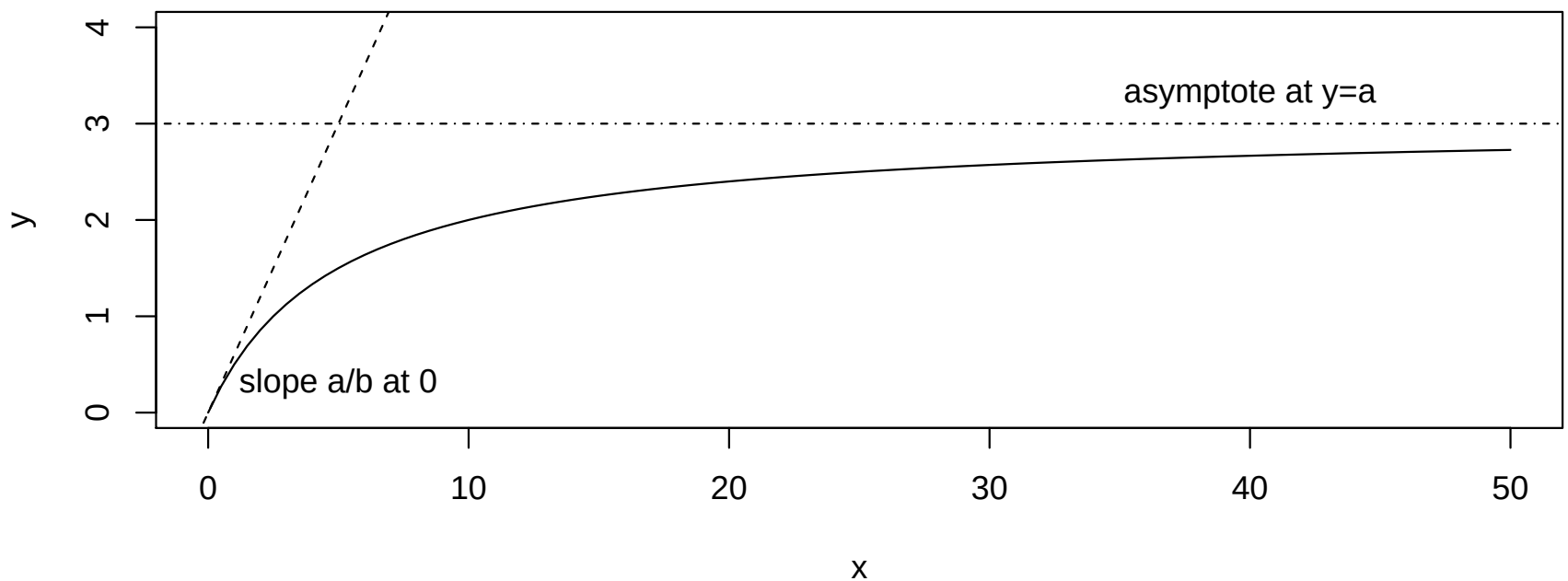
# Rational models

The ratio of two polynomials is called a **rational function**. They can have asymptotes. Not generally linearizable.

Example: Michaelis-Menten/ Holling (McNickle and Brown (2014))

$$f(x) = \frac{ax}{b + x}$$

```
curve(3*x/(5+x), from = 0, to = 50, ylim = c(0, 4), ylab = "y")
abline(h=3, lty = 4); abline(0, 3/5, lty = 2)
text(5, 0.3, "slope a/b at 0"); text(40, 3.3, "asymptote at y=a")
```



# Exponential models

Exponential growth and decay are very common.

- $\frac{dy}{dx}$ means change in $y$ as $x$ changes.
- $\frac{dy}{dx} = k \cdot y$ means $y$ changes by a fixed fraction ($k$) of itself.

The solution is

$$y = a\, e^{kx} + \epsilon$$

Growth if $k > 0$, decline if $k < 0$.

- Exponential growth is usually bad for extrapolation. Something else tends to take over.
- With a little algebra, exponential decay can be used to model convergence to any asymptote.

