QTM 347 Machine Learning

Lecture 3: KNN

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Suggested reading: ISL Chapters 2 and 4

EMORY

Lecture plan

- K-nearest neighbors (KNN) regression

- K-nearest neighbors (KNN) classification

K-nearest neighbors regression

- A non-parametric approach

- K is a user-defined constant
  - K is an integer, e.g., $1,2,3,\cdots$

- Given a value for K and a prediction point x_0, $\hat{f}(x_0)$ is the average of the responses of K nearest neighbors

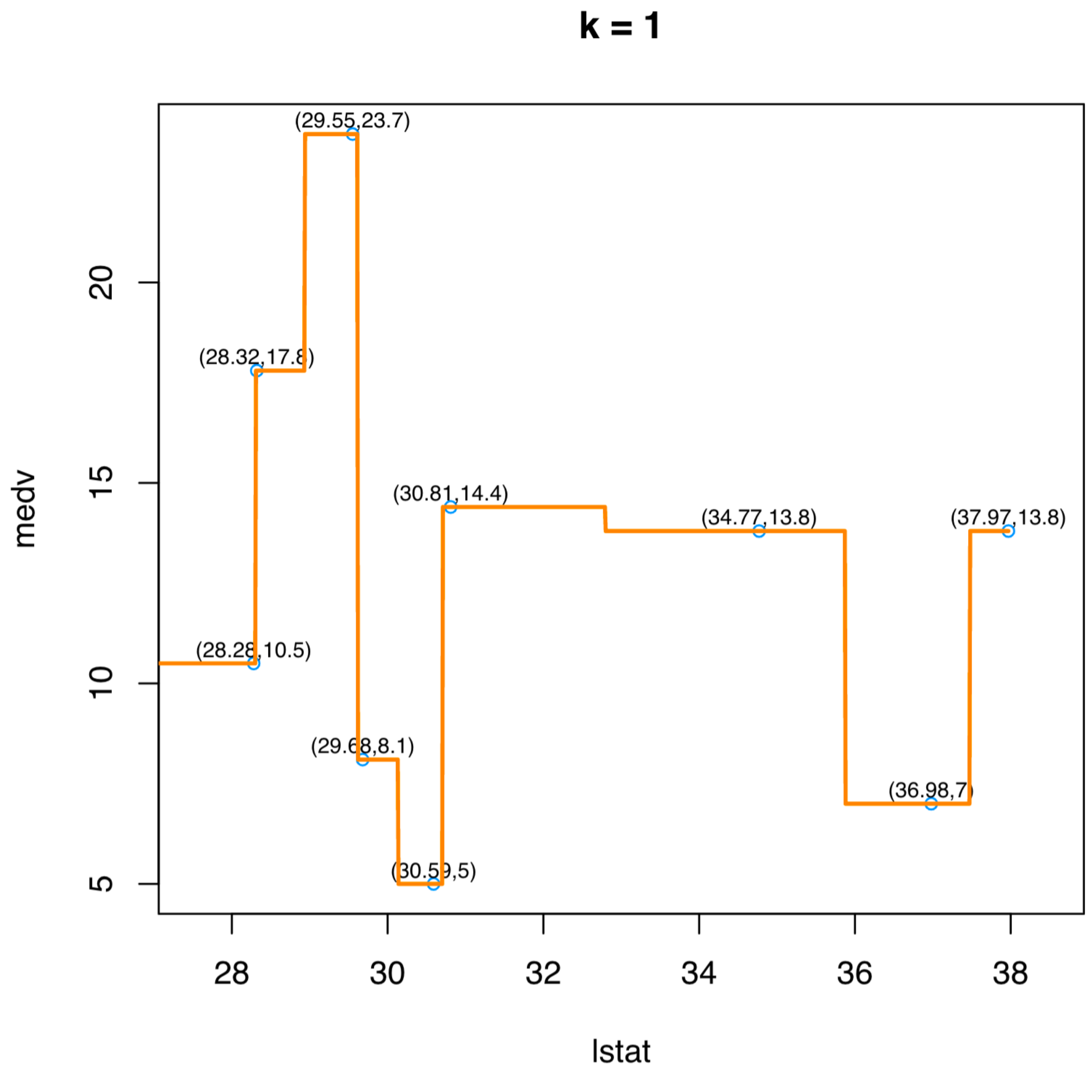
$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_i \in N_K(x_0)} y_i$$

  - $N_K(x_0)$ is the set of K training observations that are closest to x_0

Example: 1-nearest neighbor regression

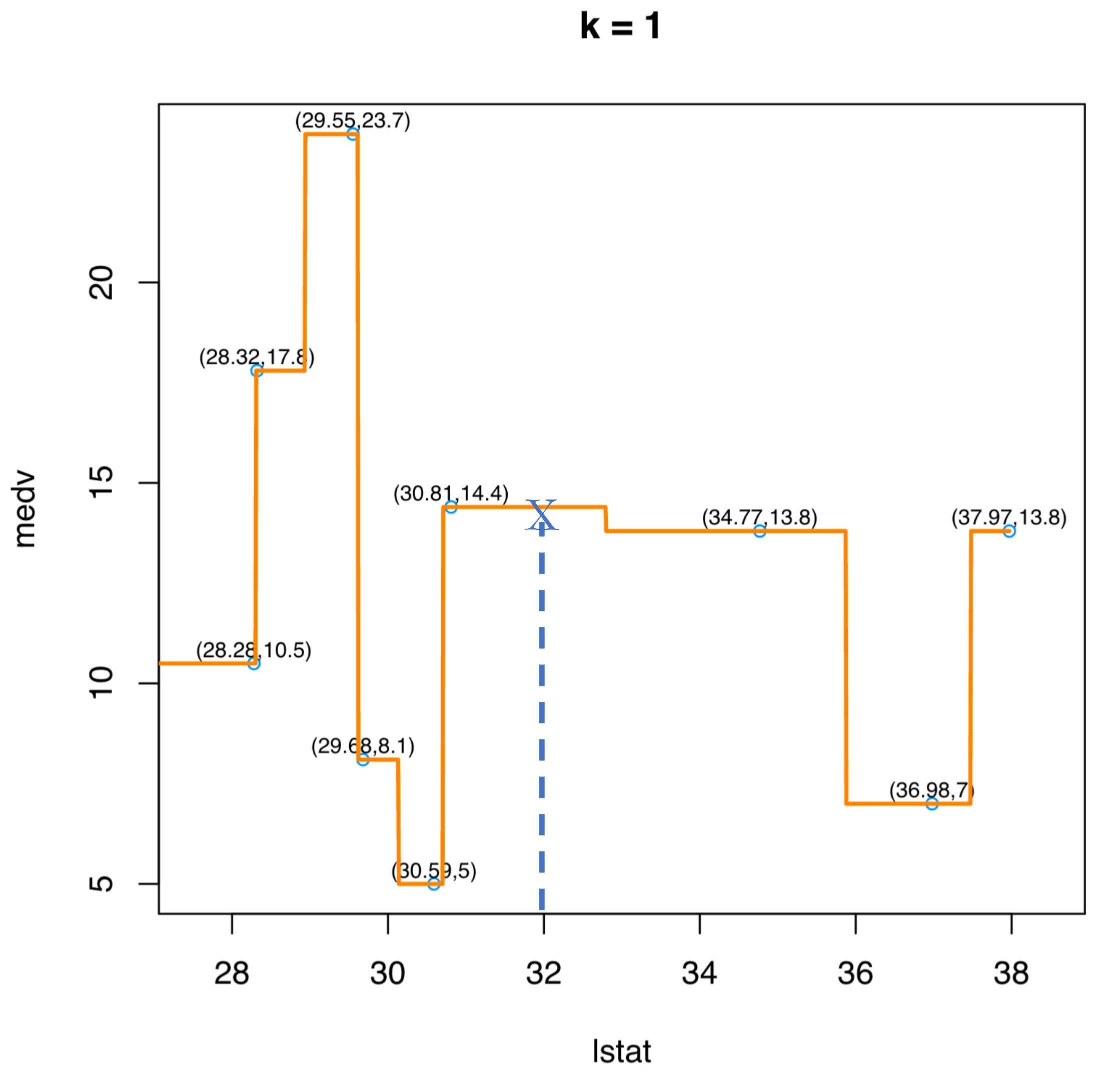
- Prediction of the median house value of a neighbor given the percentage of households with low socioeconomic status (lstat)

- Orange curve: $\hat{f}(x_0)$
  - $\hat{f}(x_0)$ equals to the response of x_0's nearest neighbor
  - $\hat{f}(x_0)$ is a step function



