Bias-variance tradeoff

David Puelz
The University of Austin

Fitting a function to data

Let's go back to fitting functions with data.

Question ... How wiggly (or not wiggly) should my function be to generate reasonable predictions?

The answer is crucial for how we discover and build functions in the real-world.

Remember the framing of our "function fitting" problem

Predict a target variable Y with input variables X.

Remember the framing of our "function fitting" problem

Predict a target variable Y with input variables X.

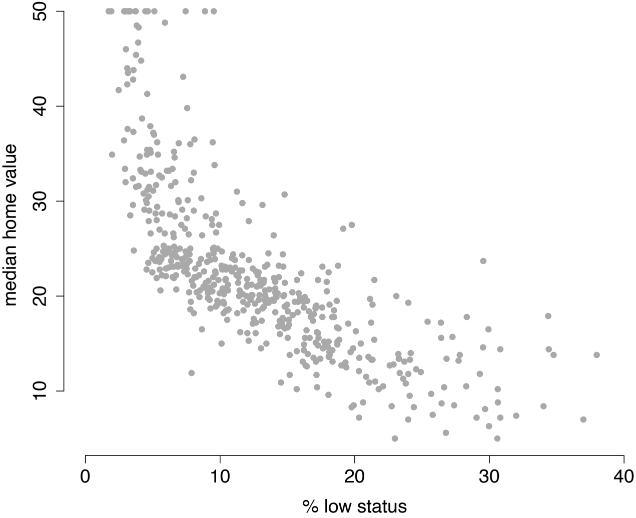
We can frame the problem by supposing Y and X are related in the following way:

$$Y_i = f(X_i) + \epsilon_i$$

To achieve our goal, we need to: *Learn or estimate* $f(\cdot)$ from data.

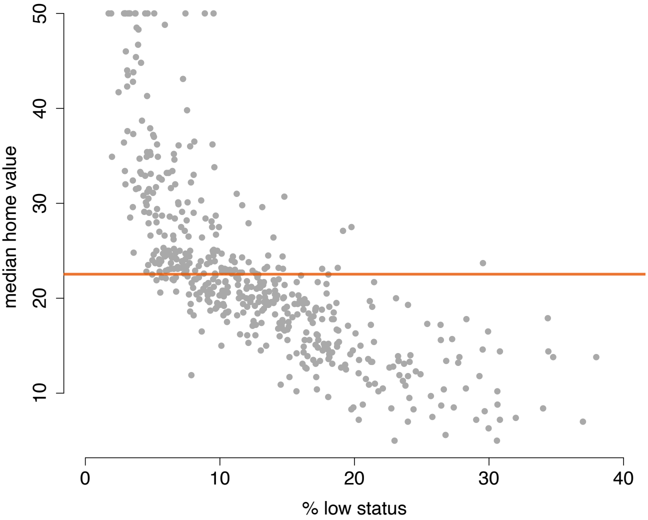
Boston housing data

Predict median home value with percent low economic status.



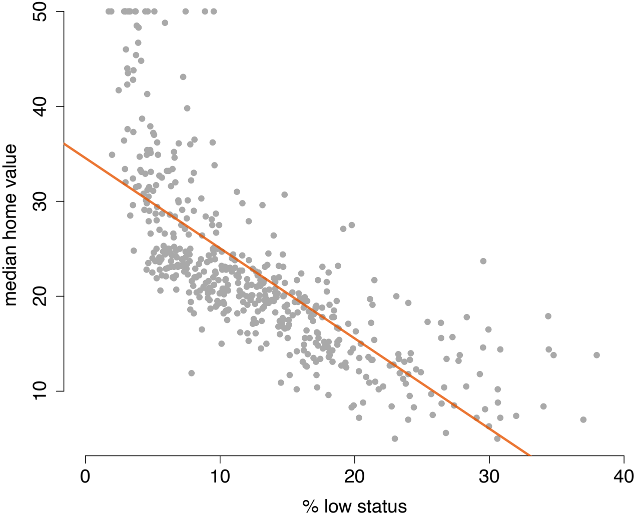
Boston housing data

Prediction at % low status = 30?



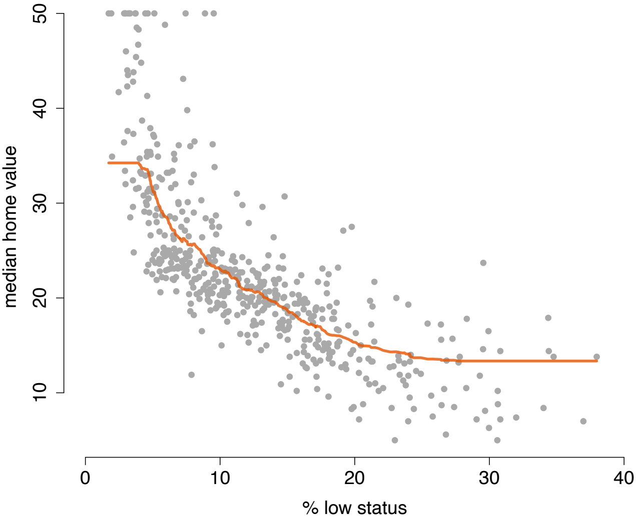
Boston housing data

Prediction at % low status = 30?