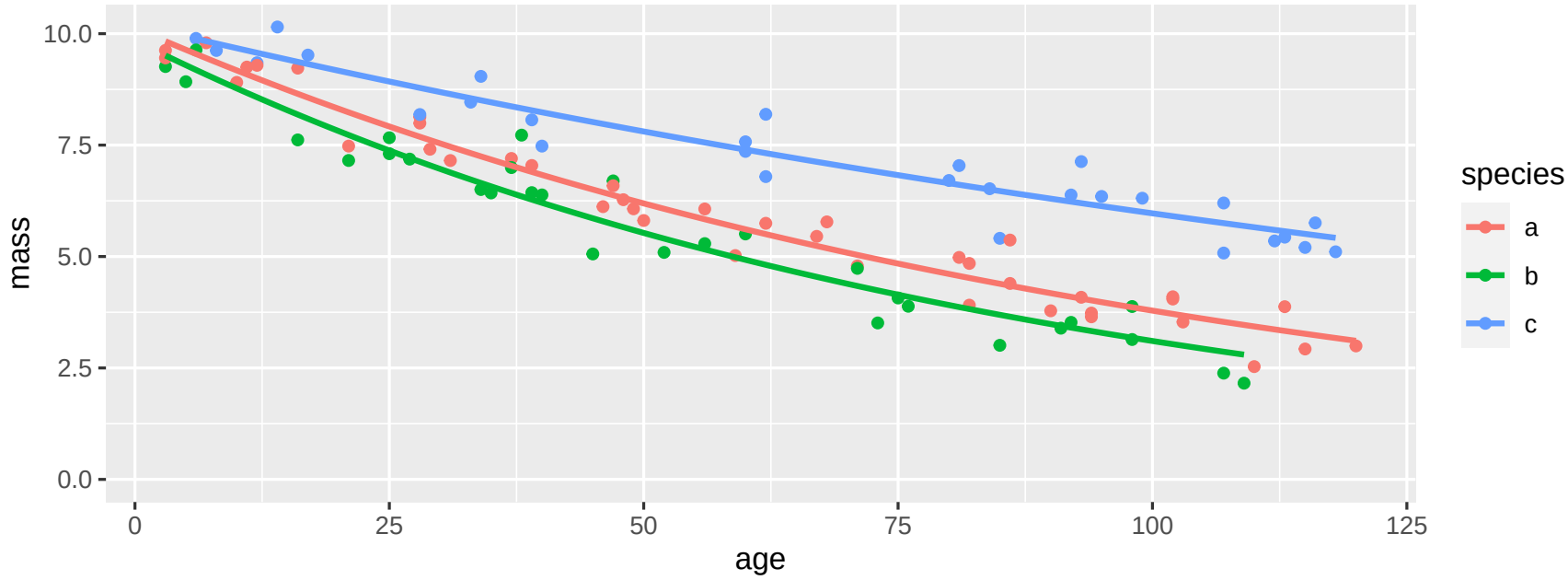
These models are not linear, but taking logs make them so:

$$\hat{y} = a\, e^{kx} \qquad \Longleftrightarrow \qquad \log(\hat{y}) = \log(a) + kx$$

# Exponential decay example

Exponential decay has long been used to model decomposition of biotic material. Olson (1963)

```
# Simulated data, see RMarkdown for code.
ggplot(decay, aes(age, mass, color=species))+
  expand_limits(y=0)+
  geom_point()+
  geom_smooth(method="glm",
              method.args = list(family=gaussian(link="log")),
              se=FALSE)
```



# Decay model using log-transformed mass

In this model speciesb and speciesc are not significant at $\alpha = 0.05$ but the interaction terms are, so their initial quantities do not appear to differ from species a, but their decay rates do.

```
lm2 <- lm(log(mass)~age*species, data=decay)
round(summary(lm2)$coefficients,4)
```

```
##                Estimate Std. Error  t value Pr(>|t|)
## (Intercept)      2.3225     0.0283  81.9712   0.0000
## age             -0.0100     0.0004 -24.5589   0.0000
## speciesb        -0.0059     0.0434  -0.1363   0.8919
## speciesc         0.0019     0.0455   0.0410   0.9674
## age:speciesb    -0.0023     0.0007  -3.3980   0.0010
## age:speciesc     0.0046     0.0006   7.5162   0.0000
```

```
round(var(lm2$residuals),4)
```

```
## [1] 0.008
```

The model for the mean is:

$$\text{mass} = 10.242 \times e^{(-0.01-0.0023\chi_b+0.0046\chi_c)\text{age}} \times \epsilon$$

$10.242 = e^{2.3225+0.008/2}$ and $\chi_b$ and $\chi_c$ are indicator functions.