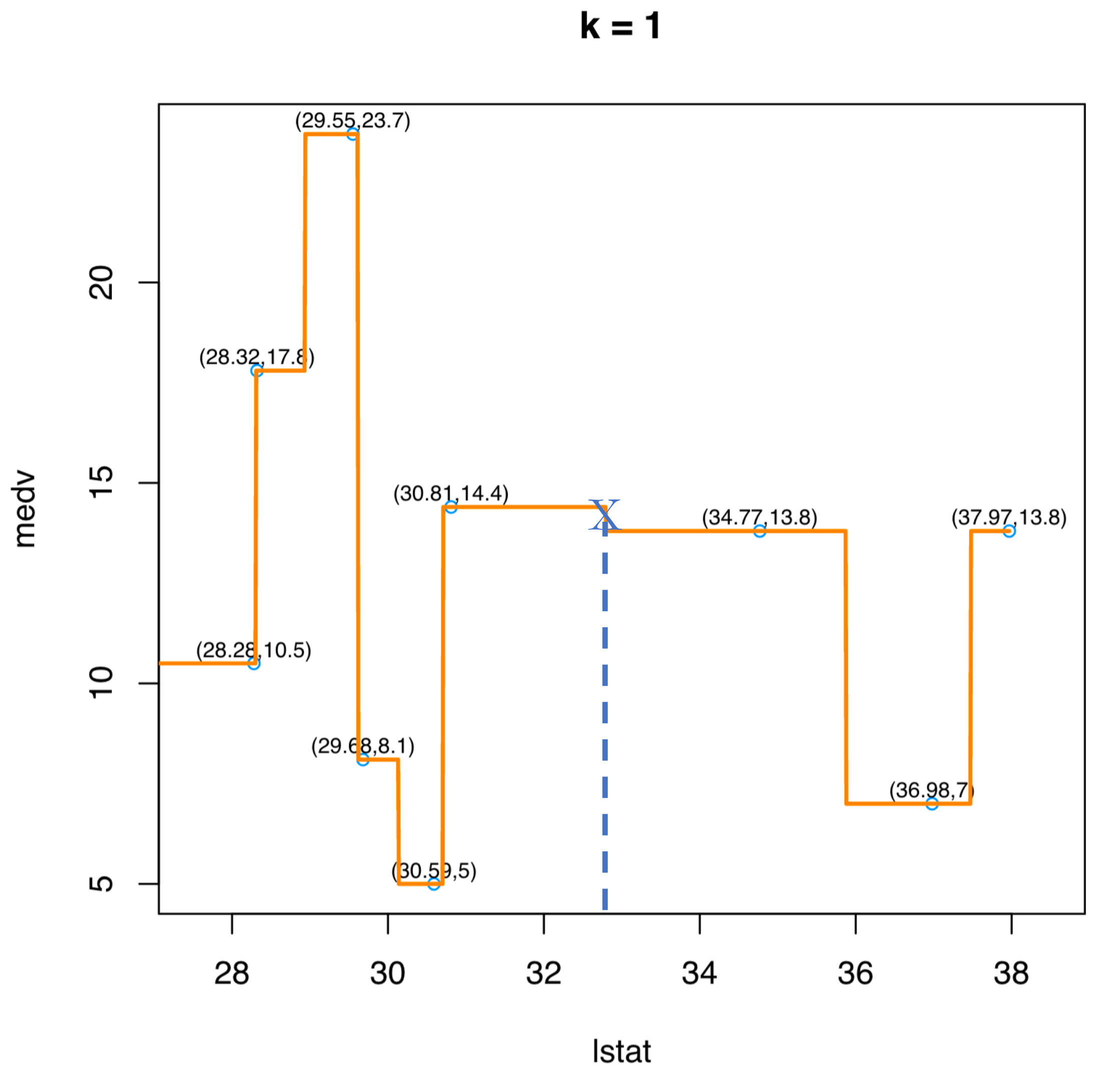
Prediction at $x_0 = 32$ $(K = 1)$

- $x_0 = 32$
- $N_K(x_0) = \{30.81\}$
- $\hat{f}(x_0 = 32) = 14.4$



Now let us understand why $\hat{f}(x_0)$ is a step function

- $x_0 = 32.79$
  - It is a switching point!
- $N_K(x_0) = \{30.81\}$ or $N_K(x_0) = \{34.77\}$
  - Note that $32.79 - 30.81 = 1.98 = 34.77 - 32.79$
- $\hat{f}(x_0 = 32.79) = 14.4$ or $\hat{f}(x_0 = 32.79) = 13.8$

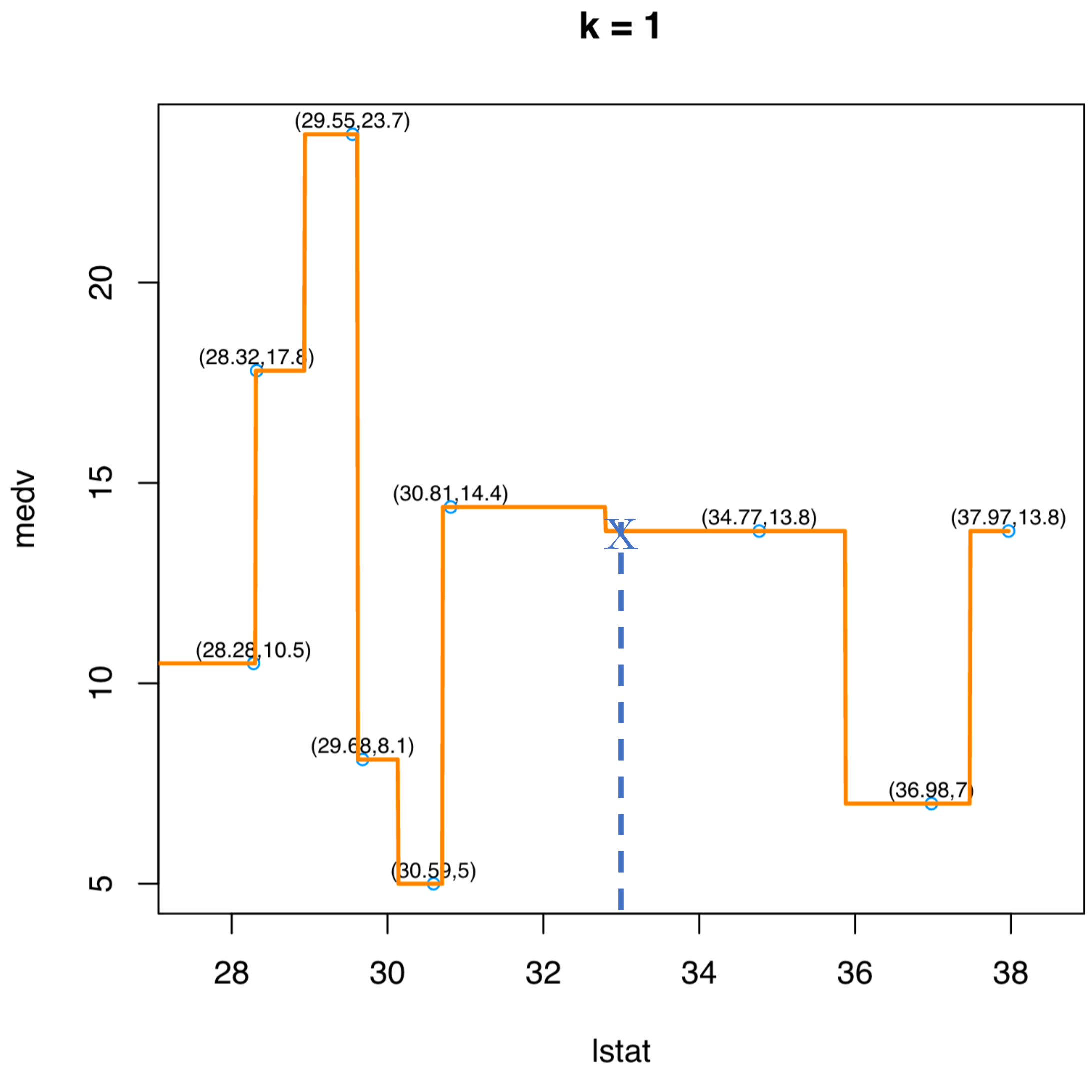


Prediction at $x_0 = 33$ $(K = 1)$

- $x_0 = 33$

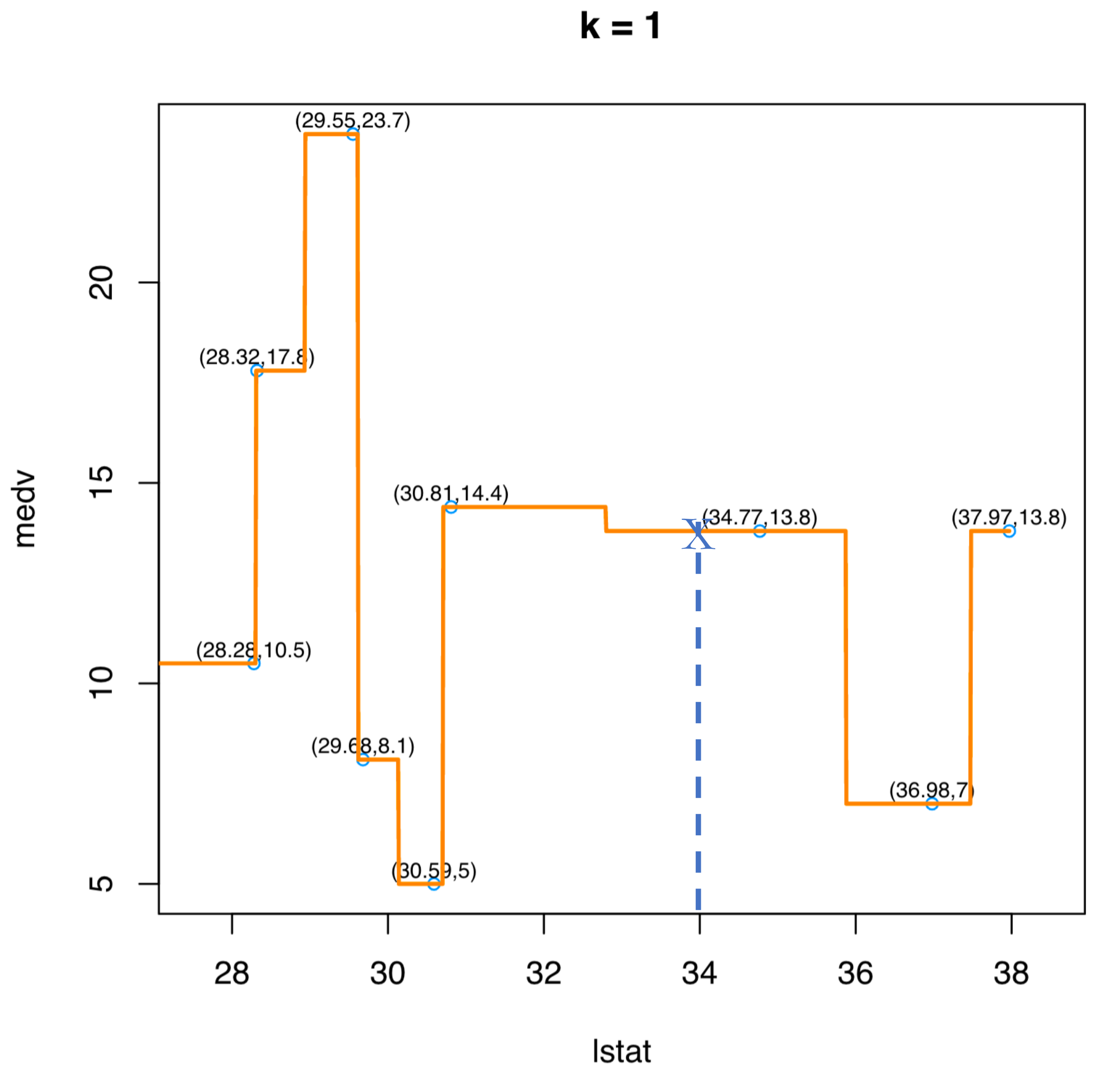
- $N_K(x_0) = \{34.77\}$
  - Note that $34.77 - 33 = 1.77 < 33 - 30.81 = 2.19$