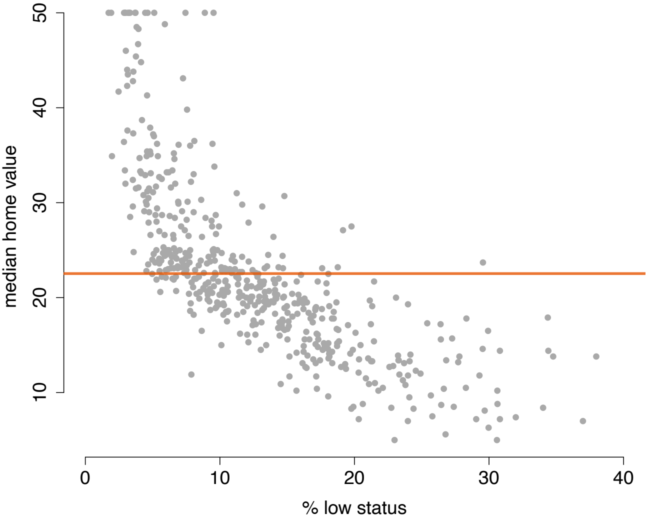
Boston housing data

Prediction at % low status = 30?



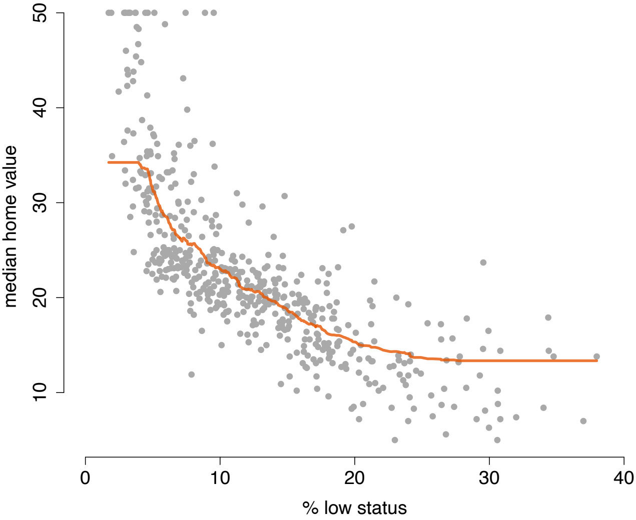
How do we estimate $f(\cdot)$?

restrictive fit, but simple interpretation.



How do we estimate $f(\cdot)$?

flexible fit, but complex interpretation.



The challenge when estimating predictions $\widehat{f(\cdot)}$

Balancing restrictiveness of function fit with simplicity of interpretation.

Let's look at k-nearest-neighbors (knn)

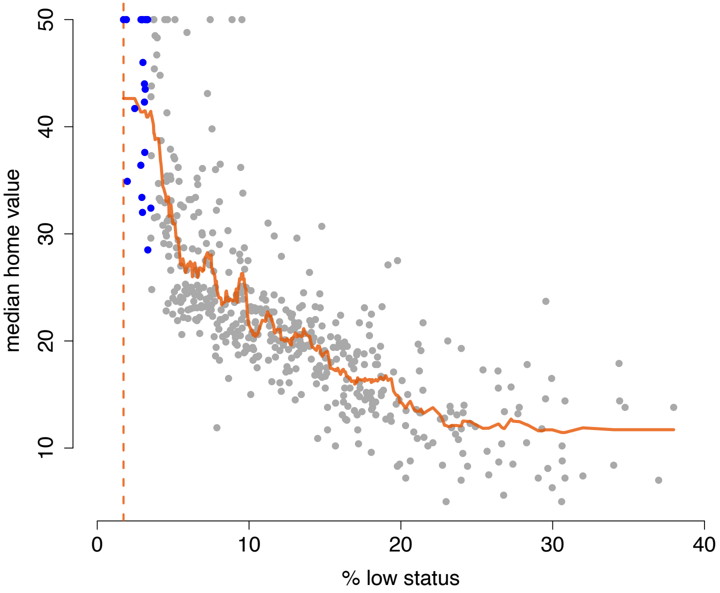
Prediction at point x, $\widehat{f(x)} =$ average of k nearest points around x.