# Link functions

Most people who fit models to log transformed variables don't do the back-transformation. But this means that they aren't actually talking about the variables in the system they want to model.

**Generalized linear models** (GLMs) offer a solution: link functions. The mathematics of computing the parameters is more complicated, but they give a model that for untransformed variables.

A GLM with a log link for $y$ in terms of $x$ fits:

$$\log(\mu_y) = \beta_0 + \beta_1 x$$

or equivalently

$$\mu_y = e^{\beta_0 + \beta_1 x}$$

and the error is homoscedastic, as we like it.

Using GLMs and link functions means we can talk about our variables, not their transforms.

# Decay model using `glm` and log link

Specifying a link function for a GLM in R is done in the `family` argument, which is used to describe the shape of the error. For normally distributed error, use `family=gaussian`.

```
lm2a <- glm(mass~age*species, family=gaussian(link=log), data=decay)
round(summary(lm2a)$coefficients, 4)
```

```
##                Estimate Std. Error  t value Pr(>|t|)
## (Intercept)      2.3150     0.0185 125.4186   0.0000
## age             -0.0098     0.0004 -25.8990   0.0000
## speciesb        -0.0280     0.0300  -0.9342   0.3526
## speciesc         0.0082     0.0278   0.2947   0.7689
## age:speciesb    -0.0017     0.0007  -2.5257   0.0132
## age:speciesc     0.0045     0.0005   8.9756   0.0000
```

Note the increase in the p-value for the `age:speciesb` term.

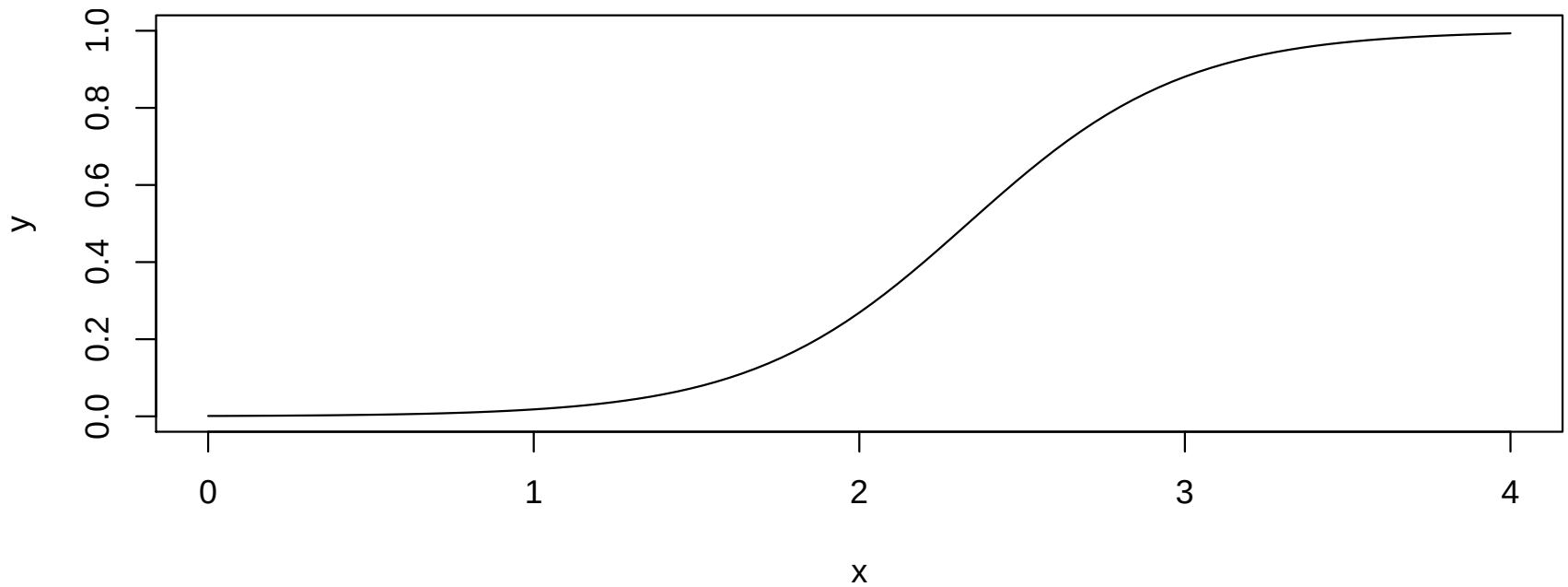
- It is possible that a difference between groups can appear significant for log transformed variables but not when we look at the variables directly.