- $\hat{f}(x_0 = 33) = 13.8$



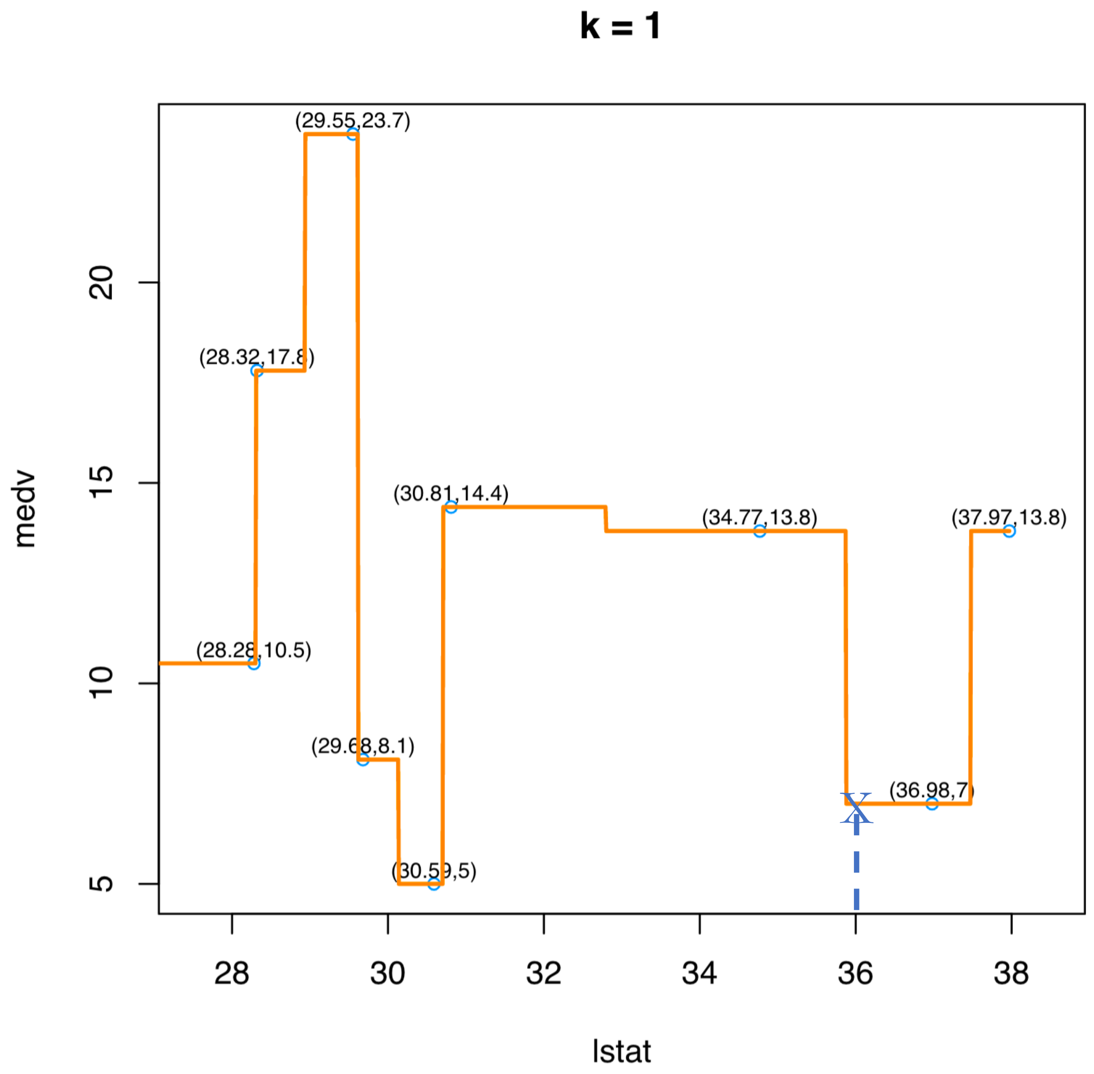
Prediction at $x_0 = 34$ $(K = 1)$

- $x_0 = 34$
- $N_K(x_0) = \{34.77\}$
- $\hat{f}(x_0 = 34) = 13.8$



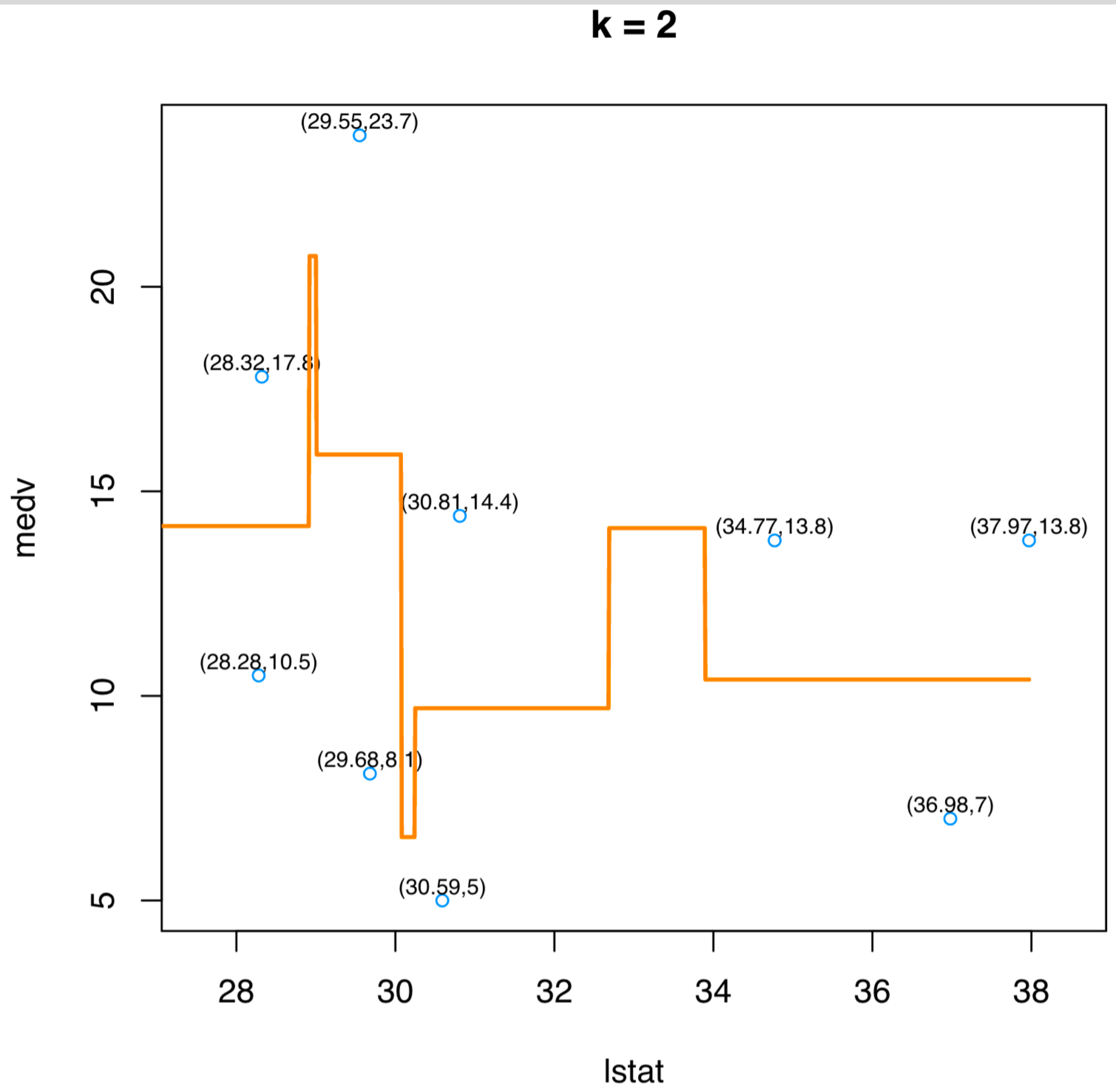
Prediction at $x_0 = 36$ $(K = 1)$

- $x_0 = 36$
- $N_K(x_0) = \{36.98\}$
- $\hat{f}(x_0 = 36) = 7$



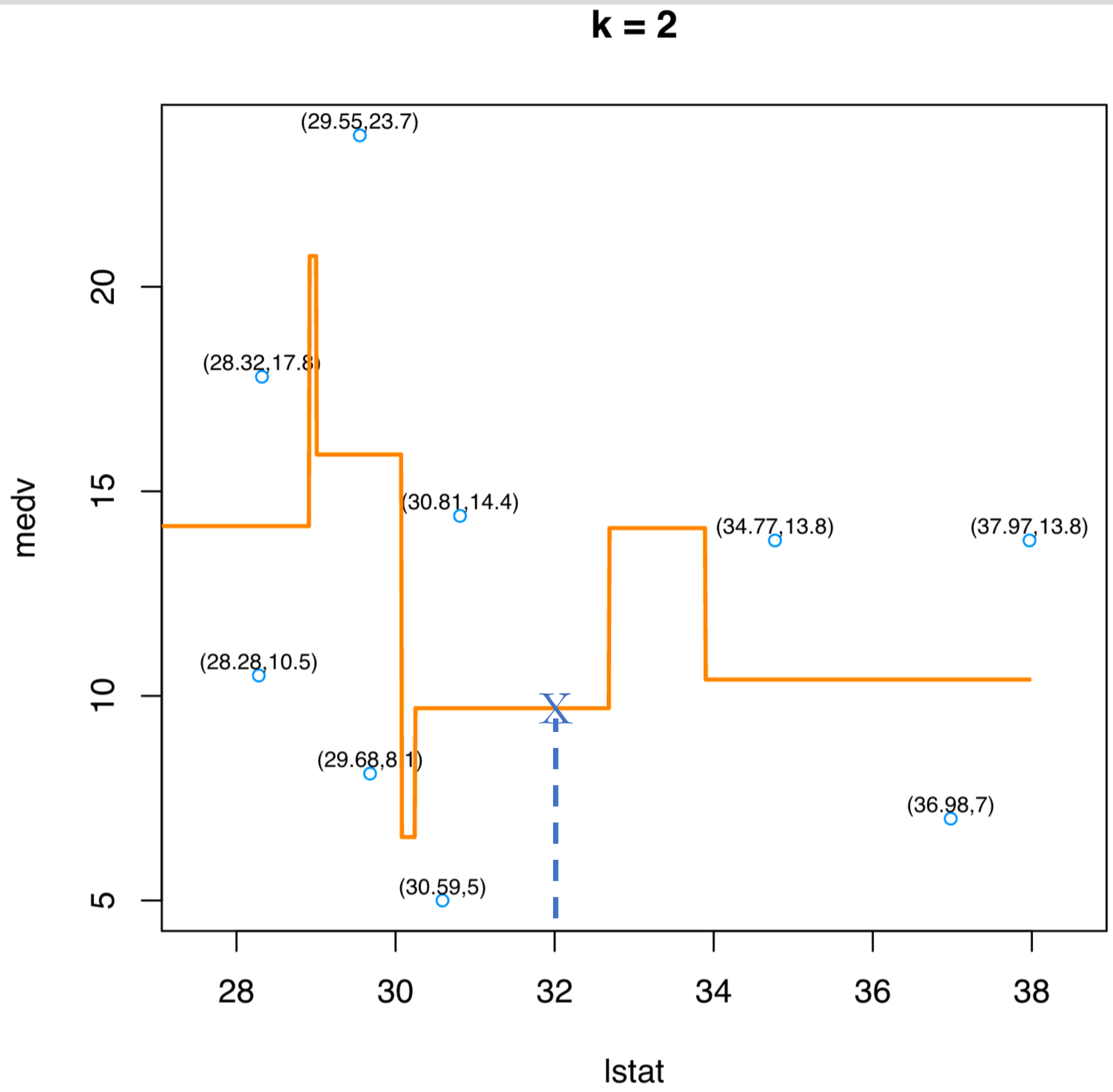