Let's look at k-nearest-neighbors (knn)

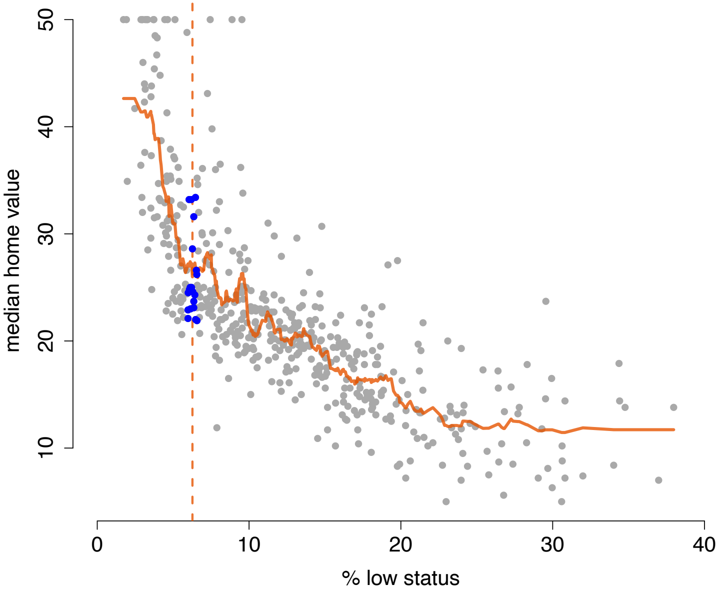
Prediction at point x, $\widehat{f(x)} =$ average of k nearest points around x.

Let's look at $k = 20$ ...

