

# Linear models

SDS 323

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Reference: Introduction to Statistical Learning Chapter 3

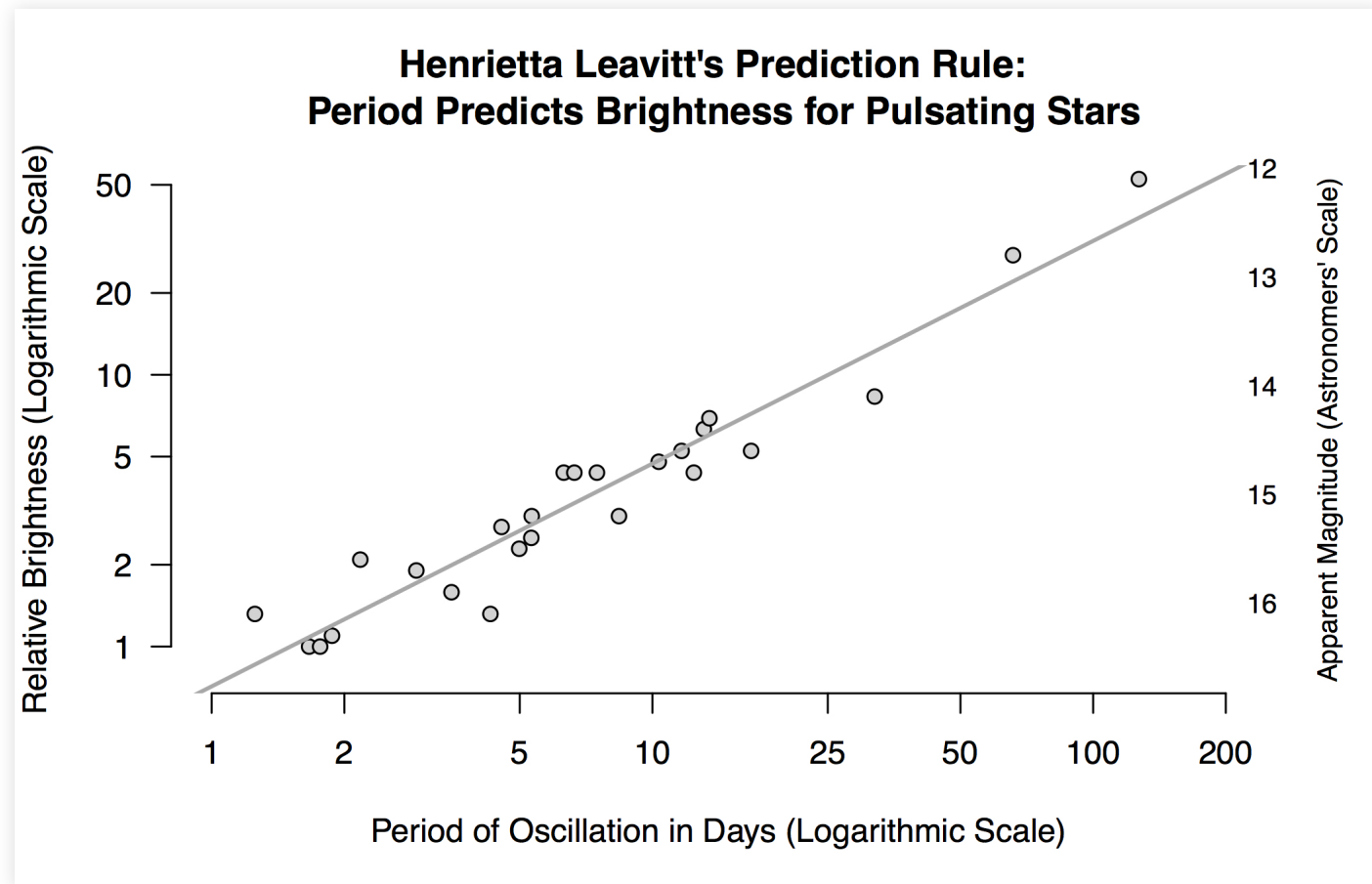
# Linear models

Linear modeling is the most widely used tool in the world for fitting a predictive model of the form  $y = f(x) + e$ .

They are used throughout the worlds of science and industry.

They have been at the heart of some of history's greatest scientific discoveries.

