# Modeling with Deterministic Functions - Capturing Signal

Zack Treisman

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WESTERN COLORADO UNIVERSITY
MATHEMATICS & COMPUTER SCIENCE DEPARTMENT

## Philosophy

Our basic scenario: $x$ is a **predictor** and $y$ the **response**. We want

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

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

- Making good models means choosing an appropriate $f(x)$ and an appropriate $\epsilon$.
- These choices are interdependent, but this week we'll focus more on signal than noise.

## xkcd

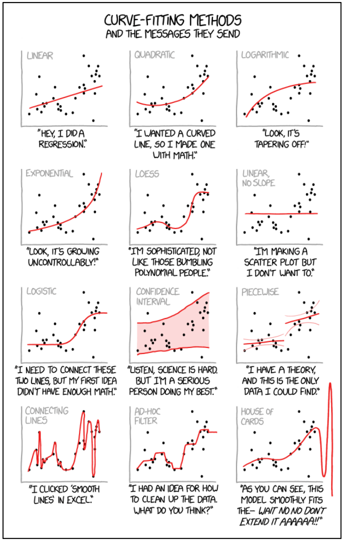

CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
"HEY, I DID A REGRESSION."
QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
"LOOK, IT'S TAPERING OFF!"
EXPONENTIAL
"LOOK, IT'S GROWING UNCONTROLLABLY!"
LOESS
"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
LINEAR, NO SLOPE
"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."
LOGISTIC
"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."
CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
CONNECTING LINES
"I CLICKED 'SMOOTH LINES' IN EXCEL."
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE- WAIT NO NO DON'T EXTEND IT AAAAAA!!"

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

## Model misuse is not a joke

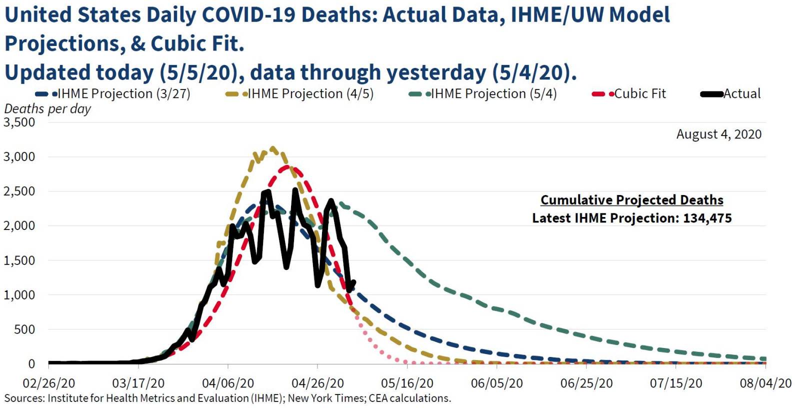


Figure 2:
https://twitter.com/WhiteHouseCEA/status/1257680258364555264

## 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.

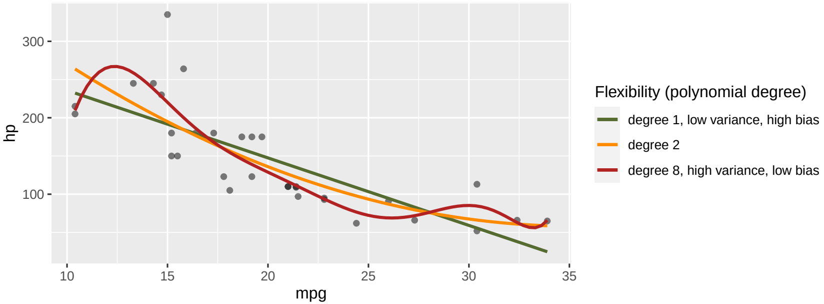
Any actual model function that we come up with will differ from this optimal function. Suppose we have a model function $f(x)$. We call the difference $f(x) - \mu(x)$ the **reducible error**. With a better $f$ we can reduce the reducible error.

## Bias and Variance

The reducible error can be broken down into two parts.