# Logistic models

The logistic function makes a transition from $y = 0$ to $y = 1$.

$$y = \frac{e^{a+bx}}{1 + e^{a+bx}}$$

```
curve(exp(-7+3*x)/(1+exp(-7+3*x)), from=0, to=4, ylim=c(0, 1), ylab="y")
```

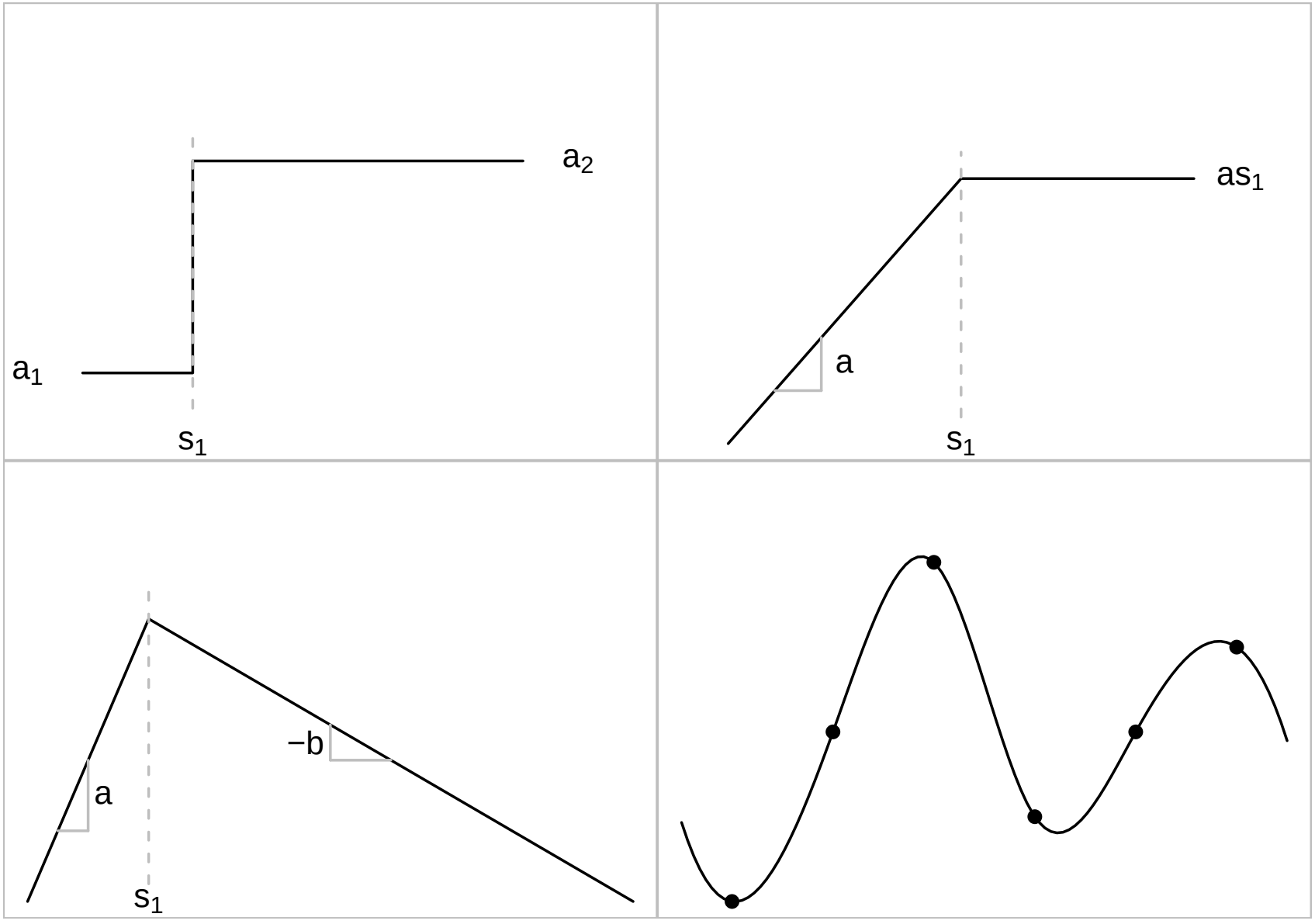