Example: 2-nearest neighbor regression

- $\hat{f}(x_0)$ equals to the average of responses of x_0's 2 nearest neighbors



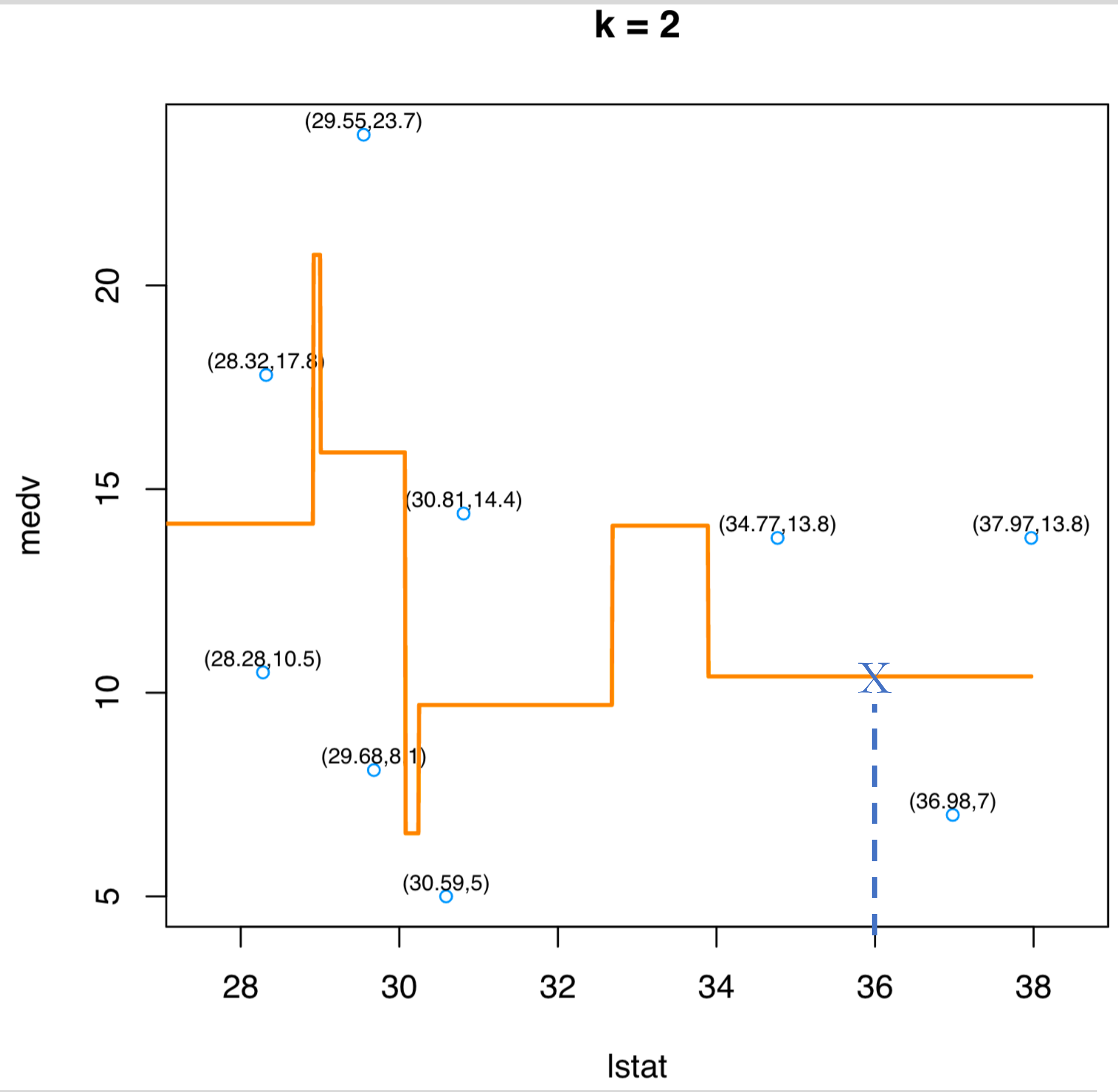
Prediction at $x_0 = 32$ $(K = 2)$

- $x_0 = 32$
- $N_K(x_0) = \{30.59, 30.81\}$
- $\hat{f}(x_0 = 32) = \frac{5+14.4}{2}$



Prediction at $x_0 = 36$ ($K = 2$)