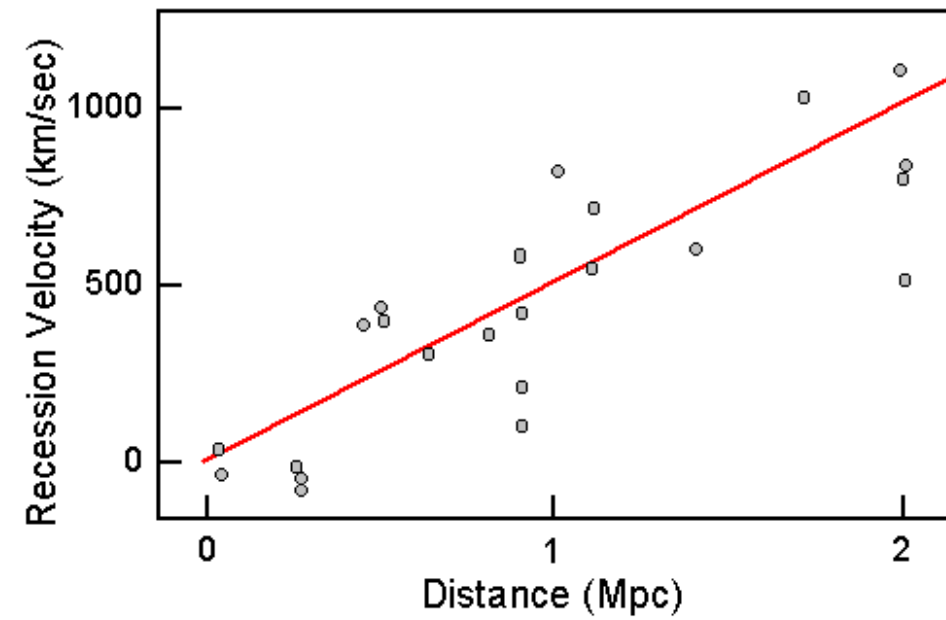
# Linear models



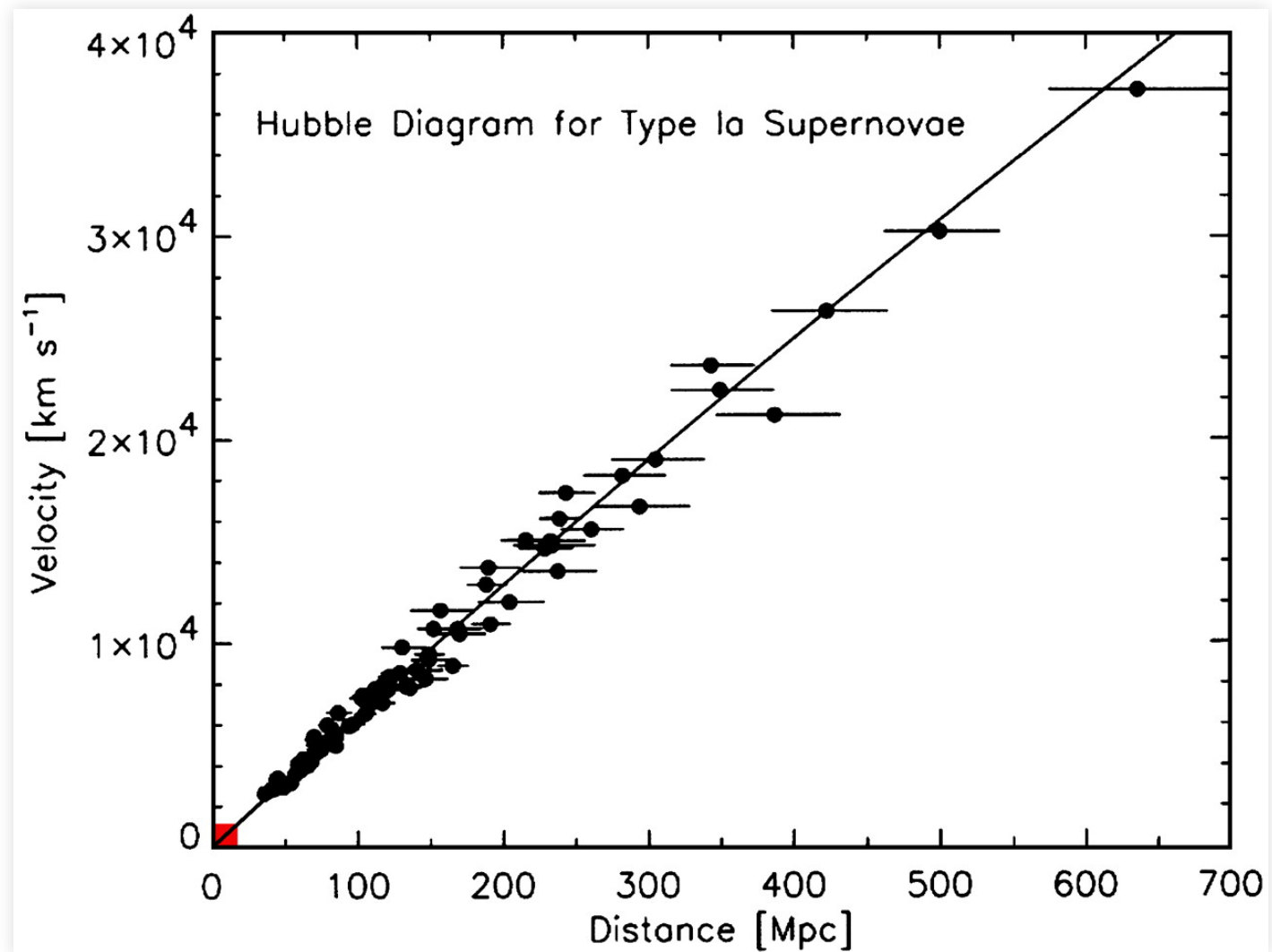
*From AIQ: How People and Machines are Smarter Together*