- **Bias** is that part of the reducible error that comes from a model function's inability to change when it needs to.
- **Variance** is that part of the reducible error that comes from a model function's flexibility to match particular data.

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 coefficients, exponents *et cetera* defining the function are called the **parameters**.
  - Parametric models can be more interpretable and meaningful, especially if there are some deterministic processes in play.
  - In principle, any function can be used, but a great deal of the work in statistics is done by linear functions and a few others.
- 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, random forests, neural networks and most other are also non-parametric models.
  - Non-parametric models often have better predictive power and can fit data more effectively.

## 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.

## Multiple predictors, categorical predictors

As we discussed last week, extending to multiple predictor variables or categorical predictors is relatively straightforward.

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

- $\beta_i$ is expected change in $y$ as $x_i$ changes and all else is fixed.
- If a predictor variable is categorical:
  - 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. My typical notation for an indicator variable is $\chi_i$.
  - The coefficient $\beta_i$ is the expected effect from observing level $i$ instead of the reference level.
- If the $x_i$ are correlated, these models can be unreliable.

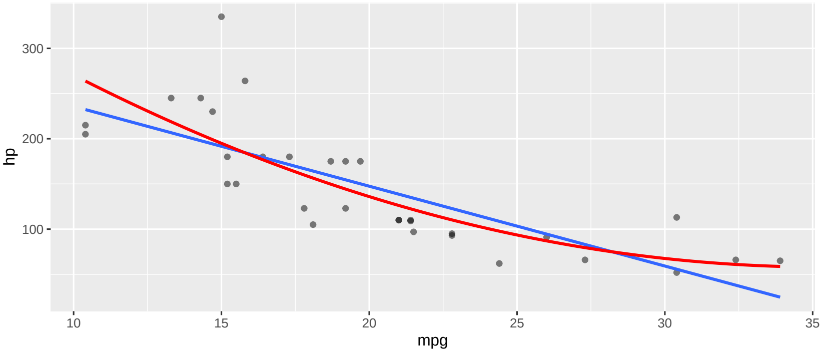
## Polynomial functions

Powers of $x$ such as $x^2$ or $x^3$ **reduce bias** but **increase variance**.

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

This is still a linear model even though it includes the $x^2$ term. The parameters $\beta_i$ appear linearly.

```
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 looks like

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

- $k$ 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, for example 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:

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

Then the prediction for the mean of $y$ is

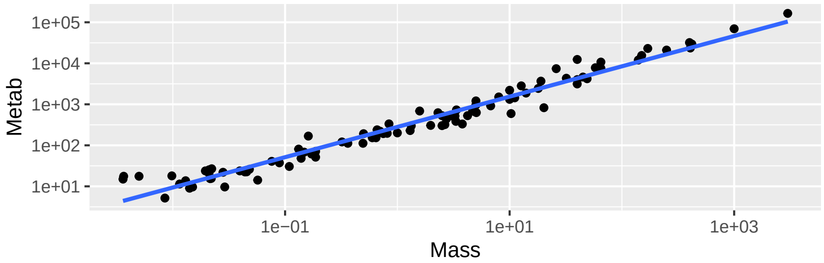
$$e^{\hat{\beta}_0 + \hat{\beta}_1 \log(x) + \sigma^2/2} = e^{\hat{\beta}_0 + \sigma^2/2} x^{\hat{\beta}_1}$$

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
```

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

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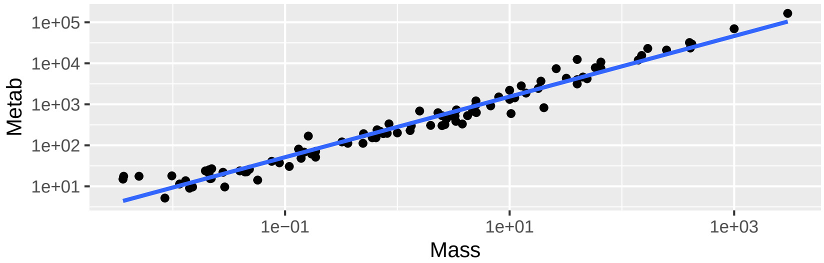

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## Exponential models

Exponential growth and decay are very common.