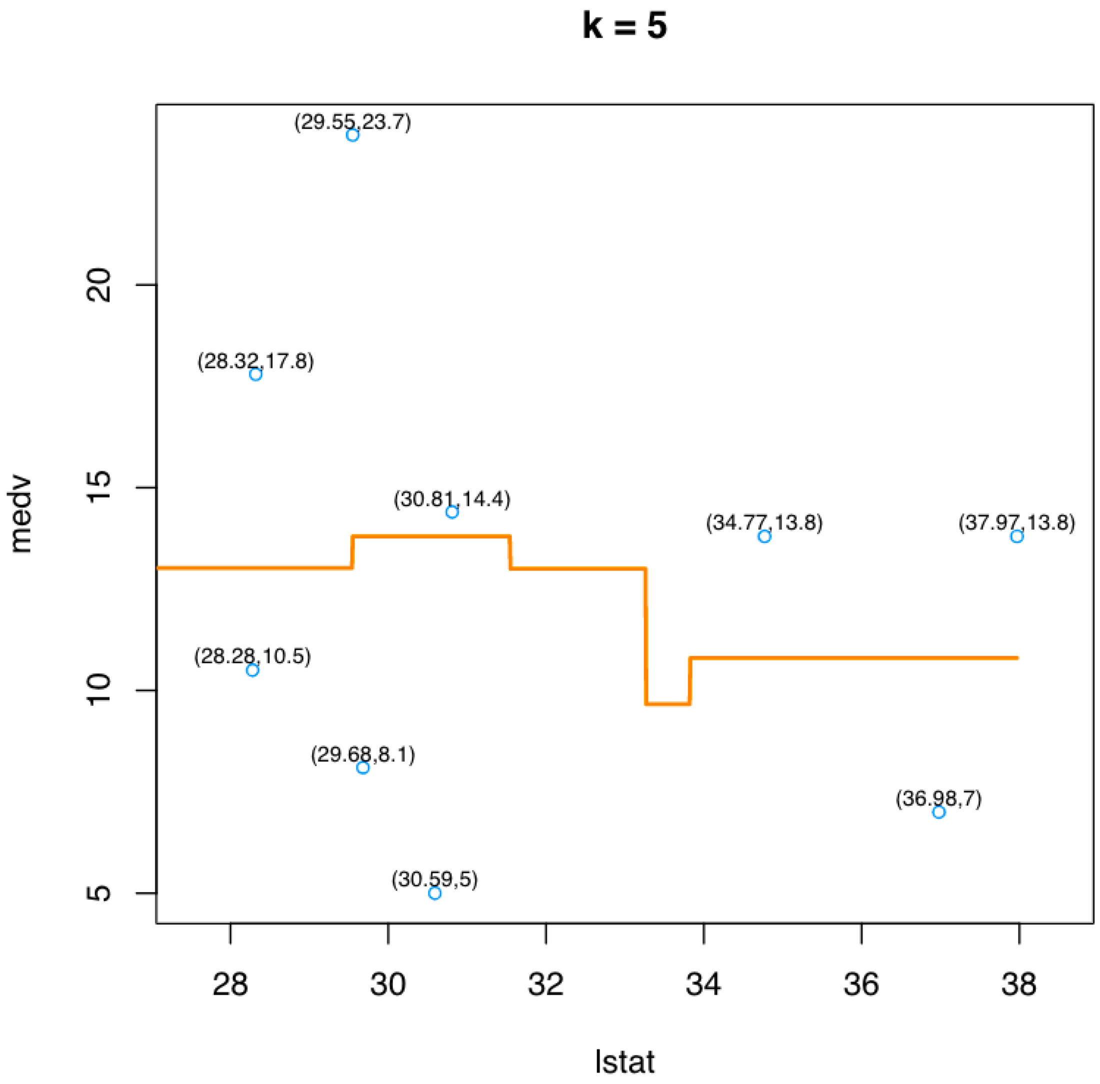
- $x_0 = 36$
- $N_K(x_0) = \{34.77, 36.98\}$
- $\hat{f}(x_0 = 36) = \frac{13.8+7}{2}$



Example: 5-nearest neighbor regression

- $\hat{f}(x_0)$ equals to the average of responses of x_0's 5 nearest neighbors

- $\hat{f}(x_0)$ is smoother as K increases

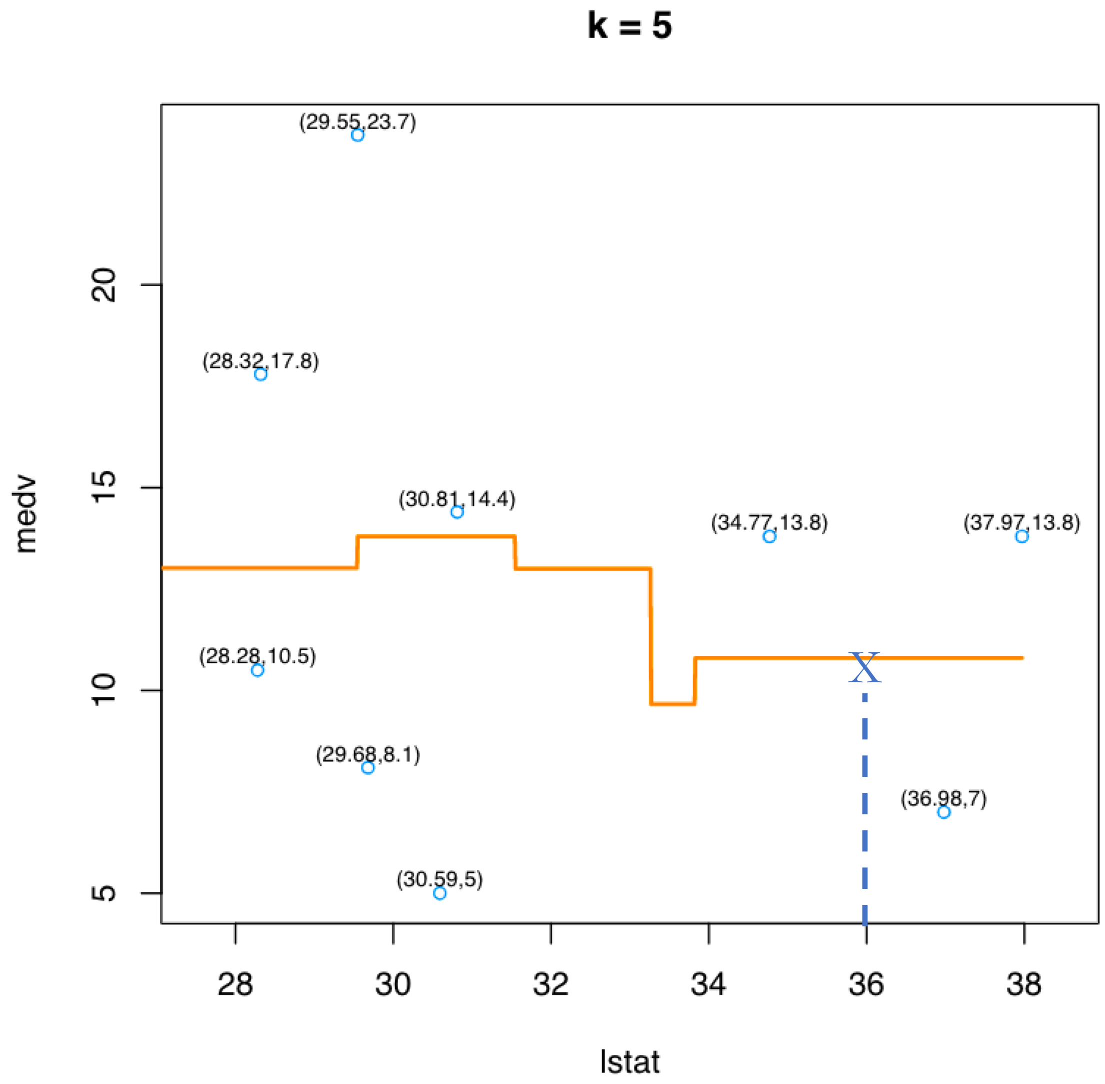


Prediction at $x_0 = 36$ ($K = 5$)