- Mostly used for binary classification. (logistic regression)
- Also useful for populations with a carrying capacity.

Model with `link=logit` in `glm`. Default for `family=binomial`.

# Piecewise models

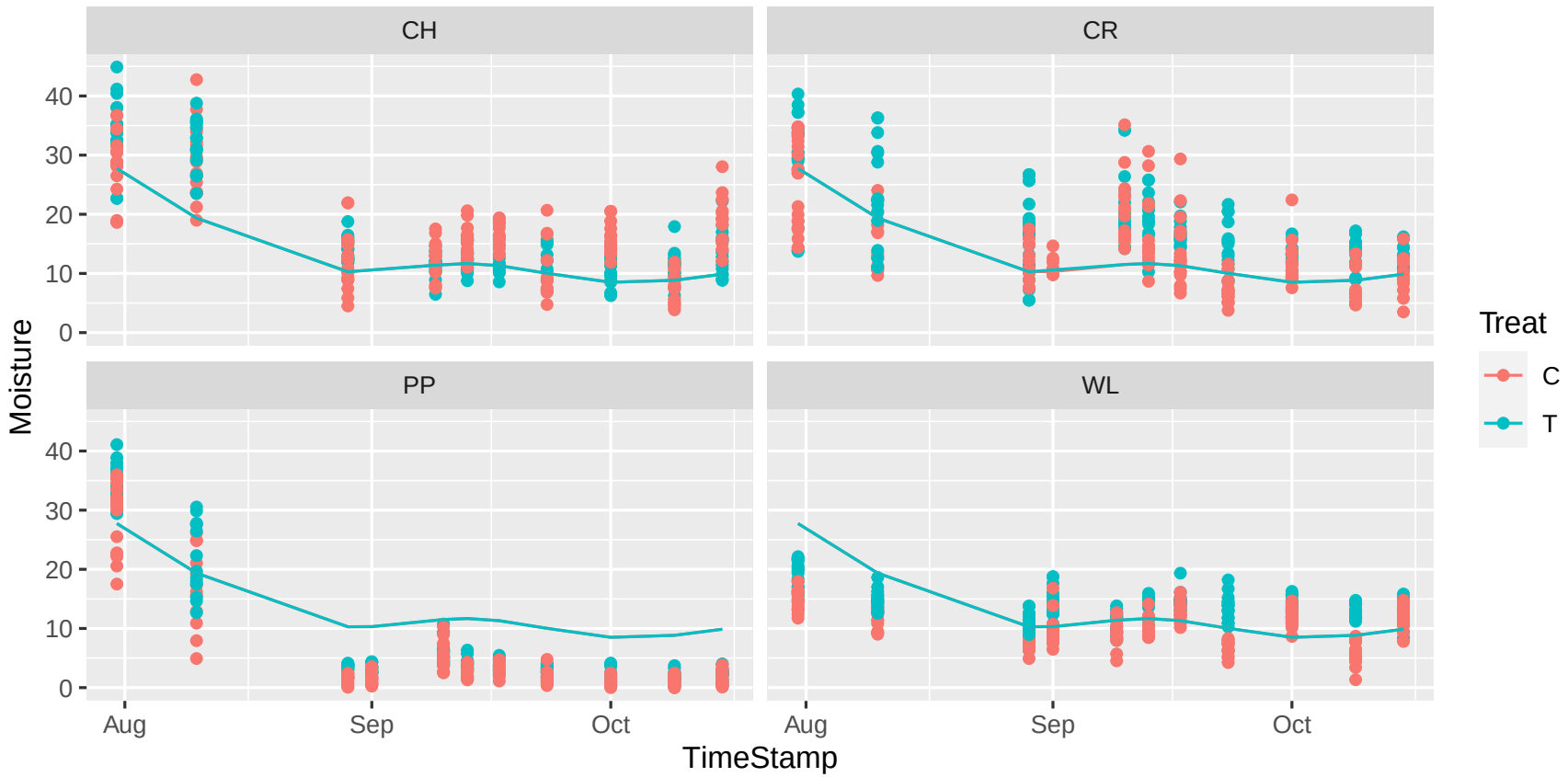
Bolker (2008) Figure 3.7.