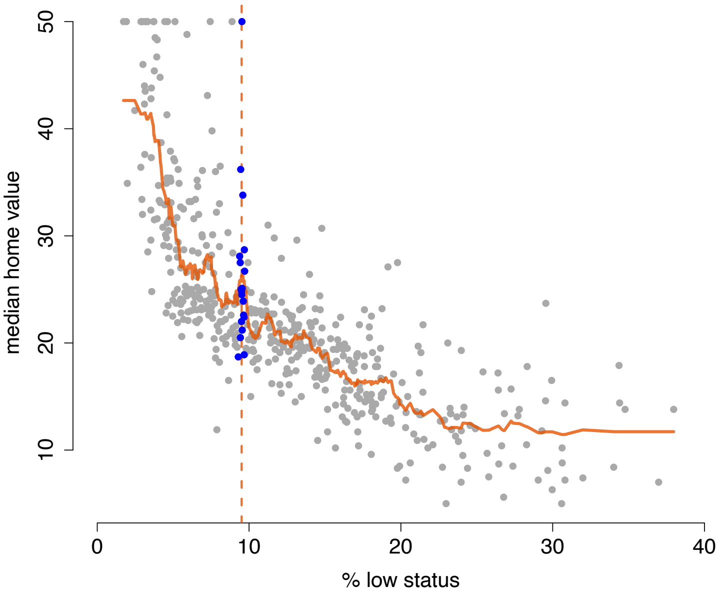
knn with $k = 20$



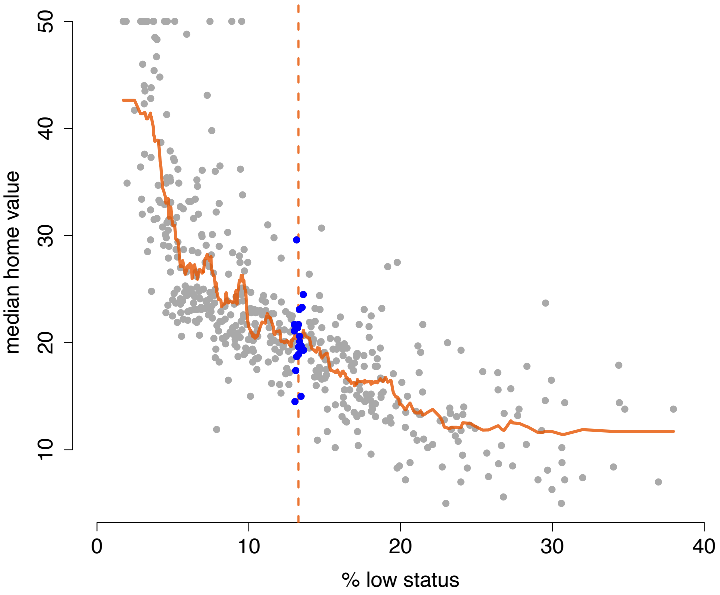
knn with $k = 20$



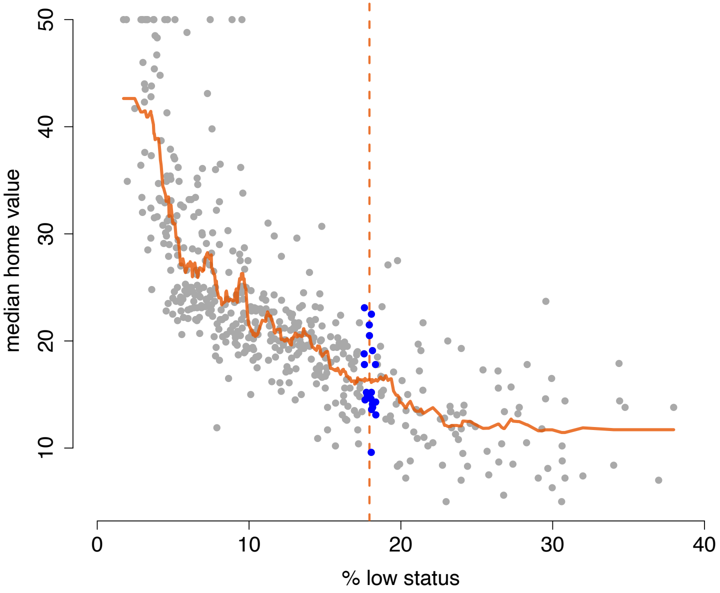
knn with $k = 20$



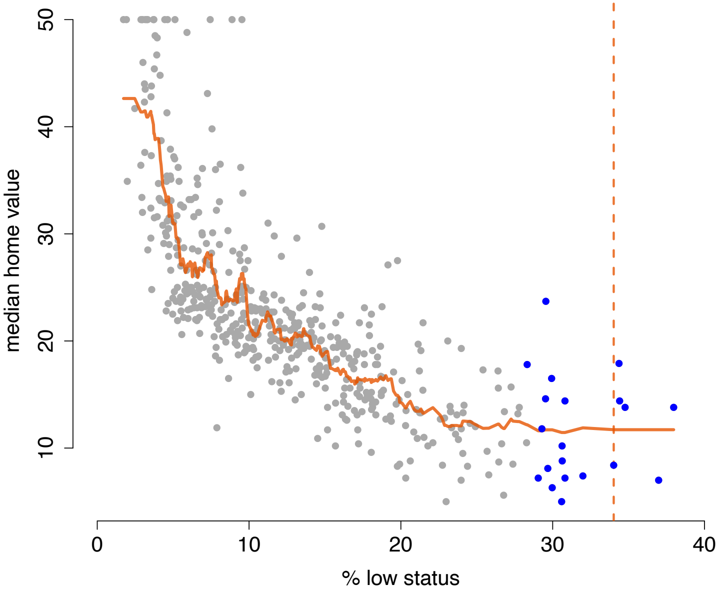
knn with $k = 20$



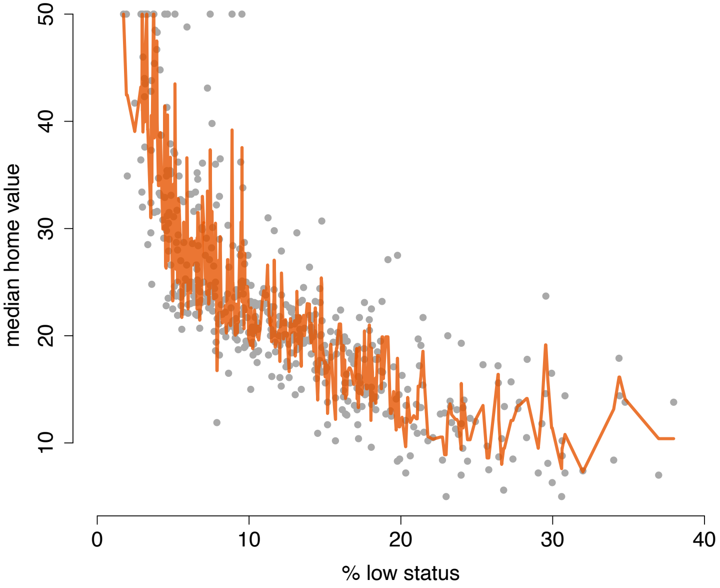