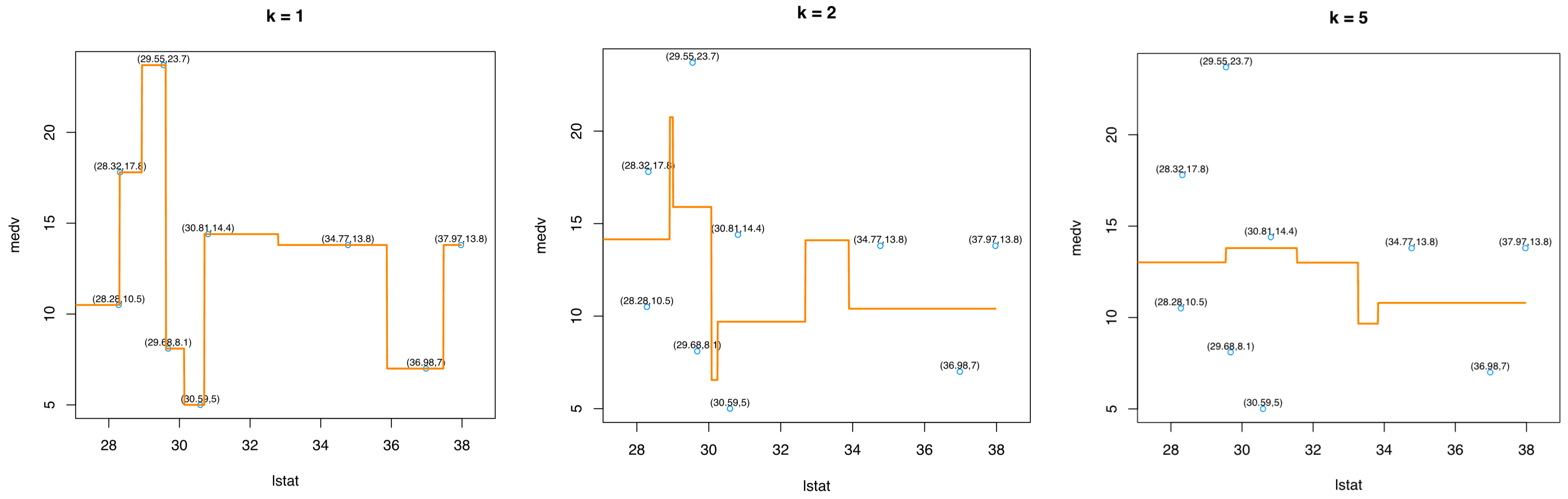
- $x_0 = 36$

- $N_K(x_0) = \{30.59, 30.81, 34.77, 36.98, 37.97\}$

- $\hat{f}(x_0 = 36) = \frac{5+14.4+13.8+7+13.8}{5}$



$\hat{f}(x_0)$ is smoother for a larger K

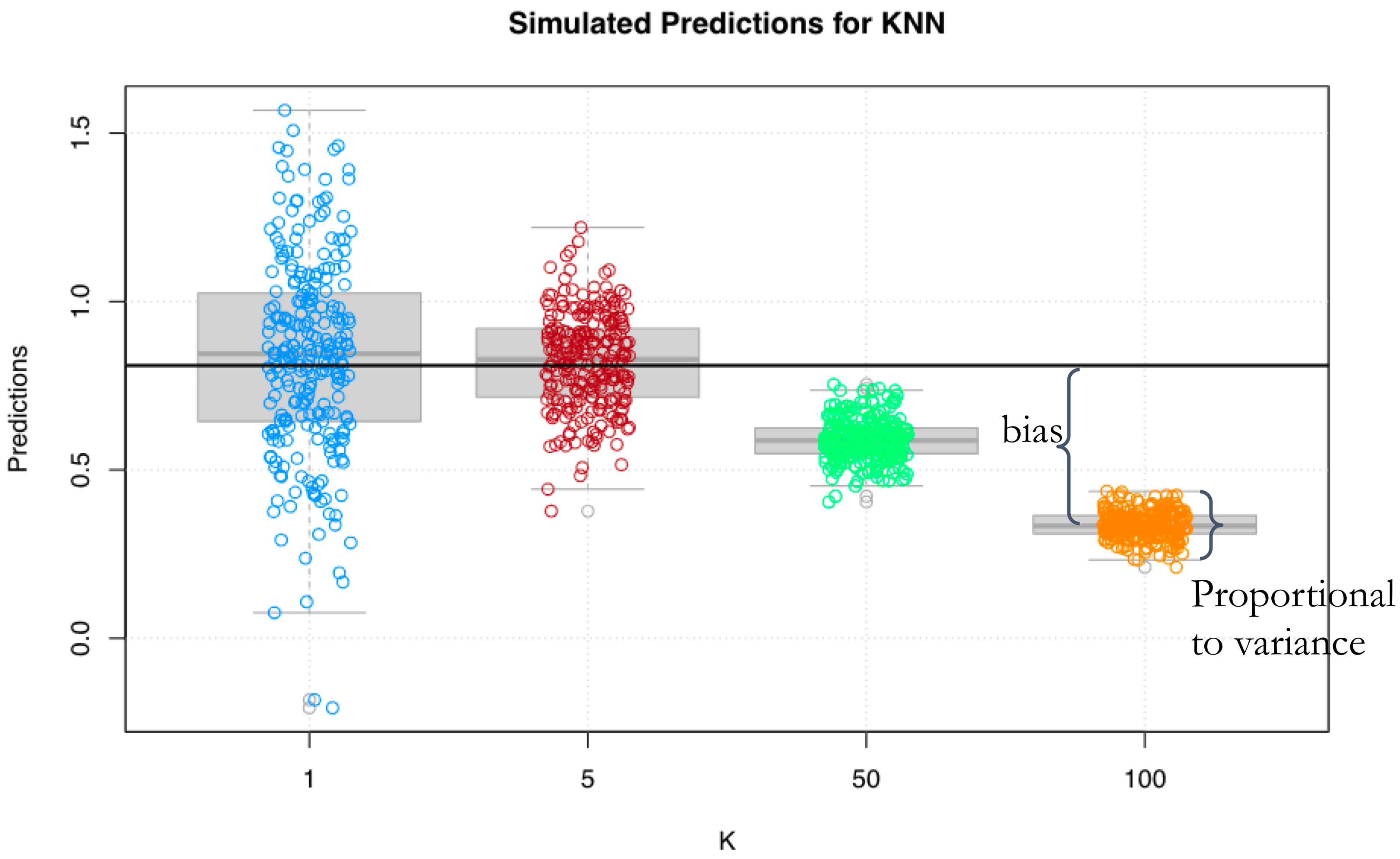


- *Question: Is the model more flexible or less flexible for a larger K?*

Bias-variance tradeoff for the optimal

- Train a KNN model to learn the true function $f(x) = x^2$ (x is a scalar)

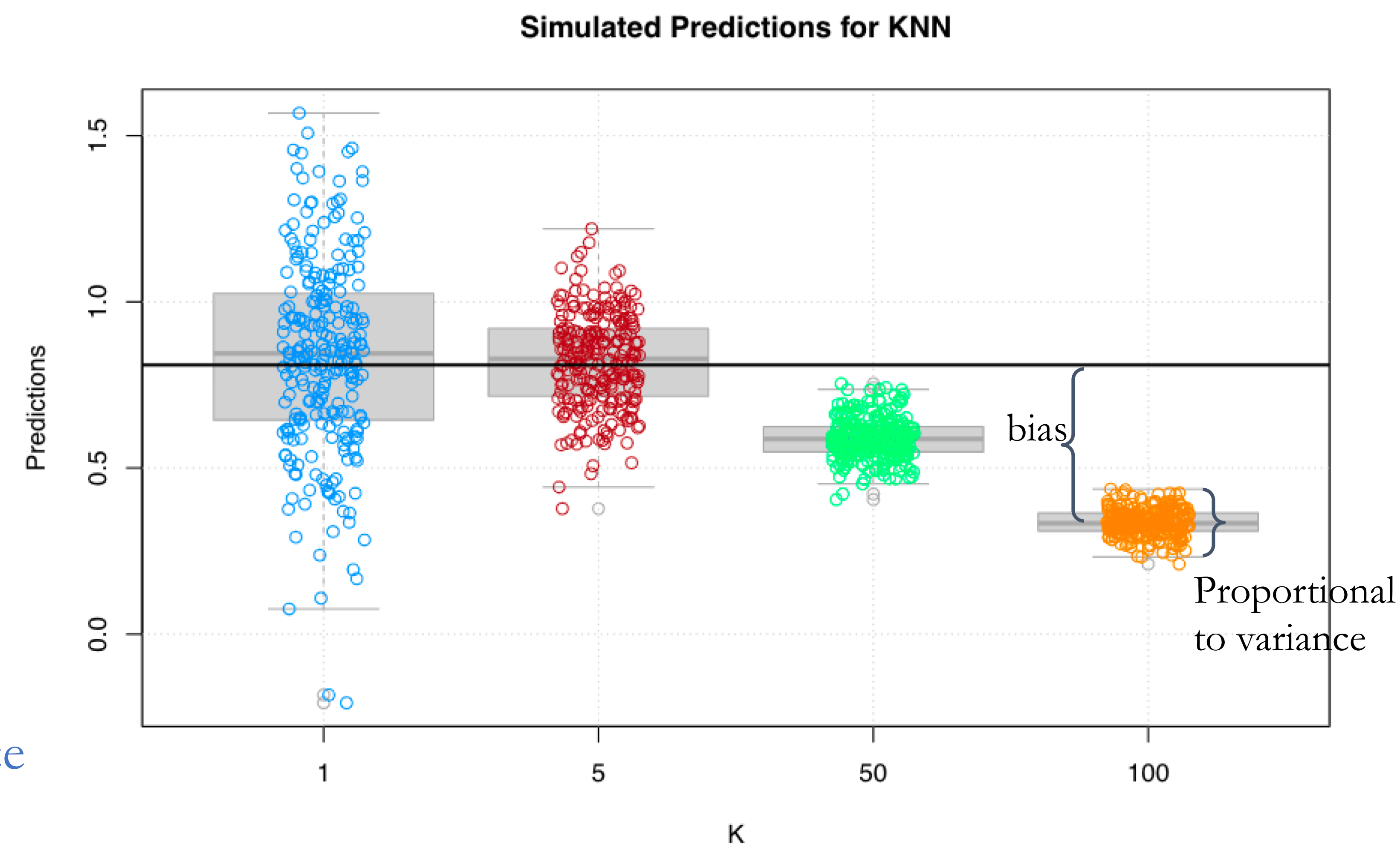
- $x_0 = 0.9$
- The truth, $f(x_0 = 0.9) = x_0^2 = 0.81$
- We have 250 datasets
- For each dataset, we fit KNN with $K = 1, 5, 50, 100$, and plot $\hat{f}(x_0 = 0.9)$



Bias-variance tradeoff for the optimal

- The square of bias
  $\hat{f}_5(x) \approx \hat{f}_1(x) < \hat{f}_{50}(x) < \hat{f}_{100}(x)$
  ➢Increasing K increases bias

- Variance
  $\hat{f}_{100}(x) < \hat{f}_{50}(x) < \hat{f}_5(x) < \hat{f}_1(x)$
  ➢Increasing K reduces variance