# Linear models

Hubble's Data (1929)



# Linear models



# Linear models

A linear model is parametric model; we can write down  $f(x)$  in the form of an equation:

$$\begin{aligned} y &= \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + e \\ &= x \cdot \beta + e \end{aligned}$$

A notational convenience: the intercept gets absorbed into the vector of predictors by including a leading term of 1:

- $x = (1, x_1, x_2, \dots, x_p)$
- $\beta = (\beta_0, \beta_1, \beta_2, \dots, \beta_p)$

# Linear models: major pros

- They often work pretty well for prediction.
- They're a simple foundation for more sophisticated techniques.
- They're easy to estimate, even for extremely large data sets.

# Linear models: major pros

- They have lower estimation variance than most nonlinear/nonparametric alternatives.
- They're easier to interpret than nonparametric models.
- Techniques for feature selection (choosing which  $x_j$ 's matter) are very well developed for linear models.



# Linear models: major cons

- Linear models are pretty much always *wrong*, sometimes subtly and sometimes spectacularly. If the truth is nonlinear, then the linear model will provide a biased estimate.
- Linear models depend on which transformation of the data you use (e.g.  $x$  versus  $\log(x)$ ).
- Linear models don't handle *interactions* among the predictors unless you explicitly build them in.

# Huh? What's an interaction?

We use the term **interaction** in statistical learning to describe situations where the effect of some feature  $x$  on the outcome  $y$  is **context-specific**:

- Biking in a low gear: easy (say 2 out of 10)
- Biking in a high gear: a bit hard (say 4 out of 10)
- Biking uphill in a low gear: a bit hard (say 5 out of 10)
- Biking uphill in a high gear: very hard (say 9 out of 10)

# Huh? What's an interaction?

So what's the “effect” of change the gear from low to high? There is no one answer... **it depends on context!**

- On flat ground: “high gear” effect =  $4 - 2 = 2$ .
- Uphill: “high gear” effect =  $9 - 5 = 4$ .

One feature (slope) changes how another feature (gear) affects  $y$ .

**That's an interaction.**

# Other simple examples

What's the effect of a 5 mph breeze on comfort? It depends!

- When it's hot outside, a 5 mph breeze makes things more pleasant.
- What about the effect of the same breeze when it's cold outside?

# Other simple examples

What's the effect of a 5 mph breeze on comfort? It depends!

- When it's hot outside, a 5 mph breeze makes things more pleasant.
- What about the effect of the same breeze when it's cold outside?

What's the effect of two Tylenol pills on a headache? It depends!

- This dose will help a headache in a 165 pound adult human being.
- What about the effect of that same dose on a 13,000 pound African elephant?

# Linear models and interactions

Interactions are about capturing these context-specific effects by correctly modeling the *joint effect* of more than one feature at once.

The real world is full of interactions!

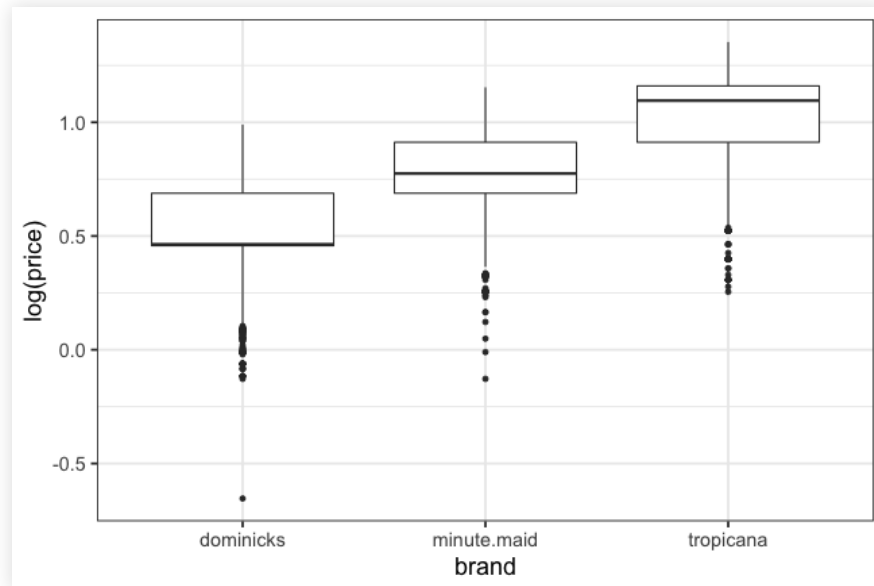
- house price versus (square footage, location)
- college GPA versus (SAT Math score, college major)
- health outcomes vs (ACE inhibitors, pregnancy)

Linear models *can* accommodate interactions among feature variables—**but only** if we build these interaction terms in “by hand.”