# Splines

Weather drives the response. A spline can help account for this.

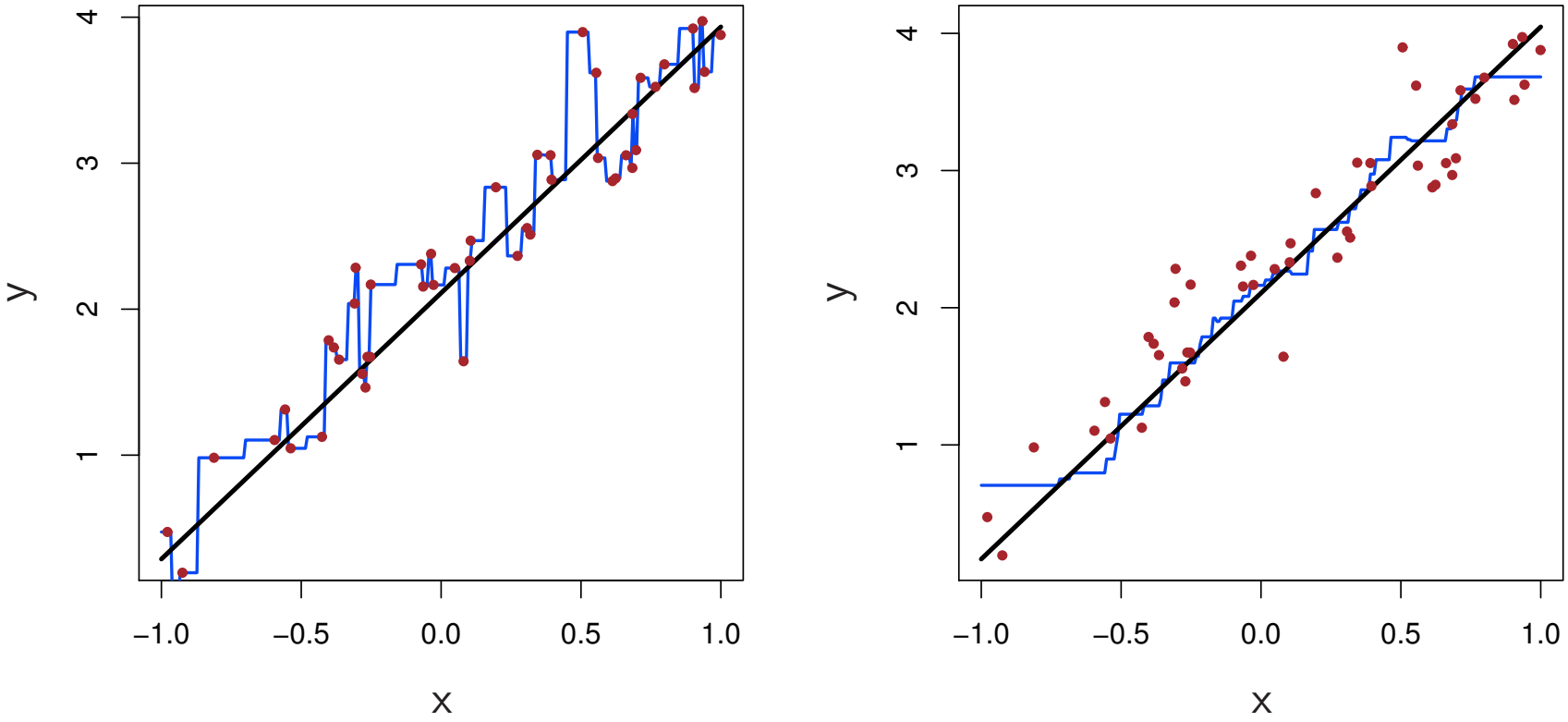
```
SoilMoist <- read.csv("data/SoilMoisture_ALL.csv") # Alexia Cooper's data
SoilMoist$TimeStamp <- mdy(SoilMoist$TimeStamp)
splinemod <- lm(Moisture~ns(TimeStamp,4), data=SoilMoist)
SoilMoist$pred <- predict(splinemod)
ggplot(SoilMoist, aes(TimeStamp,Moisture, color = Treat))+
  facet_wrap(~Site)+geom_point()+geom_line(aes(y=pred))
```



