CEE 697M: Probabilistic Machine Learning

M4 Nonparametric Methods: L4a: Exemplar-based methods

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Outline

Nonparametric modeling

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- Other names: instance-based learning, memory-based learning

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- K-nearest neighbors (KNN)
- Kernel density estimation
- Kernel [local] regression

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Illustration of KNN

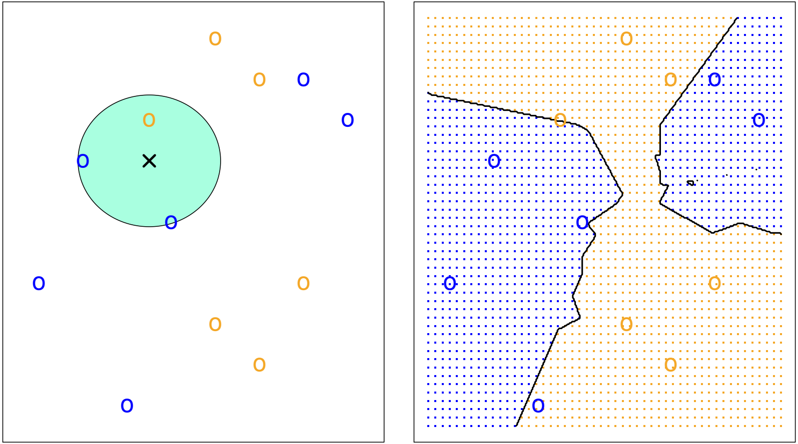

Figure: Illustration of the KNN approach on a training set of 12 observations and the resulting decision boundary. (ESL Fig 2.14)

Bias-variance trade-off in KNN

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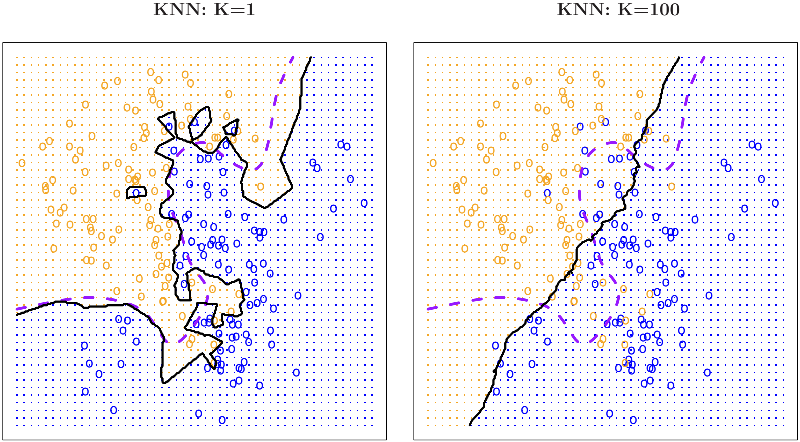

Figure: Comparing decision boundaries $K = 1$ and $K = 100$ for a dataset of 100 observations. Which model has lower bias? Which one gives a higher variance? The Bayes decision boundary is the purple dashed line (ESL Fig 2.16)

Approximating Bayes decision boundary with KNN

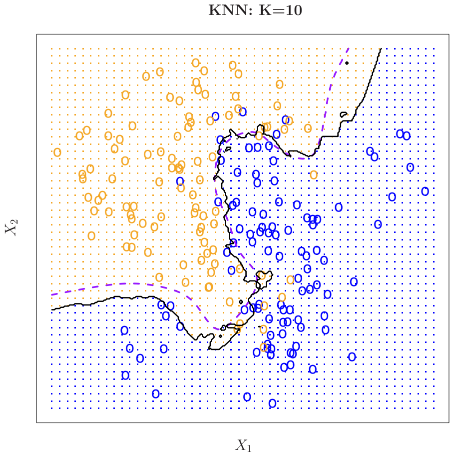

Figure: KNN decision boundary with $K = 10$ on the same training data set. (ESL Fig 2.15)

Training and test error rates for KNN

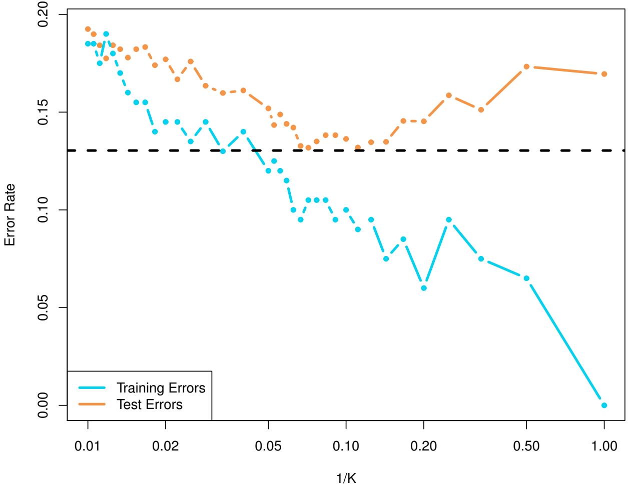

Figure: KNN training error rate (blue, 200 observations) and test error rate (orange, 5000 observations). Flexibility increases as K decreases. Which K should you choose? (ESL Fig 2.17)