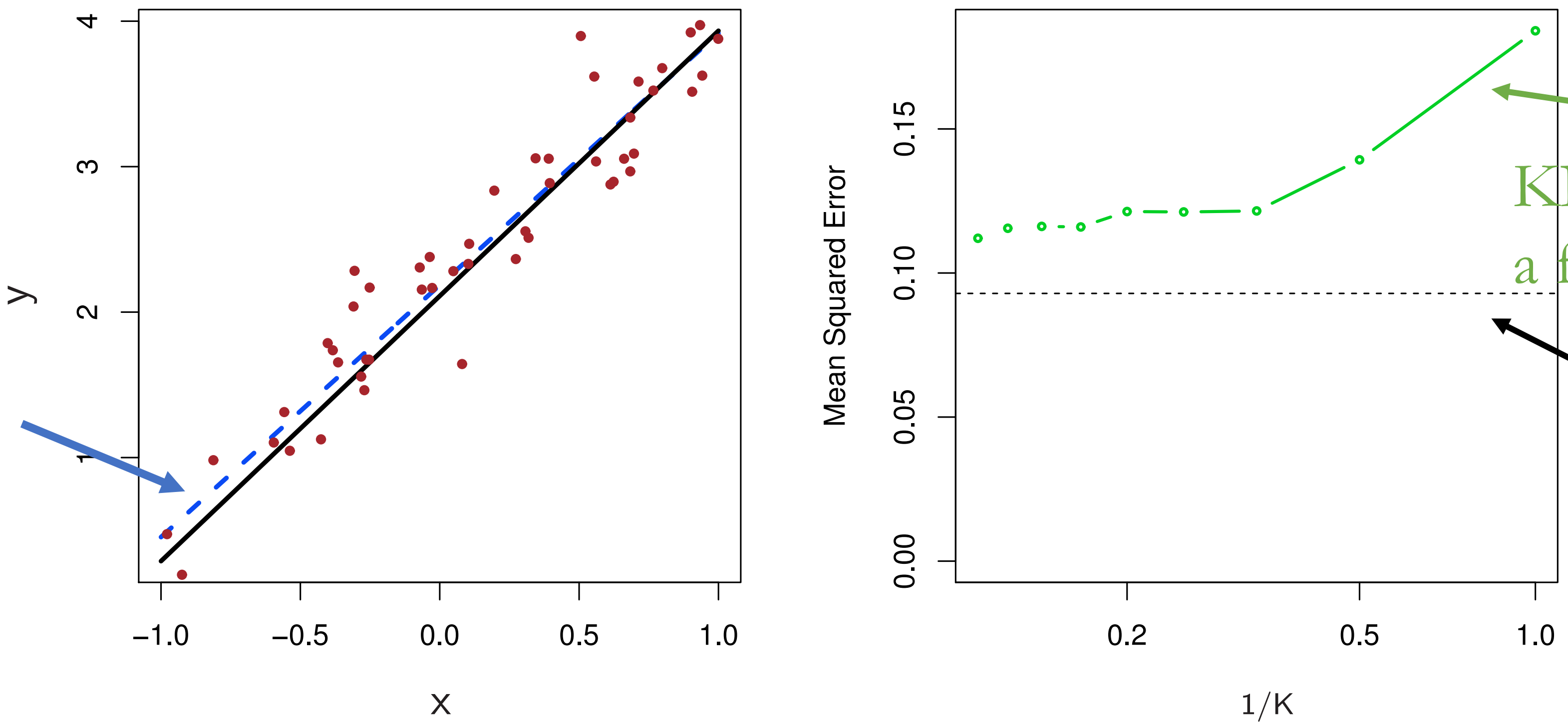
Linear regression vs K-nearest neighbors

- KNN is only better when the function f is far from linear (in which case linear model is *misspecified*)
- When n is not much larger than p, even if f is nonlinear, linear regression can outperform KNN
- KNN has smaller bias, but this comes at a price of higher variance

Linear models can dominate KNN

- Truth is linear, plot of test MSE vs. $1/K$ shows KNN worse than linear regression.

linear
regression



KNN test MSE as a function of $1/K$

linear
regression
test MSE

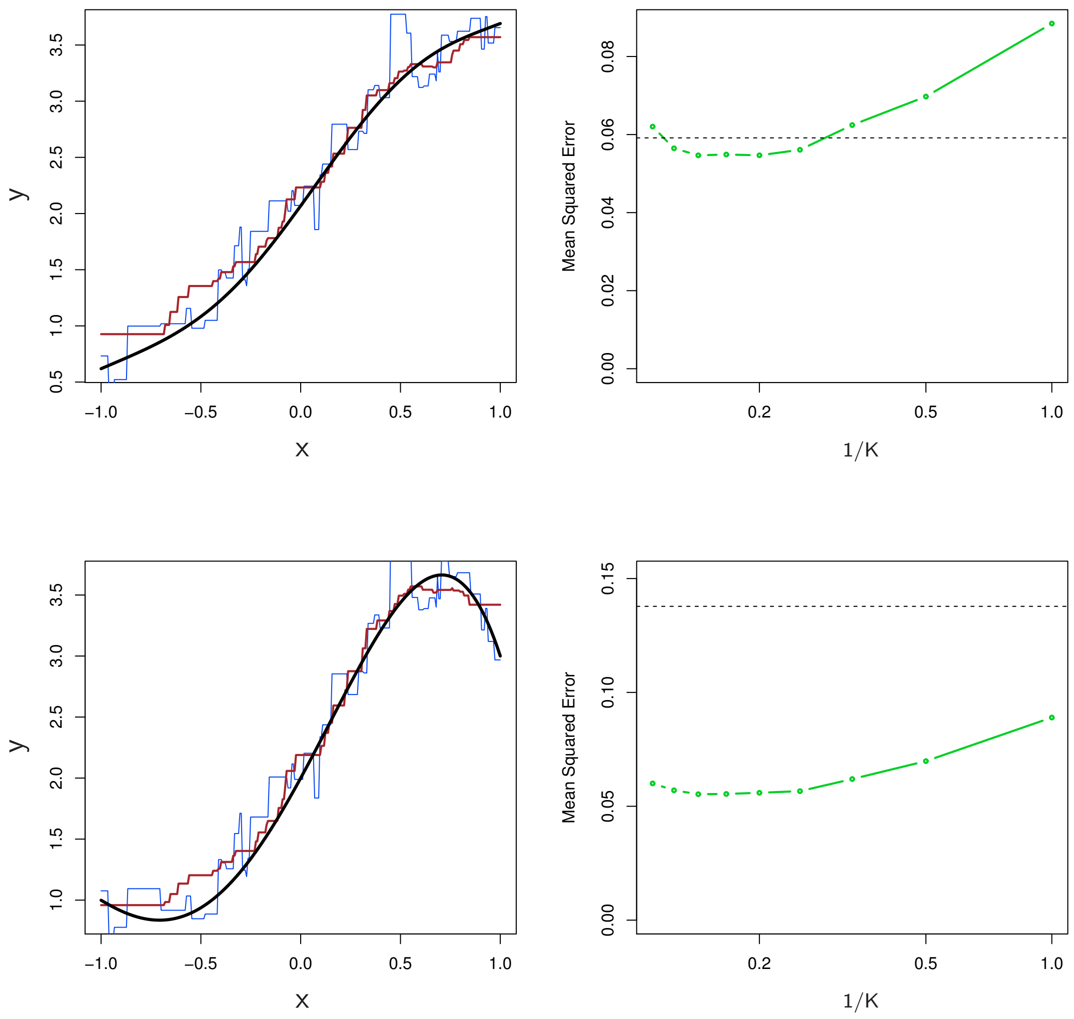
Increasing deviations from linearity

Slightly nonlinear relationship between X and Y

Blue: $K = 1$

Red: $K = 9$

Strongly nonlinear relationship between X and Y

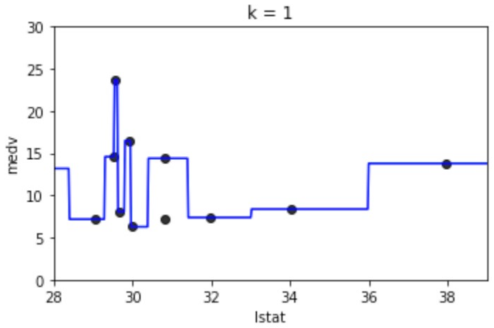


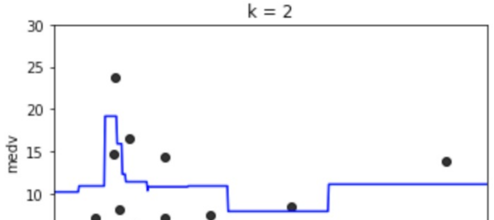
K-nearest neighbors regression in Python

```
In [3]: from sklearn.neighbors import KNeighborsRegressor
        import pandas as pd
        import seaborn as sns
```

```
In [4]: df_train = pd.DataFrame({'lstat': X_train.reshape(-1,), 'medv': y_train.reshape(-1,)})

        fig, axes = plt.subplots(3, 1, figsize = (5,10))

        n_neighbors = [1, 2, 5]

        T = np.linspace(28, 39, 500)[:, np.newaxis] # For graphing

        for i, n in enumerate(n_neighbors):
            knn = KNeighborsRegressor(n, weights = 'uniform')
            y_pred = knn.fit(X_train, y_train).predict(T)
            fit_df = pd.DataFrame({"T": T.reshape((-1,)), "y_pred": y_pred.reshape((-1,))})

            sns.lineplot(data = fit_df, x = 'T', y = 'y_pred', color = 'blue', ax = axes[i])
            sns.regplot(data = df_train, x = 'lstat', y = 'medv', ax = axes[i], fit_reg = False, scatter_kws={"color": "black"}

            axes[i].set_xlim([28, 39])
            axes[i].set_ylim([0, 30])


        fig.tight_layout()
```

Alternatively, weights = 'distance', where weight points by the inverse of their distance





Lecture plan

- K-nearest neighbors (KNN) regression

- K-nearest neighbors (KNN) classification

Classification problem

- Classification is a form of supervised machine learning

- The response variable Y is categorical, as opposed to numerical for regression

- Our goal is to find a function C which takes feature(s), x, as input, and outputs a category which is the same as the true category as frequently as possible

Input
x
numerical or categorical

$\rightarrow$

function
$\hat{C}(x)$

$\rightarrow$

Output
$\hat{y}$
categorical

K-nearest neighbors classification

- Given a value for K and a prediction point x_0
  - The predicted probability of class g is the fraction of responses of K nearest neighbors in class g

$$\hat{P}(Y = g|X = x_0) = \frac{1}{K} \sum_{x_i \in N_K(x_0)} 1(y_i = g)$$

    - $1(\cdot)$: indicator function
    - $N_K(x_0)$ is the set of K training observations that are closest to x_0

  - The predicted class is the class with maximum predicted probability

$$\hat{C}(x_0) = \text{argmax}_g \hat{P}(Y = g|X = x)$$

K-nearest neighbors classification

- Given a value for K and a prediction point x_0
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$$\hat{P}(Y = g | X = x_0) = \frac{1}{K} \sum_{x_i \in N_K(x_0)} 1(y_i = g)$$