- $\frac{dy}{dx} = k \cdot y$
- Change in $y$ is proportional (with coefficient $k$) to $y$ itself.

The solution is

$$y = a\, e^{kx} + \epsilon, , \quad a = \text{initial value}, \quad k = \text{growth or decay rate}$$

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:

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

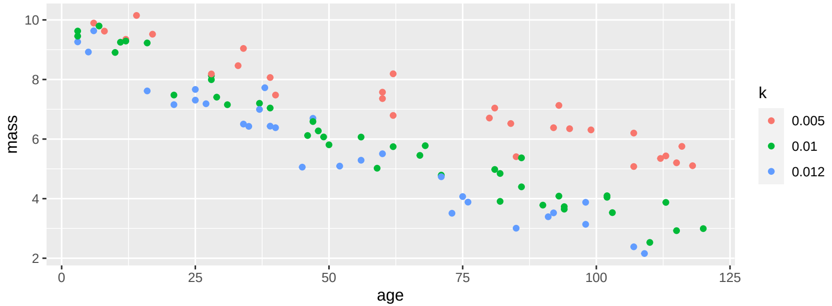
## Exponential decay example

Exponential decay can model decomposition, radioactive decay, temperature changes, and many other scenarios.

Simulate: $a = 10, k = 0.005 + 0.005\chi_{green} + 0.007\chi_{blue}, \sigma = 0.5$

$$\hat{\texttt{mass}} = 10\, e^{(0.005+0.005\chi_{green}+0.007\chi_{blue})\texttt{age}}, \quad \text{or}$$
$$\log(\hat{\texttt{mass}}) = \log 10 + (0.005 + 0.005\chi_{green} + 0.007\chi_{blue})\texttt{age}$$

```
# Simulated data, see RMarkdown for code.
ggplot(decay, aes(age, mass, color=k))+geom_point()
```



## Option 1: model using log-transformed `mass`

Take logs of all the `mass` values and then make a linear model.

```
lm2 <- lm(log(mass)~age*k, data=decay)
```

```
##              Estimate Std. Error  t value Pr(>|t|)
## (Intercept)   2.3243     0.0356  65.2844   0.0000
## age          -0.0054     0.0005 -11.7842   0.0000
## k0.01        -0.0019     0.0455  -0.0410   0.9674
## k0.012       -0.0078     0.0485  -0.1606   0.8728
## age:k0.01    -0.0046     0.0006  -7.5162   0.0000
## age:k0.012   -0.0069     0.0007  -9.7919   0.0000
```

Residual variance is 0.008. At $\alpha = 0.05$ this model says . . .

- Significant intercept: the initial value for the `mass` for red points is not 1. (Its log is not 0.)
- Significant coefficient on age: $k \neq 0$ for the red points.
- No significant coefficients on indicator variables: initial `mass` does not appear to depend on color.
- Significant coefficients of the interaction terms for age and the indicator variables: decay rates differ by color.

## Option 1 (continued)

```
##                Estimate Std. Error  t value Pr(>|t|)
## (Intercept)     2.3243     0.0356  65.2844   0.0000
## age            -0.0054     0.0005 -11.7842   0.0000
## k0.01          -0.0019     0.0455  -0.0410   0.9674
## k0.012         -0.0078     0.0485  -0.1606   0.8728
## age:k0.01      -0.0046     0.0006  -7.5162   0.0000
## age:k0.012     -0.0069     0.0007  -9.7919   0.0000
```

Plugging the significant coefficients in and simplifying, the model is:

$$\log(\texttt{mass}) = 2.3243 + (-0.0054 - 0.0046\chi_{green} - 0.0069\chi_{blue})\text{age} + \epsilon$$

Where $\epsilon \sim N(0, \sqrt{0.008})$. Transforming back to the original scale[1]:

$$\texttt{mass} = 10.26048 \times e^{(-0.0054 - 0.0046\chi_{green} - 0.0069\chi_{blue})\text{age}} \times e^{\epsilon}$$

This is pretty close to the actual model, but there is a potential issue. The error has become multiplicative instead of additive, and it follows this “exponential normal” distribution.