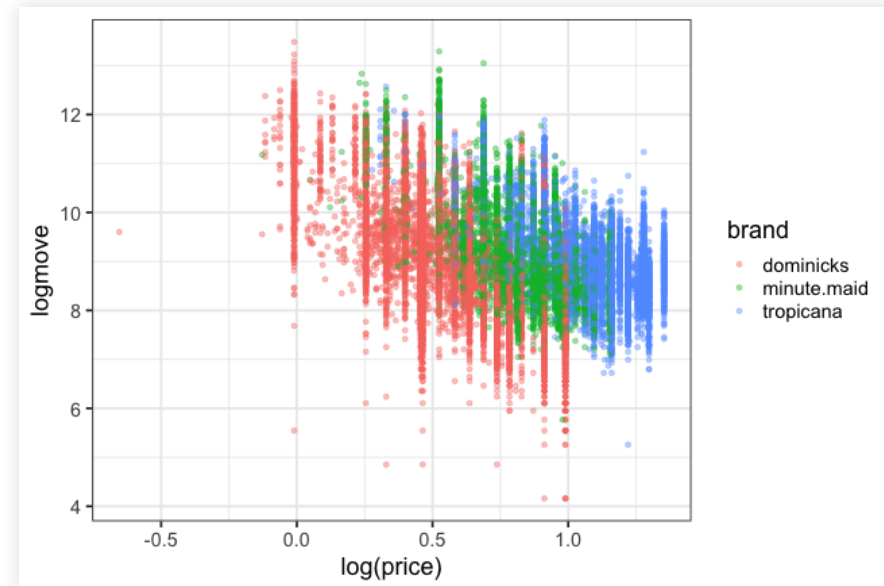
# Example: orange juice sales

- Three brands of OJ: Tropicana, Minute Maid, Dominicks
- 83 Chicago-area stores
- Demographic info for each store
- Price, sales (log units moved), and whether advertised (`feat`)
- data in `oj.csv`, code in `oj.R`.

# Example: orange juice sales



Each brand occupies a well-defined price range.



Sales decrease with price (duh).



# OJ: price elasticity

A simple “elasticity model” for orange juice sales  $y$  might be:

$$\log(y) = \gamma \log(\text{price}) + x \cdot \beta$$

The rough interpretation of a log-log regression like this: for every 1% increase in price, we can expect a  $\gamma\%$  change in sales, holding variables in  $x$  constant.

Let's try this in R, using `brand` as a feature ( $x$ ):

```
reg = lm(logmove ~ log(price) + brand, data=oj)
coef(reg) ## look at coefficients
```

(Intercept)	log(price)	brandminute.maid	brandtropicana
10.8288216	-3.1386914	0.8701747	1.5299428

# OJ: model matrix and dummy variables

What happened to `branddominicks`?

Our regression formulas look like  $\beta_0 + \beta_1 x_1 + \dots$ . But `brand` is not a number, so you can't do  $\beta \cdot \text{brand}$ .

The first step of `lm` is to create a numeric “model matrix” from the input variables:

# OJ: model matrix and dummy variables

Input:

<b>Brand</b>
dominicks
minute maid
tropicana

Variable expressed  
as a factor.

Output:

<b>Intercept</b>	<b>brand=minute maid</b>	<b>brand = tropicana</b>
1	0	0
1	1	0
1	0	1

Variable coded as a set of numeric “dummy variables” that we can multiply against  $\beta$  coefficients. This is done using `model.matrix`.

# OJ: model matrix and dummy variables

Our OJ model used `model.matrix` to build a 4 column matrix:

```
> x <- model.matrix( ~ log(price) + brand, data=oj)
> x[1,]
Intercept log(price) branBDminute.maid brandtropicana
1.00000    1.353255         0.000000         1.000000
```

Each factor's reference level is absorbed by the intercept.  
Coefficients are “change relative to reference level” (dominicks here).

To check the reference level of your factors, use

```
levels(oj$brand)
```

```
[1] "dominicks"    "minute.maid" "tropicana"
```

The first level is reference.

# OJ: model matrix and dummy variables

To *change* the reference level, use `relevel`:

```
oj$brand2 = relevel(oj$brand, 'minute.maid')
```

Now if you re-run the regression, you'll see a different baseline category. But crucially, the price coefficient doesn't change:

```
reg2 = lm(logmove ~ log(price) + brand2, data=oj)
coef(reg) # old model
```

(Intercept)	log(price)	brandminute.maid	brandtropicana
10.8288216	-3.1386914	0.8701747	1.5299428

```
coef(reg2) # new model
```

(Intercept)	log(price)	brand2dominicks	brand2tropicana
11.6989962	-3.1386914	-0.8701747	0.6597681

# Interactions

Remember: an interaction is when one feature changes how another feature acts on  $y$ .