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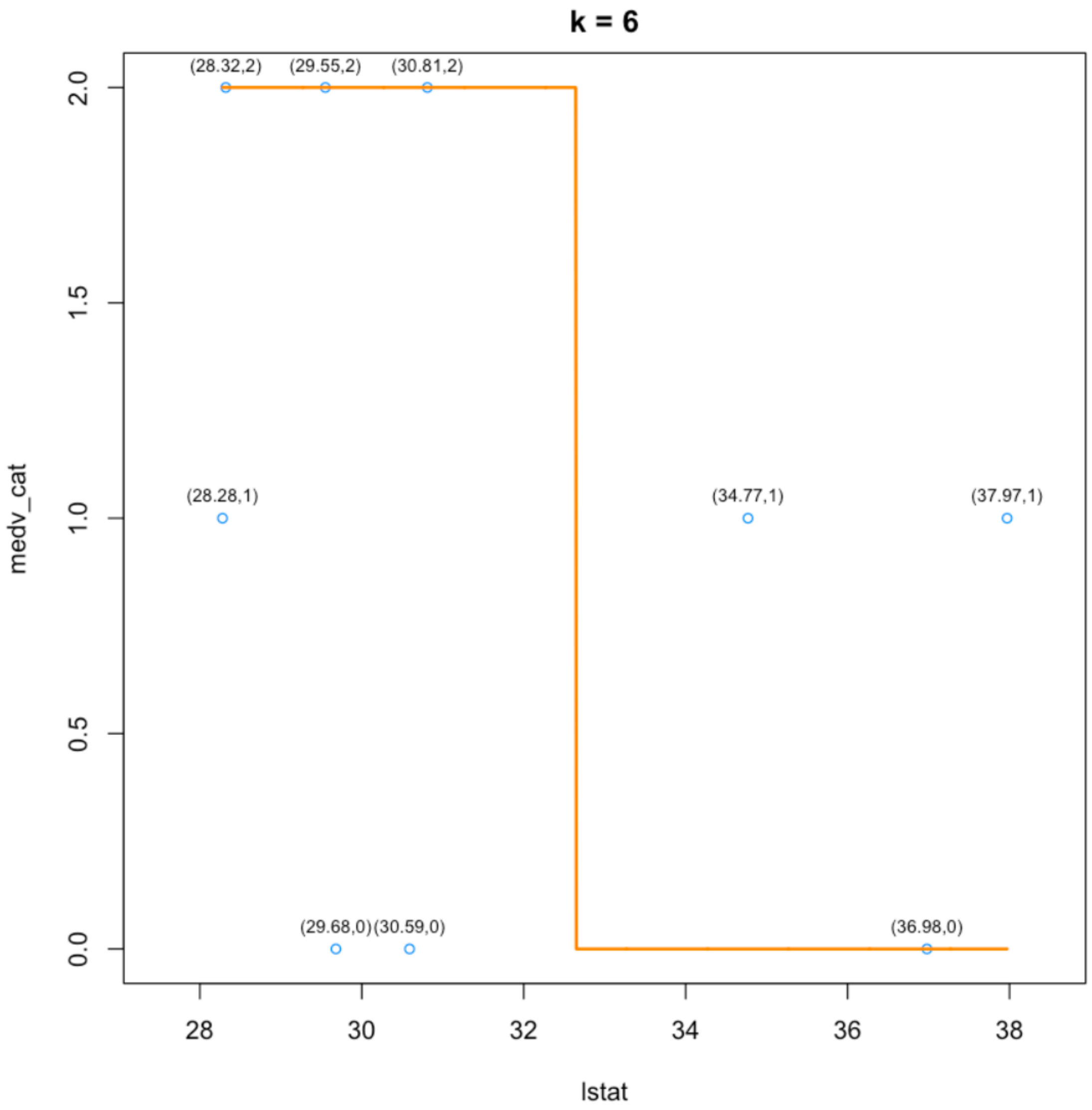
  - The predicted class is the class with maximum predicted probability

$$\hat{C}(x_0) = \text{argmax}_g \hat{P}(Y = g | X = x)$$

Example: 6-nearest neighbors classification

- Prediction of the category of median house value (0: low, 1: medium, 2: high) given the percentage of households with low socioeconomic status (lstat)

- Orange curve: $\hat{C}(x_0)$



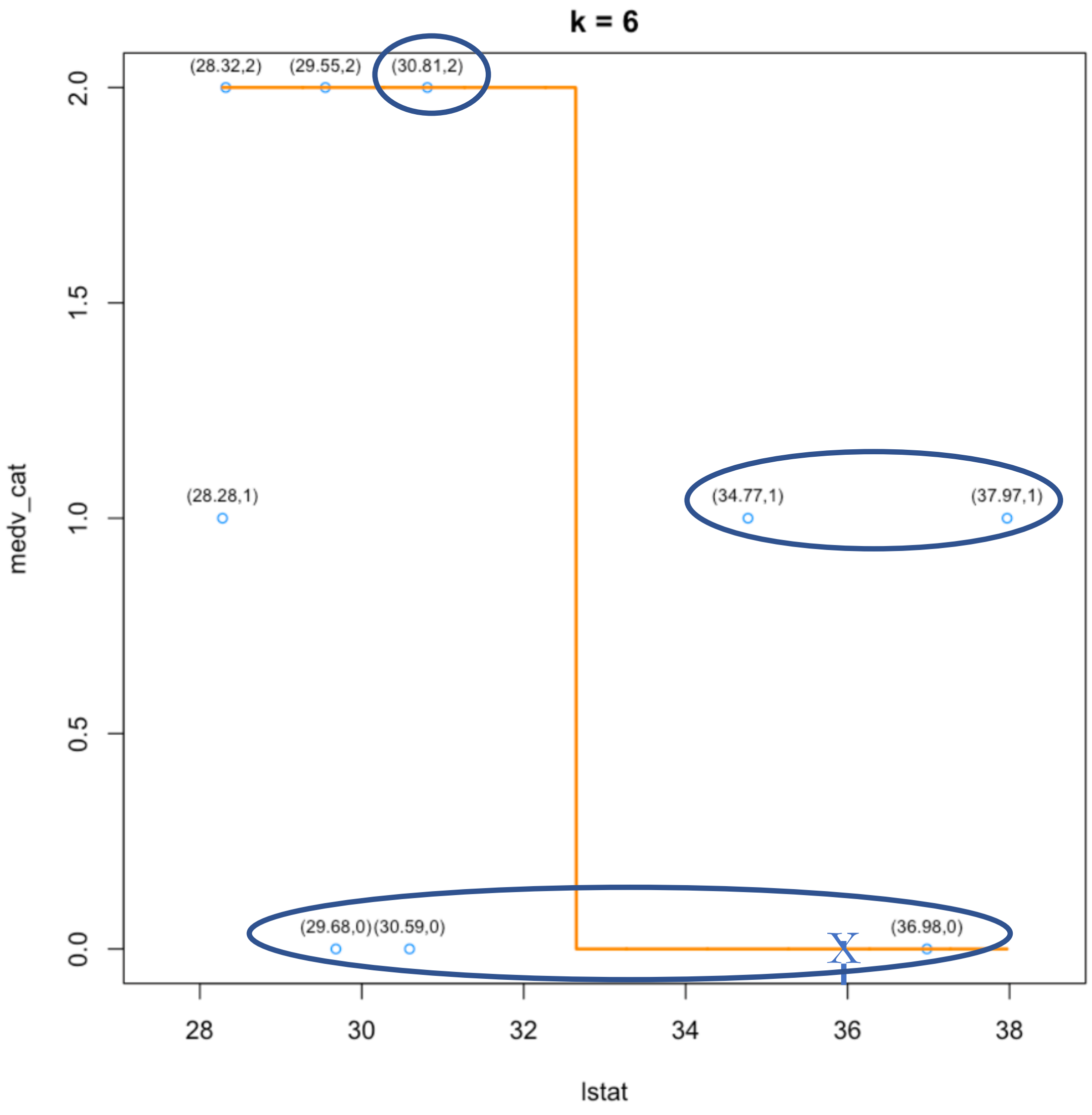
Example: 6-nearest neighbors classification

- $x_0 = 36$

- $N_K(x_0) = \{29.68, 30.59, 30.81, 34.77, 36.98, 37.97\}$

- $\hat{P}(Y = 0|X = x_0) = \frac{1}{2}$
- $\hat{P}(Y = 1|X = x_0) = \frac{1}{3}$
- $\hat{P}(Y = 2|X = x_0) = \frac{1}{6}$

- $\hat{C}(x_0) = 0$



K-nearest neighbors classification in Python

KNN as classification problem

In [6]:
```
from sklearn.neighbors import KNeighborsClassifier
```

In [7]:
```
df = load_data("Boston")

X_train, X_test, y_train, y_test = train_test_split(df[['lstat']], df[['medv']], train_size=250, random_state=42) # We

X_train = X_train.to_numpy()
y_train = y_train.to_numpy()

y_train_cat = (y_train >= 14) * 2 + ((y_train < 14) * (y_train >= 10)) * 1
y_train_cat = y_train_cat.reshape((-1,))
```

In [8]:
```
df_train = pd.DataFrame({'lstat': X_train.reshape(-1,), 'medv': y_train_cat.reshape(-1,)})

T = np.linspace(28, 39, 500)[:, np.newaxis] # For graphing

n = 2
knn = KNeighborsClassifier(n, weights = 'uniform')
y_pred = knn.fit(X_train, y_train_cat).predict(T)
fit_df = pd.DataFrame({'T': T.reshape((-1,)), 'y_pred': y_pred.reshape((-1,))})

sns.lineplot(data = fit_df, x = 'T', y = 'y_pred', color = 'blue')
sns.regplot(data = df_train, x = 'lstat', y = 'medv', fit_reg = False, scatter_kws={"color": "black"}).set(title = f'k

plt.xlim([28, 39])
plt.show()
```