knn with $k = 20$



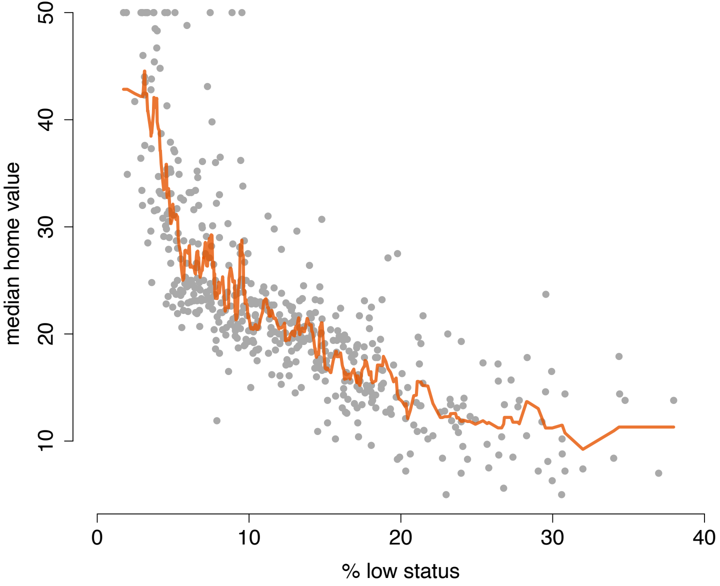
knn with $k = 20$



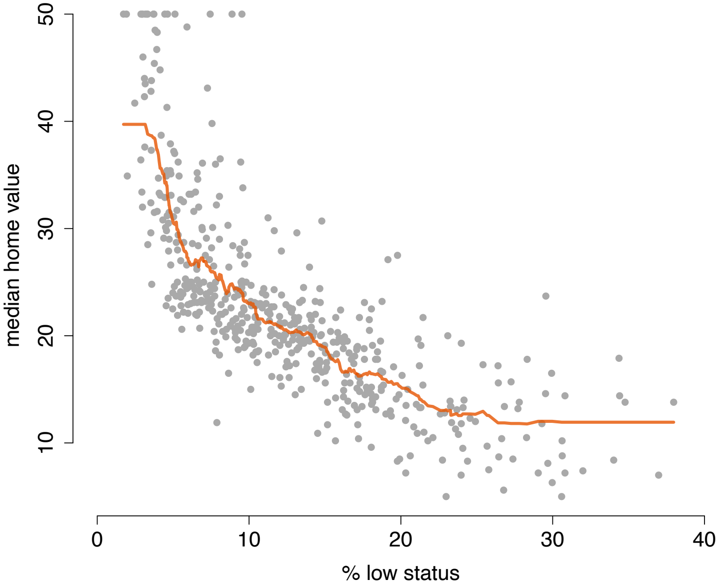
Why don't I choose $k = 2$ instead?



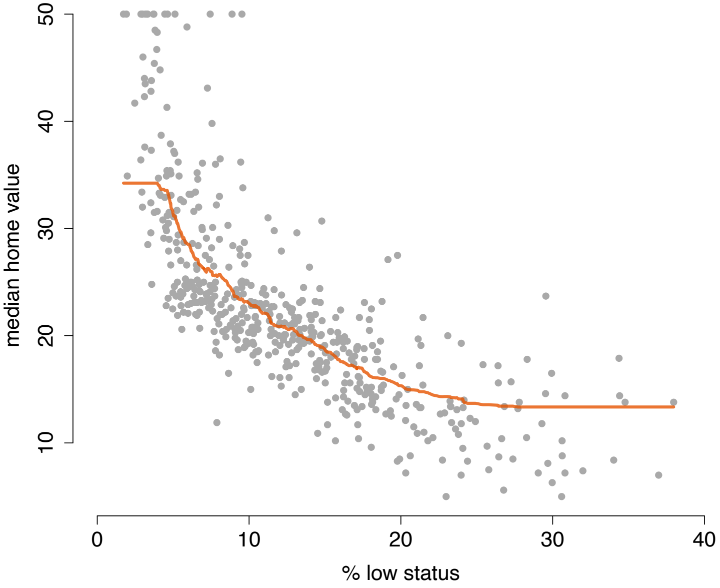
or $k = 10$ ...



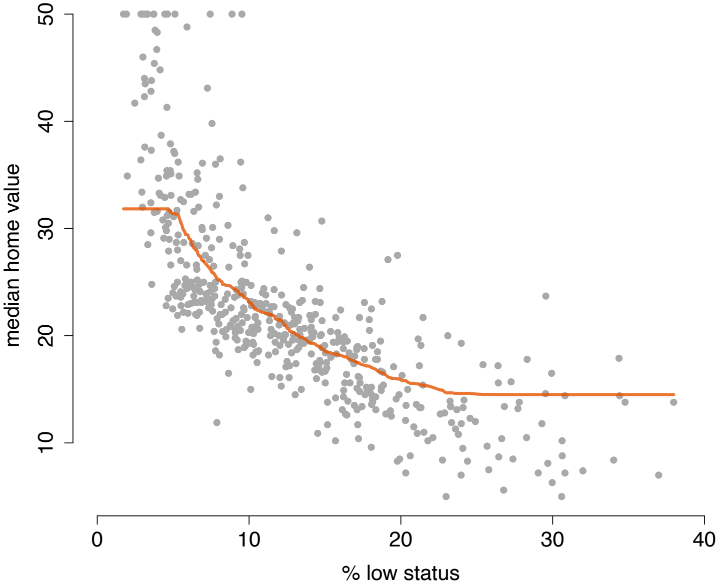
or $k = 50$ ...