In regression, an interaction is expressed as the product of two features:

$$E(y \mid x) = f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \dots$$

so that the effect on  $y$  of a one-unit increase in  $x_1$  is  $\beta_1 + \beta_{12} x_2$ . (It depends on  $x_2$ !)

# Interactions

Interactions play a *massive* role in statistical learning. They are important for making good predictions, and they are often central to social science and business questions:

- Does gender change the effect of education on wages?
- Do patients recover faster when taking drug A?
- How does brand affect price sensitivity?

# Interactions in R: use \*

This model statement says: elasticity (the `log(price)` coefficient) is different from one brand to the next:

```
reg3 = lm(logmove ~ log(price)*brand, data=oj)
coef(reg3)
```

(Intercept)	log(price)
10.95468173	-3.37752963
brandminute.maid	brandtropicana
0.88825363	0.96238960
log(price):brandminute.maid	log(price):brandtropicana
0.05679476	0.66576088

This output is telling us that the elasticities are:

dominicks: -3.4      minute maid: -3.3      tropicana: -2.7

Where do these numbers come from? Do they make sense?



# Interactions: OJ

- A key question: what changes when we feature a brand? Here, this means in-store display promo or flier ad (`feat` in `oj.csv`):
  1. Maybe `feat` changes sales, but doesn't affect price sensitivity (no interaction)...
  2. Or maybe `feat` changes sales and also affects price sensitivity, but in the same way for all brands (two-way interaction)...
  3. Or maybe `feat` changes sales and affects price sensitivity in *different ways for different brands* (three-way interaction!)
- Let's see the R code in `oj.R` for all three models. Goal: connect the regression formula to a specific assumption about the underlying system.

# Brand-specific elasticities

	<b>Dominicks</b>	<b>Minute Maid</b>	<b>Tropicana</b>
Not featured	-2.8	-2.0	-2.0
Featured	-3.2	-3.6	-3.5

## Findings:

- Ads always decrease elasticity.
- Minute Maid and Tropicana elasticities drop 1.5% with ads, moving them from less to more price sensitive than Dominicks.

Why does marketing increase price sensitivity? And how does this influence pricing/marketing strategy?

# Brand-specific elasticities

Before including feat, Minute Maid behaved like Dominicks.

```
reg_interact = lm(logmove ~ log(price)*brand, data=oj)
coef(reg_interact)
```

(Intercept)	log(price)
10.95468173	-3.37752963
brandminute.maid	brandtropicana
0.88825363	0.96238960
log(price):brandminute.maid	log(price):brandtropicana
0.05679476	0.66576088

(Compare the elasticities!)

# Brand-specific elasticities

With feat, Minute Maid looks more like Tropicana. Why?

```
reg_ads3 <- lm(logmove ~ log(price)*brand*feat, data=oj)
coef(reg_ads3)
```

(Intercept)	10.40657579	log(price)	-2.77415436
brandminute.maid	0.04720317	brandtropicana	0.70794089
feat	1.09440665	log(price):brandminute.maid	0.78293210
log(price):brandtropicana	0.73579299	log(price):feat	-0.47055331
brandminute.maid:feat	1.17294361	brandtropicana:feat	0.78525237
log(price):brandminute.maid:feat	-1.10922376	log(price):brandtropicana:feat	-0.98614093

(Again, compare the elasticities!)

# What happened?

Minute Maid was more heavily promoted!

	brand		
feat	dominicks	minute.maid	tropicana
0	0.743	0.711	0.834
1	0.257	0.289	0.166

Because Minute Maid was more heavily promoted, AND promotions have a negative effect on elasticity, we were confounding the two effects on price when we estimated an elasticity without accounting for `feat`.

Including `feat` helped deconfound the estimate!

# Take-home messages: dummy variables

- Categorical variables are encoded using dummies. Happens behind the scenes, but to interpret the output correctly, it's important to know how it works.

<b>Intercept</b>	<b>brand=minute maid</b>	<b>brand = tropicana</b>
1	0	0
1	1	0
1	0	1

- One category is arbitrarily chosen as the baseline/intercept. Any baseline is as good as another:
  - JJ Watt is 6'5", Yao Ming is +13 inches, Simone Biles is -21 inches.
  - Simone Biles is 4'8", Yao Ming is +34 inches, JJ Watt is +21 inches.

# Take-home messages: interactions

- An interaction is when one variable changes the effect of another variable on  $y$ .
- In linear models, we express interactions as products of variables:

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \dots$$

so that the effect on  $y$  of a one-unit increase in  $x_1$  is  $\beta_1 + \beta_{12} x_2$ .