[1] using $10.26048 = e^{2.3243 + 0.008/2}$

## Link functions

Many 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:

Assume there is an invertible function $g(x)$ and define a model

$$y = g(\beta_0 + \beta_1 x) + \epsilon.$$

The function $g^{-1}$ is called the **link**. For example, a GLM with a log link finds:

$$\log(\hat{y}) = \hat{\beta}_0 + \hat{\beta}_1 x$$

or equivalently

$$\hat{y} = e^{\hat{\beta}_0 + \hat{\beta}_1 x}.$$

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

## Option 2: model using `glm` and log link

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

```
lm2a <- glm(mass~age*k, family=gaussian(link=log), data=decay)
```

```
##              Estimate Std. Error  t value Pr(>|t|)
## (Intercept)   2.3232     0.0208 111.5830   0.0000
## age          -0.0054     0.0003 -16.6556   0.0000
## k0.01        -0.0082     0.0278  -0.2947   0.7689
## k0.012       -0.0362     0.0315  -1.1500   0.2531
## age:k0.01    -0.0045     0.0005  -8.9756   0.0000
## age:k0.012   -0.0062     0.0006  -9.5910   0.0000
```

The resulting model is

$$\texttt{mass} = 10.20829 \times e^{(-0.0054-0.0045\chi_{green}-0.0062\chi_{blue})\text{age}} + \epsilon$$

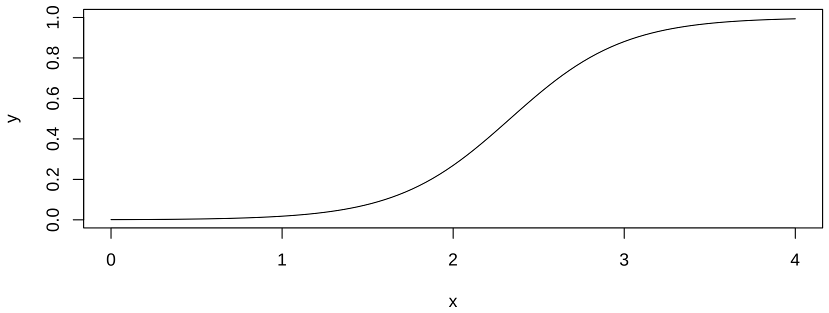
where $\epsilon$ is normally distributed with standard deviation 0.4594.

## 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.

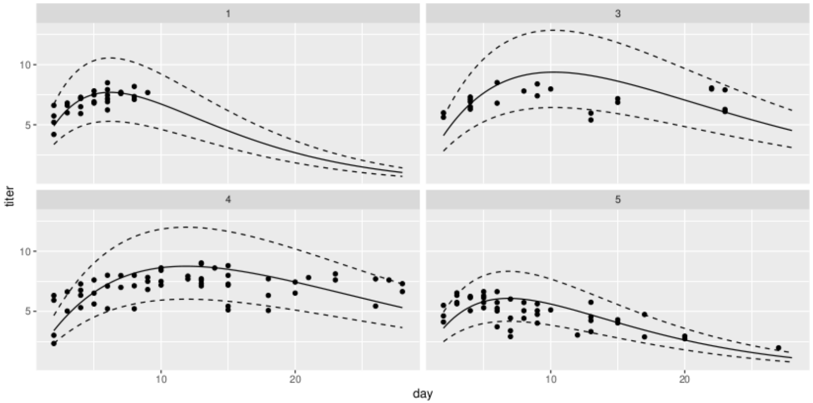
Model with `link=logit` in `glm`. Default for `family=binomial`.

## Other function models

Any function can potentially be used as a model function.