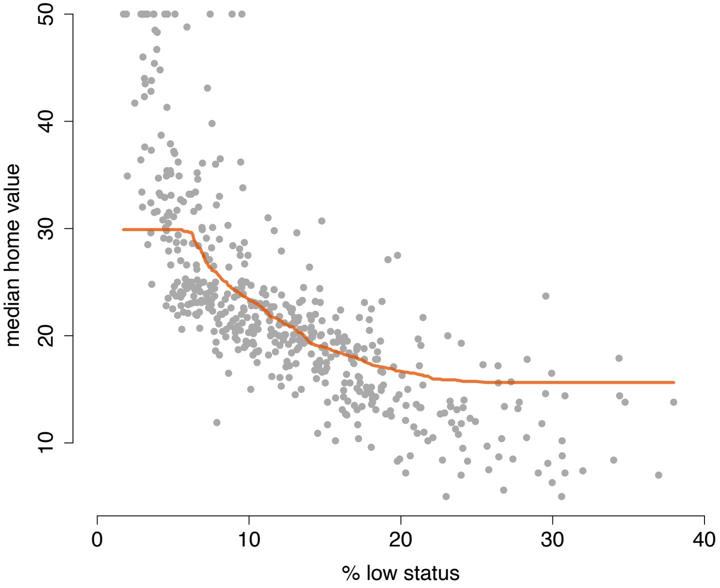
or $k = 100$ ...



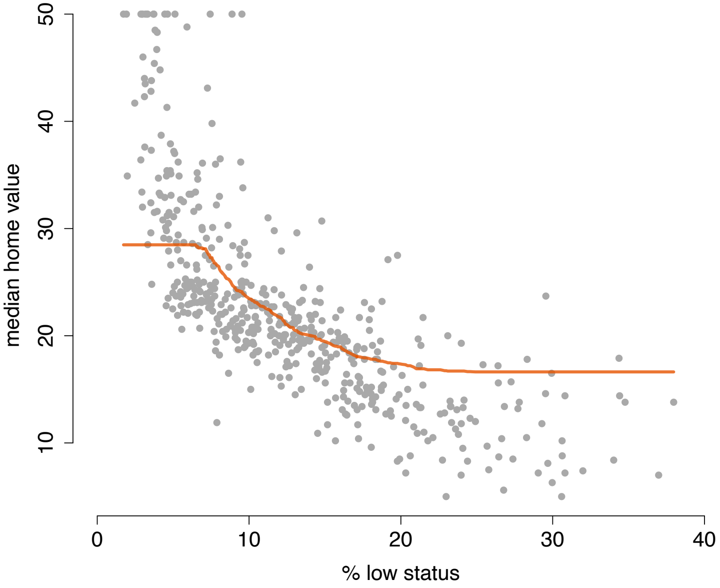
or $k = 150$ …



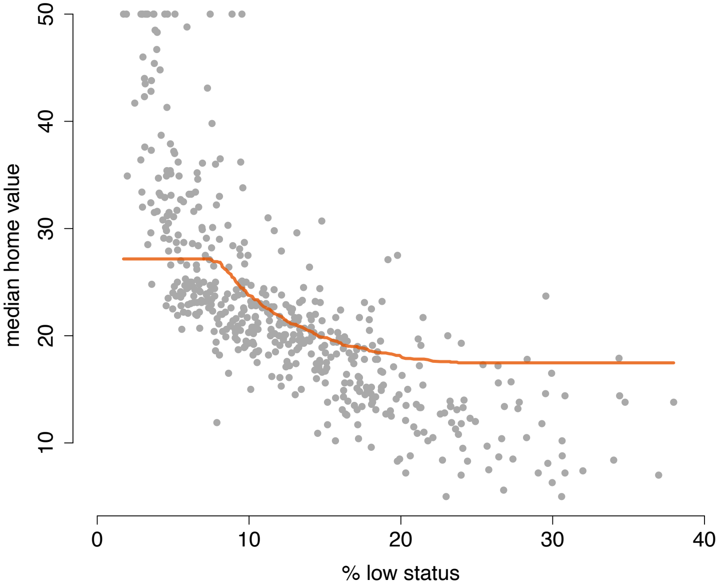
or $k = 200$ ...