# Out-of-sample fit: linear models

- Just like with K-nearest neighbors in one  $x$  variable, it's important to consider out of sample fit for a linear model.
- Especially in a model with lots of variables, the in-sample fit and out-of-sample fit can be very different.
- Let's see these ideas in practice, by comparing three predictive models for house prices in Saratoga, New York.



# Variables in the data set

- price ( $y$ )
- lot size, in acres
- age of house, in years
- living area of house, in square feet
- percentage of residents in neighborhood with college degree
- number of bedrooms
- number of bathrooms
- number of total rooms
- number of fireplaces
- heating system type (hot air, hot water, electric)
- fuel system type (gas, fuel oil, electric)
- central air conditioning (yes/no)

# Three models for house prices

We'll consider three possible models for price constructed from these 11 predictors.

- Small model: price versus lot size, bedrooms, and bathrooms (4 total parameters, including the intercept).
- Medium model: price versus all variables above, main effects only (14 total parameters, including the dummy variables).
- Big model: price versus all variables listed above, together with all pairwise interactions between these variables (90 total parameters, include dummy variables and interactions).

# Three models for house prices

A starter script is in `saratoga_lm.R`. Goals for today:

- See if you can “hand-build” a model for price that outperforms all three of these baseline models! Use any combination of transformations, polynomial terms, and interactions that you want.
- When measuring out-of-sample performance, there is *random variation* due to the particular choice of data points that end up in your train/test split. Make sure your script addresses this by averaging the estimate of out-of-sample RMSE over many different random train/test splits.

# Three models for house prices

```
# Split into training and testing sets
n = nrow(SaratogaHouses)
n_train = round(0.8*n) # round to nearest integer
n_test = n - n_train
train_cases = sample.int(n, n_train+1, replace=FALSE)
test_cases = setdiff(1:n, train_cases)
saratoga_train = SaratogaHouses[train_cases,]
saratoga_test = SaratogaHouses[test_cases,]

# Fit to the training data
lm1 = lm(price ~ lotSize + bedrooms + bathrooms, data=saratoga_train)
lm2 = lm(price ~ . - sewer - waterfront - landValue - newConstruction,
data=saratoga_train)
lm3 = lm(price ~ (. - sewer - waterfront - landValue - newConstruction)^2,
data=saratoga_train)
```

# Three models for house prices

```
# Predictions out of sample
yhat_test1 = predict(lm1, saratoga_test)
yhat_test2 = predict(lm2, saratoga_test)
yhat_test3 = predict(lm3, saratoga_test)

rmse = function(y, yhat) {
  sqrt( mean( (y - yhat)^2 ) )
}

# Root mean-squared prediction error
rmse(saratoga_test$price, yhat_test1)
```

```
[1] 76718.89
```

```
rmse(saratoga_test$price, yhat_test2)
```

```
[1] 66710.4
```

```
rmse(saratoga_test$price, yhat_test3)
```

```
[1] 79040.66
```

# Comparison with K-nearest-neighbors

- A linear model makes strong assumptions about the form of  $f(x)$ .
- If these assumptions are wrong, then a linear model can predict poorly (large bias).
- A nonparametric model like KNN is different:
  - It makes fewer assumptions (and thus can have lower bias).
  - You don't have to “hand build” interactions into the model.
  - But it typically has higher estimation variance.
- Which approach leads to a more favorable spot along the bias-variance tradeoff?

# Comparison with K-nearest-neighbors

Let's fit a KNN model to the Saratoga house-price data using all the same variables we used in our “medium” model. Recall the basic recipe:

- Given a value of  $K$  and a point  $x_0$  where we want to predict, identify the  $K$  nearest training-set points to  $x_0$ . Call this set  $\mathcal{N}_0$ .
- Then estimate  $\hat{f}(x_0)$  using the average value of the target variable  $y$  for all the points in  $\mathcal{N}_0$ .

$$\hat{f}(x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} y_i$$

(The summation over  $i \in \mathcal{N}_0$  means “sum over all data points  $i$  that fall in the neighborhood.”)

# Measuring closeness

There's a caveat here: how do we measure which  $K$  points are the closest to  $x_0$ ? To see why this is trickier than it sounds at first, consider three houses:

- House A: 4 bedrooms, 2 bathrooms, 2200 sq ft
- House B: 4 bedrooms, 2 bathrooms, 2300 sq ft
- House C: 2 bedrooms, 1.5 bathrooms, 2125 sq ft

Which house (B or C) should be “closer to” A?



# Measuring closeness

Most people would think that A and B are the most similar: they both have 4 BR/2 BA, and their size is similar. House C has only 2BR/1.5 BA; it's *enormous* for a house with that number of bedrooms. Yet if we naively try to calculate pairwise Euclidean distances, we find the following:

$$\begin{aligned}d(A, B) &= \sqrt{(4 - 4)^2 + (2 - 2)^2 + (2200 - 2300)^2} \\ &= 100\end{aligned}$$

$$\begin{aligned}d(A, C) &= \sqrt{(4 - 2)^2 + (2 - 1.5)^2 + (2200 - 2125)^2} \\ &\approx 75.03\end{aligned}$$

So A's nearest neighbor is C, not B!