# Nearest neighbor averaging (knn)

- Assume the actual expected value function doesn't change too quickly: $\mu(x-h) \approx \mu(x) \approx \mu(x+h)$.

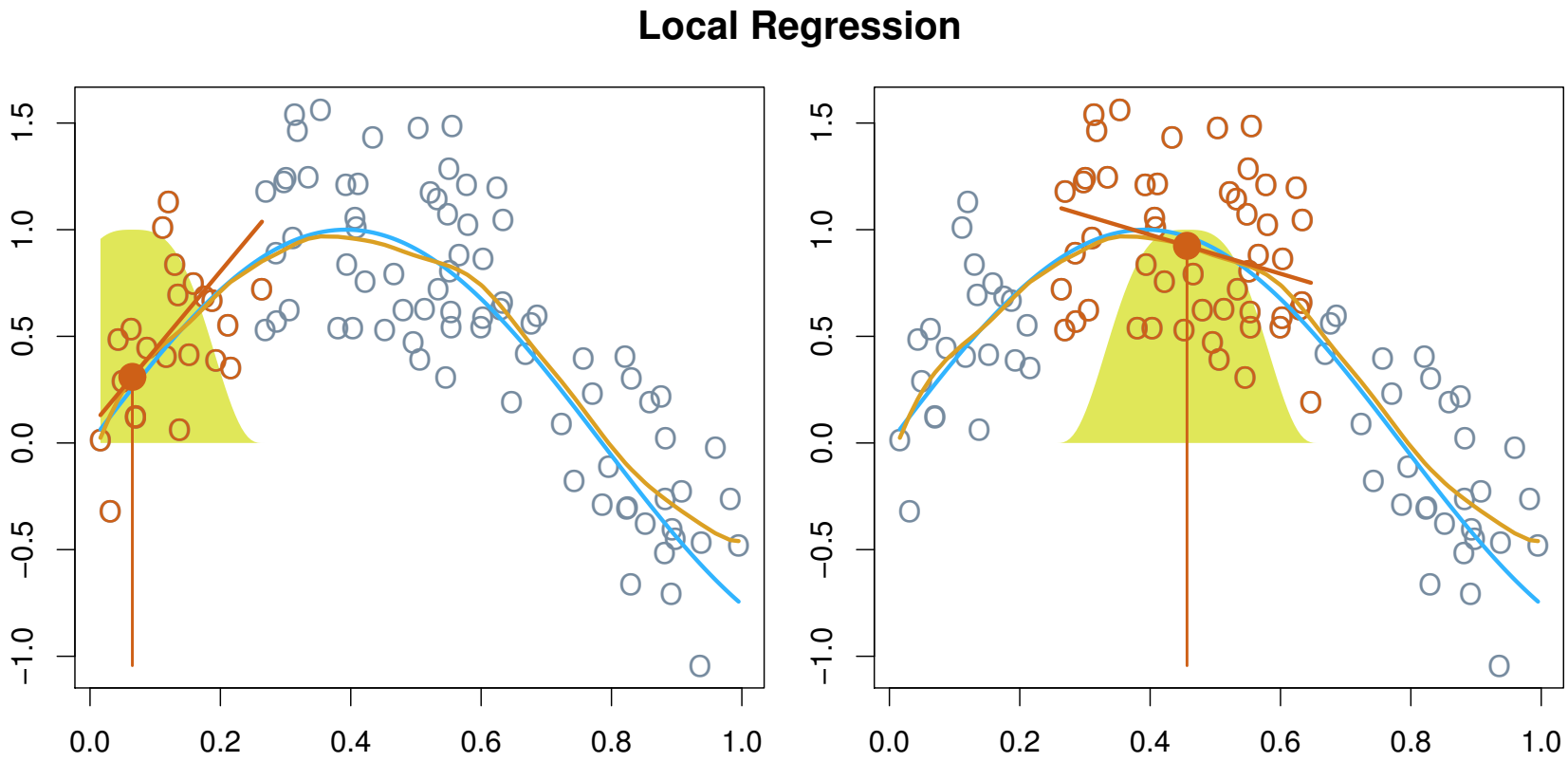
Choose a positive integer $k$ and define $f(x)$ as the average of $y_i$ for the points $(x_i, y_i)$ where $x - x_i$ is among the $k$ smallest.