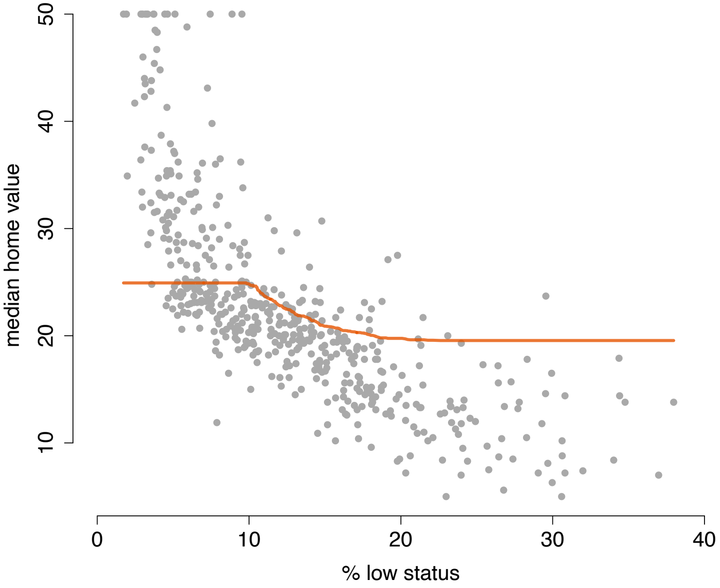
or $k = 250$ ...



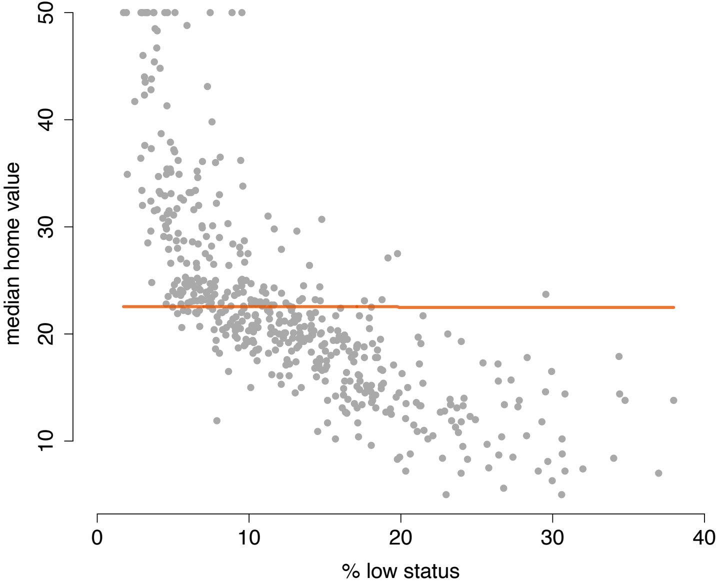
Or $k = 300$ ...



or $k = 400$ ...



or $k = 505$ ...



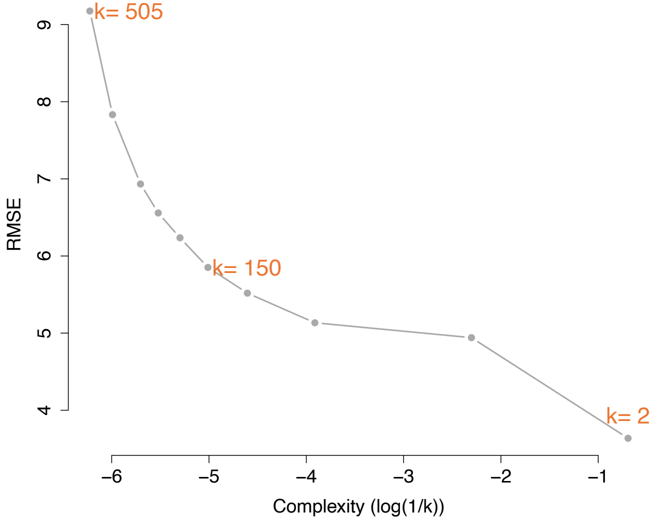
A rigorous way to select

- The root mean squared error measures how accurate my predictions are, on average.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[Y_i - \widehat{f(X_i)}\right]^2}$$

In sample RMSE

It looks like $k = 2$ is the best. Should we choose this model?