- Several pre-packaged link functions are available and work well with particular choices of error distribution.
- More complicated functions require more complicated code.

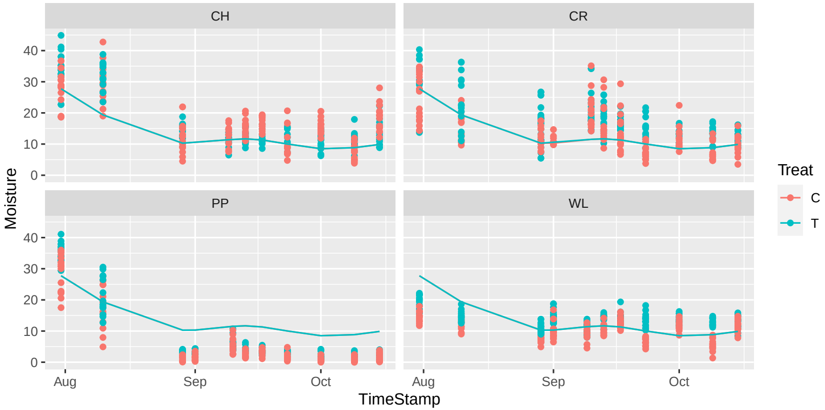
$$\mu_{titer} = a_g t e^{-b_g t}$$



## Splines

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

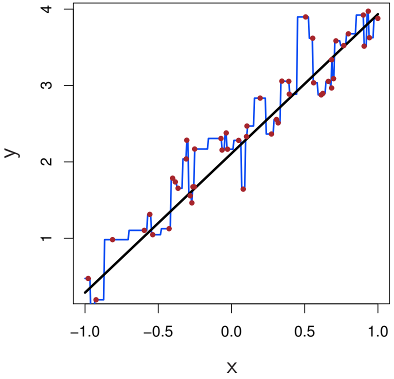
```
SoilMoist <- read.csv("data/SoilMoisture_ALL.csv") # A. Cooper's data
SoilMoist$TimeStamp <- mdy(SoilMoist$TimeStamp) # from lubridate package
splinemod <- lm(Moisture~ns(TimeStamp,4), data=SoilMoist)
SoilMoist$pred <- predict(splinemod)
ggplot(SoilMoist, aes(TimeStamp,Moisture, color = Treat))+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

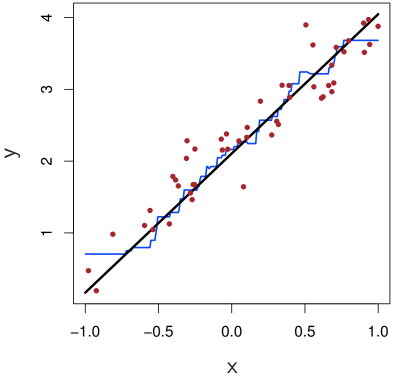


## Nearest neighbor averaging (knn)

- 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.

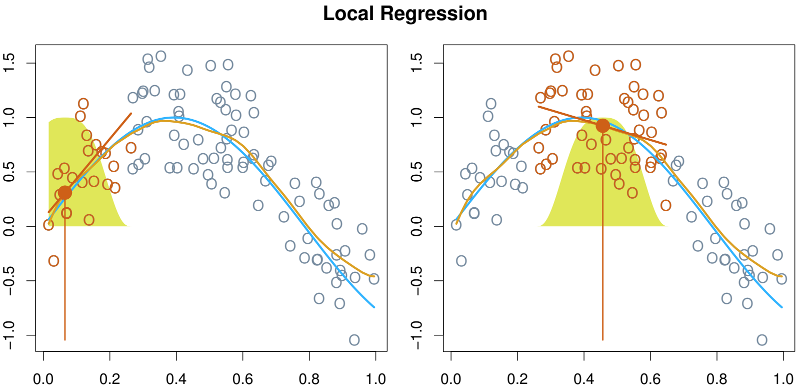




Left: knn with $k = 1$. Variance is high. Right: knn with $k = 9$.

# 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/.