# Measuring closeness

- What happened here is that the `sqft` variable completely overwhelmed the BR and BA variables in the distance calculations.
- The root of the problem: square footage is measured on an *entirely different scale* than bedrooms or bathrooms. Treating them as if they're on the same scale leads to counter-intuitive distance calculations.
- The simple way around this: weighting. That is, we treat some variables as more important than others in the distance calculation.

# Weighting

Ordinary Euclidean distance:

$$d(x_1, x_2) = \sqrt{\sum_{j=1}^p \{x_{1,j} - x_{2,j}\}^2}$$

Weighted Euclidean distance:

$$d_w(x_1, x_2) = \sqrt{\sum_{j=1}^p \{w_j \cdot (x_{1,j} - x_{2,j})\}^2}$$

This depends upon the choice of weights  $w_1, \dots, w_p$  for each feature variable.

# Weighting

We can always choose the scales/weights to reflect our substantive knowledge of the problem. For example:

- a “typical” bedroom is about 200 square feet (roughly 12x16).
- a “typical” bathroom is about 50 square feet (roughly 8x6).

This might lead us to scales like the following:

$$d_w(x, x') = \sqrt{(x_1 - x'_1)^2 + \{200(x_2 - x'_2)\}^2 + \{50(x_3 - x'_3)\}^2}$$

where  $x_1$  is square footage,  $x_2$  is bedrooms, and  $x_3$  is bathrooms.  
Thus a difference of 1 bedroom counts 200 times as much as a difference of 1 square foot.

# Weighting by scaling

But choosing weights by hand can be a real pain.

A “default” choice of weights that requires no manual specification is to weight by the inverse standard deviation of each feature variable:

$$d_w(x_1, x_2) = \sqrt{\sum_{j=1}^p \left( \frac{x_{1,j} - x_{2,j}}{s_j} \right)^2}$$

where  $s_j$  is the sample standard deviation of feature  $j$  across all cases in the training set.

# Weighting

This is equivalent to calculating “ordinary” distances using a rescaled feature matrix, where we center and scale each feature variable to have mean 0 and standard deviation 1:

$$\tilde{X}_{ij} = \frac{(x_{ij} - \mu_j)}{s_j}$$

where  $(\mu_j, s_j)$  are the sample mean and standard deviation of feature variable  $j$ .

Then we can run ordinary (unweighted) KNN using Euclidean distances based on  $\tilde{X}$ .

# Example: KNN on the house-price data

```
# construct the training and test-set feature matrices
# note the "-1": this says "don't add a column of ones for the intercept"
Xtrain = model.matrix(~ . - (price + sewer + waterfront + landValue +
newConstruction) - 1, data=saratoga_train)
Xtest = model.matrix(~ . - (price + sewer + waterfront + landValue +
newConstruction) - 1, data=saratoga_test)

# training and testing set responses
ytrain = saratoga_train$price
ytest = saratoga_test$price

# now rescale:
scale_train = apply(Xtrain, 2, sd) # calculate std dev for each column
Xtilde_train = scale(Xtrain, scale = scale_train)
Xtilde_test = scale(Xtest, scale = scale_train) # use the training set
scales!
```

# Example: KNN on the house-price data

```
head(Xtrain, 2)
```

```
      lotSize age livingArea pctCollege bedrooms fireplaces bathrooms rooms
142    0.33  32    1898         64         3         1         1.5       7
51    0.24  10    1782         52         3         0         2.5       6
      heatinghot air heatinghot water/steam heatingelectric fuelelectric
142             0             1             0             0
51             1             0             0             0
      fueloil centralAirNo
142         0             1
51         0             0
```

```
head(Xtilde_train, 2) %>% round(3)
```

```
      lotSize    age livingArea pctCollege bedrooms fireplaces bathrooms
142 -0.248  0.147    0.237    0.818    -0.17    0.731    -0.611
51  -0.394 -0.612    0.050   -0.351    -0.17   -1.091    0.911
      rooms heatinghot air heatinghot water/steam heatingelectric
142 -0.011             -1.335             2.171             -0.475
51  -0.441             0.749             -0.460             -0.475
      fuelelectric fueloil centralAirNo
142      -0.483   -0.372    0.760
51      -0.483   -0.372   -1.314
```



# Example: KNN on the house-price data

```
library(FNN)
K = 10

# fit the model
knn_model = knn.reg(Xtilde_train, Xtilde_test, ytrain, k=K)

# calculate test-set performance
rmse(ytest, knn_model$pred)
```

```
[1] 67610.25
```

```
rmse(ytest, yhat_test2) # from the linear model with the same features
```

```
[1] 66710.4
```

