Week 8– K Nearest Neighbors (KNN)

Regression

Pedram Jahangiry



- If the specified functional form is far from the truth, and prediction accuracy is our goal, then the parametric method will perform poorly. For instance, if we assume a linear relationship between X and Y but the true relationship is far from linear, then the resulting model will provide a poor fit to the data, and any conclusions drawn from it will be suspect.
- In contrast, non-parametric methods do not explicitly assume a parametric form for f(X), and thereby provide an alternative and more flexible approach for performing regression.
- KNN is one of the simplest and best-known non-parametric methods
- The KNN regression method is closely related to the KNN classifier

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

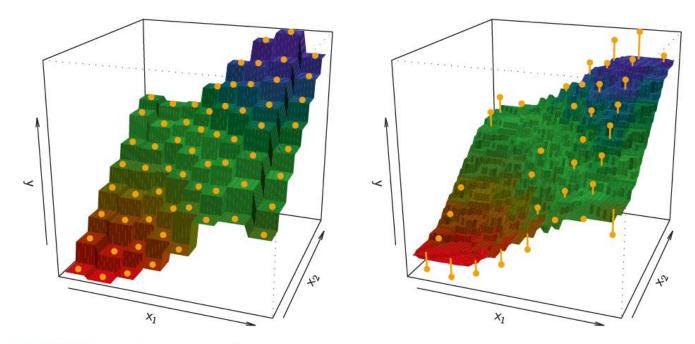


FIGURE 3.16. Plots of $\hat{f}(X)$ using KNN regression on a two-dimensional data set with 64 observations (orange dots). Left: K = 1 results in a rough step function fit. Right: K = 9 produces a much smoother fit.

In general, the optimal value for K will depend on the bias-variance tradeoff. What is the trade off? Model Flexibility?

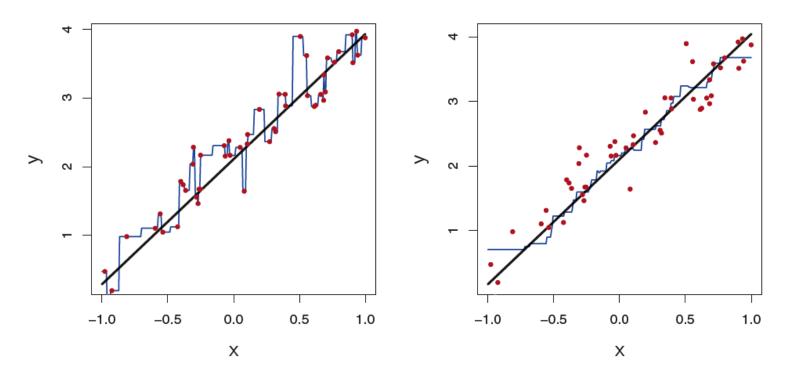


FIGURE 3.17. Plots of $\hat{f}(X)$ using KNN regression on a one-dimensional data set with 100 observations. The true relationship is given by the black solid line. Left: The blue curve corresponds to K=1 and interpolates (i.e. passes directly through) the training data. Right: The blue curve corresponds to K=9, and represents a smoother fit.

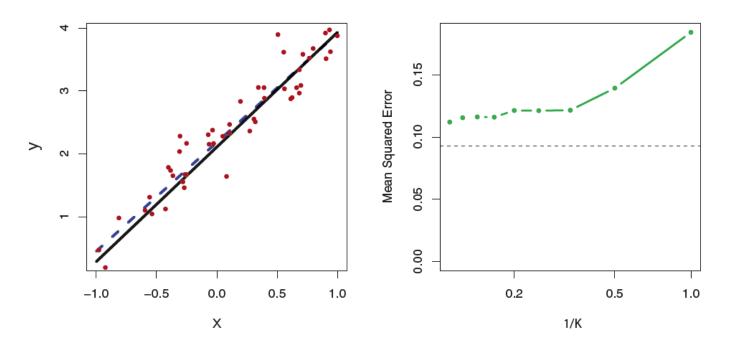


FIGURE 3.18. The same data set shown in Figure 3.17 is investigated further. Left: The blue dashed line is the least squares fit to the data. Since f(X) is in fact linear (displayed as the black line), the least squares regression line provides a very good estimate of f(X). Right: The dashed horizontal line represents the least squares test set MSE, while the green solid line corresponds to the MSE for KNN as a function of 1/K (on the log scale). Linear regression achieves a lower test MSE than does KNN regression, since f(X) is in fact linear. For KNN regression, the best results occur with a very large value of K, corresponding to a small value of 1/K.

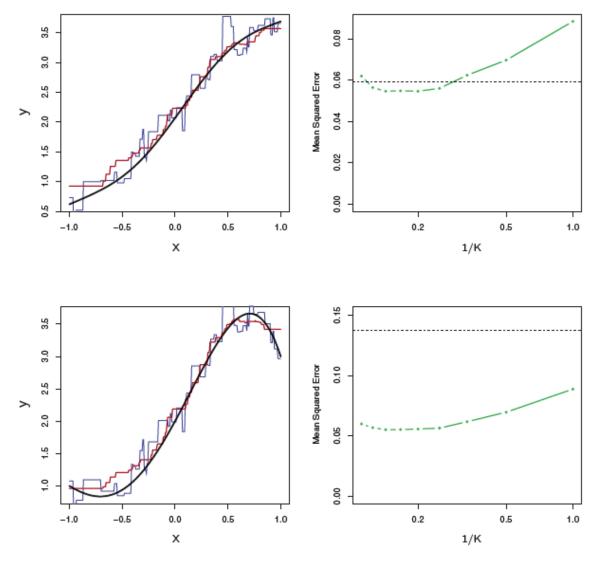


FIGURE 3.19. Top Left: In a setting with a slightly non-linear relationship between X and Y (solid black line), the KNN fits with K=1 (blue) and K=9 (red) are displayed. Top Right: For the slightly non-linear data, the test set MSE for least squares regression (horizontal black) and KNN with various values of 1/K (green) are displayed. Bottom Left and Bottom Right: As in the top panel, but with a strongly non-linear relationship between X and Y.

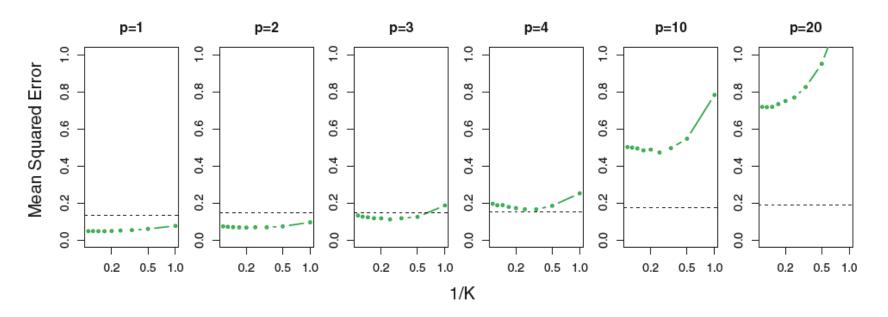


FIGURE 3.20. Test MSE for linear regression (black dashed lines) and KNN (green curves) as the number of variables p increases. The true function is non-linear in the first variable, as in the lower panel in Figure 3.19, and does not depend on the additional variables. The performance of linear regression deteriorates slowly in the presence of these additional noise variables, whereas KNN's performance degrades much more quickly as p increases.