We care about out of sample performance

- Suppose we have m additional observations (X_i^o, Y_i^o), for $i = 1, \ldots, m$, that we did not use to fit the model. Let's call this dataset the *validation set* (a.k.a *hold-out set* or *test set*)

We care about out of sample performance

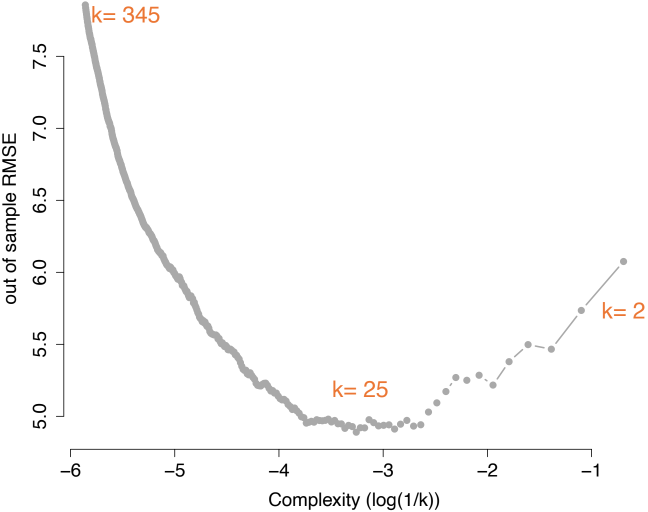
- Suppose we have m additional observations (X_i^o, Y_i^o), for $i = 1, \ldots, m$, that we did not use to fit the model. Let's call this dataset the *validation set* (a.k.a *hold-out set* or *test set*)

- We evaluate the fit with out of sample RMSE:

$$RMSE^o = \sqrt{\frac{1}{m} \sum_{i=1}^{m} \left[Y_i^o - \widehat{f(X_i^o)} \right]^2}$$

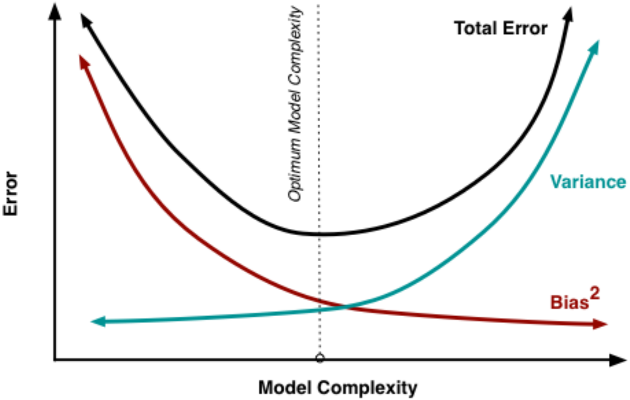
Out of sample RMSE

Fit each model on training set of size 400. Test each model (*out of sample*) on testing set of size 106. Here, we plot the out of sample performance.



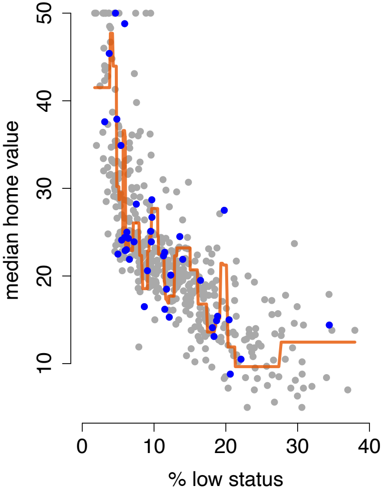
The Bias-variance tradeoff!

When fitting a predictive model, there is a tradeoff between bias and variance of predictions.



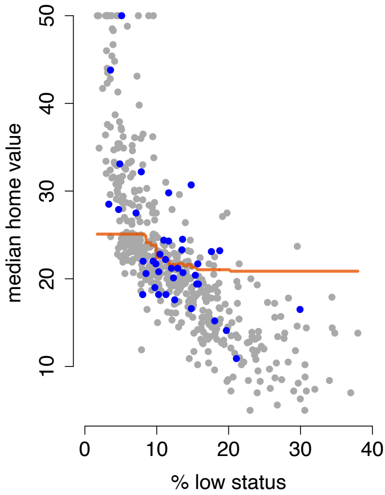
$k = 2$: low bias, high variance

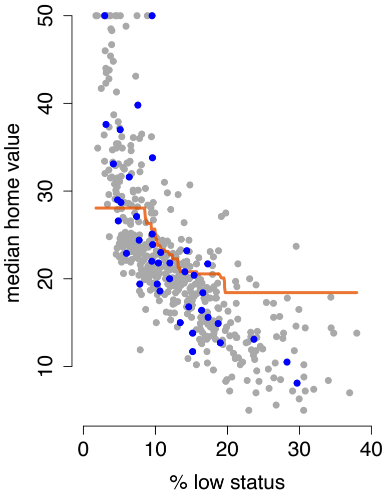
Training set of size 40.



$k = 25$: high bias, low variance

Training set of size 40.





What have we learned?

More wiggles are not always better!

A function fit to data should be "adaptive enough."

If too adaptive aka **overfit** to the observed data, it will not predict well when confronted with new data.