Left: knn with $k = 1$. Variance is high. Right: knn with $k = 9$.

# Weighted averaging and local regression (loess)

Choose a distance and define $f(x)$ by linear regression using the data within that distance of $x$ or weighted based on that distance.




Simulated data. Blue curve is the true signal, orange is the weighted local regression.

# Loess in R

One way to do loess in R is to use `gam` and `lo`.

```
moistmod0 <- gam(Moisture~lo(TimeStamp), data=SoilMoist)
moistmod1 <- gam(Moisture~lo(TimeStamp)+Site, data=SoilMoist)
moistmod2 <- gam(Moisture~lo(TimeStamp)+Site+Treat, data=SoilMoist)
moistmod3 <- gam(Moisture~lo(TimeStamp)+Site*Treat, data=SoilMoist)
anova(moistmod0, moistmod1, moistmod2, moistmod3, test="F")
```

```
## Analysis of Deviance Table
##
## Model 1: Moisture ~ lo(TimeStamp)
## Model 2: Moisture ~ lo(TimeStamp) + Site
## Model 3: Moisture ~ lo(TimeStamp) + Site + Treat
## Model 4: Moisture ~ lo(TimeStamp) + Site * Treat
##   Resid. Df Resid. Dev Df Deviance       F    Pr(>F)
## 1    1362.8      56413
## 2    1359.8      38604  3  17809.1 225.919 < 2.2e-16 ***
## 3    1358.8      36577  1   2026.9  77.138 < 2.2e-16 ***
## 4    1355.8      35627  3    950.3  12.056 8.642e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Using loess instead of a spline, we ask if `Site`, `Treat`, and their interaction are significant drivers of soil moisture after accounting for the common temporal variability. It appears that the answer is yes.

# Acknowledgements

Some figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

Other figures are created using code provided by Ben Bolker related to his text "Ecological Models and Data in R" (Princeton 2008)

# References


Bolker, Benjamin M. 2008. *Ecological Models and Data in R*. Princeton University Press.

James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani. 2013. *An Introduction to Statistical Learning: With Applications in R*. Springer. https://faculty.marshall.usc.edu/gareth-james/ISL/.

McNickle, Gordon G., and Joel S. Brown. 2014. "When Michaelis and Menten met Holling: towards a mechanistic theory of plant nutrient foraging behaviour." *AoB PLANTS* 6 (December). https://doi.org/10.1093/aobpla/plu066.

Olson, Jerry S. 1963. "Energy Storage and the Balance of Producers and Decomposers in Ecological Systems." *Ecology* 44 (2): 322–31. https://doi.org/https://doi.org/10.2307/1932179.