# Example: KNN on the house-price data

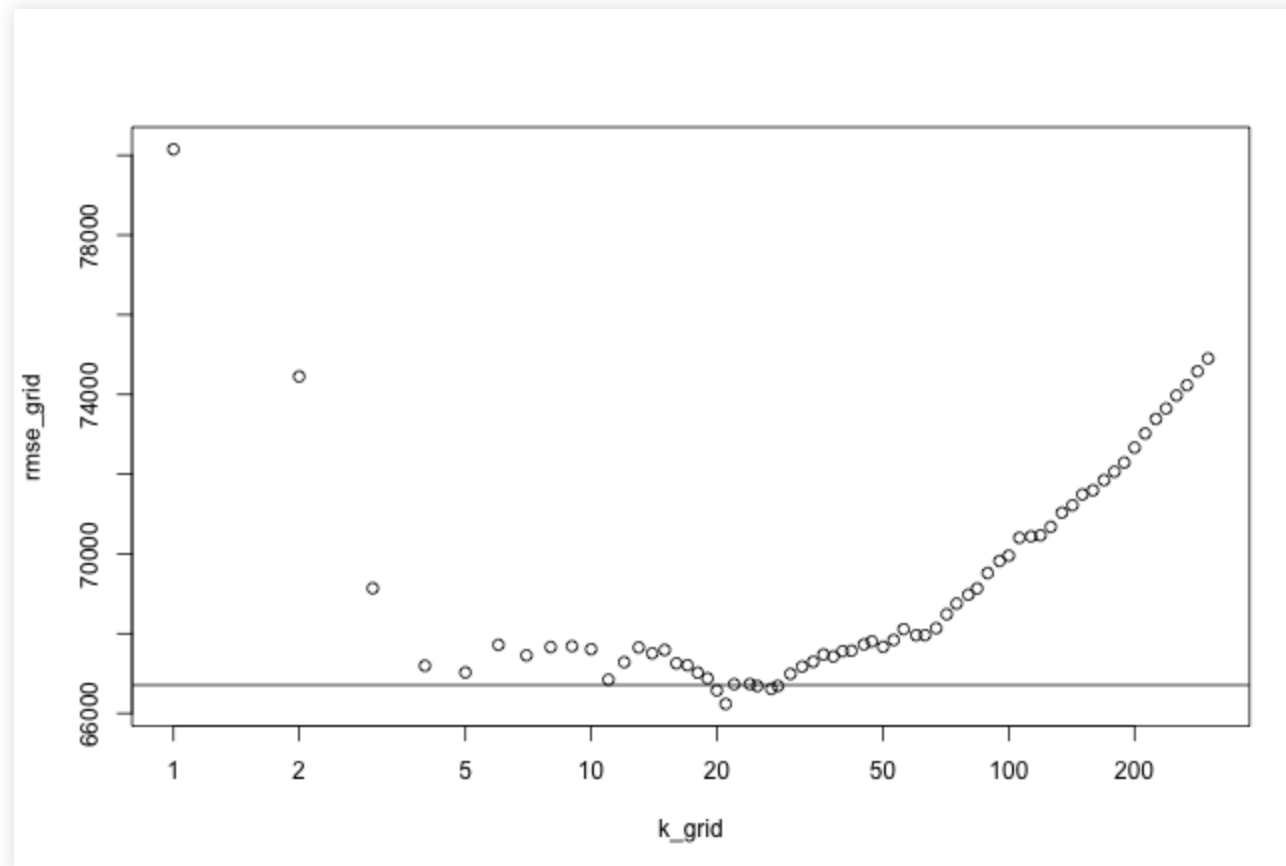
Let's try many values of  $K$ :

```
library(foreach)

k_grid = exp(seq(log(1), log(300), length=100)) %>% round %>% unique
rmse_grid = foreach(K = k_grid, .combine='c') %do% {
  knn_model = knn.reg(Xtilde_train, Xtilde_test, ytrain, k=K)
  rmse(ytest, knn_model$pred)
}
```

# Example: KNN on the house-price data

```
plot(k_grid, rmse_grid, log='x')  
abline(h=rmse(ytest, yhat_test2)) # linear model benchmark
```



# Back to your "favorite" linear model

- Return to your “hand-built” model for price, which might have included transformations, newly defined variables, etc.
- See if you can turn that linear model into a better-performing KNN model.
- Note: don't explicitly include interactions or polynomial terms in your KNN model! It is sufficiently adaptable to find them, if they are there.

# Take-home messages

- “Feature selection” is an important component of building a linear model.
- It can be used for its own sake (i.e. to build a linear predictive model) or as a pre-processing step to choose features for a non-linear model.
- But selecting features by hand is laborious, and selecting interactions by hand is even worse! Stay tuned for more automated methods :-)