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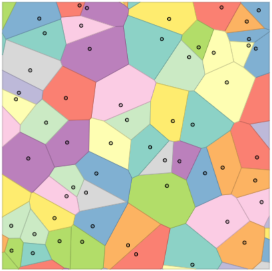

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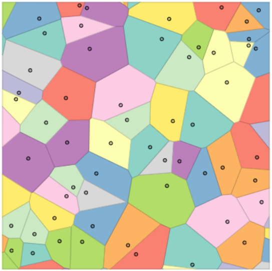

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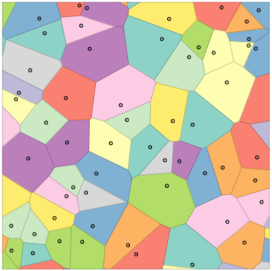

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- Memory intensive

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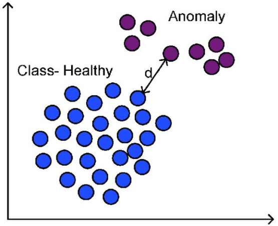

Source: https://www.intechopen.com/chapters/74393

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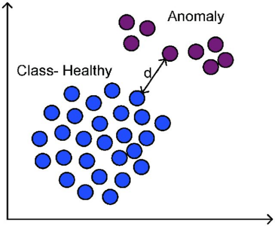

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- Few-shot classification (for person re-identification or face verification)

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- When f is a deep neural network, this process is termed **deep metric learning**

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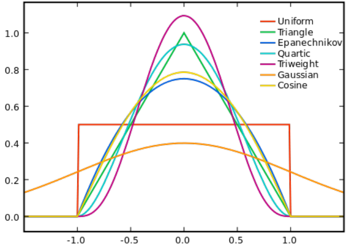

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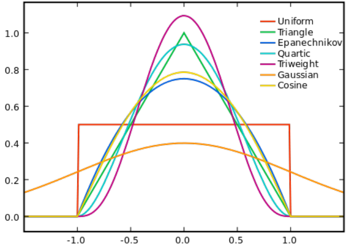

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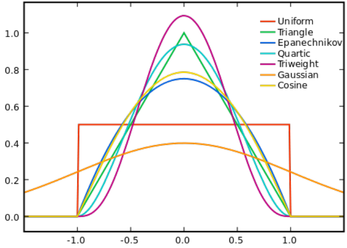

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- Triangular: $\mathcal{K}(x) = (1 - |x|)$
- Epanechnikov: $\mathcal{K}(x) = \frac{3}{4}(1 - x^2)$
- Triweight: $\mathcal{K}(x) = \frac{35}{32}(1 - x^2)^3$
- Tricube: $\mathcal{K}(x) = \frac{70}{81}(1 - |x|^3)^3$
- Gaussian: $\mathcal{K}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$

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Specifies the width of the kernel:

$$\mathcal{K}_h := \frac{1}{h}\mathcal{K}\left(\frac{x}{h}\right) \tag{8}$$

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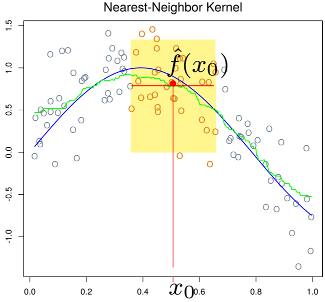

Figure: KNN equally-weighted kernel

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In D, the half-width (or *bandwidth*) of the neighborhood is given by λ.

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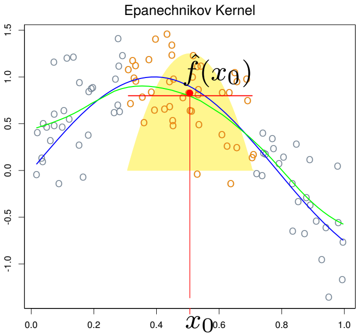

Figure: Nadaraya-Watson estimate of $\hat{f}(x)$ using the Epanechnikov kernel. Half-width is fixed at $\lambda = 0.2$

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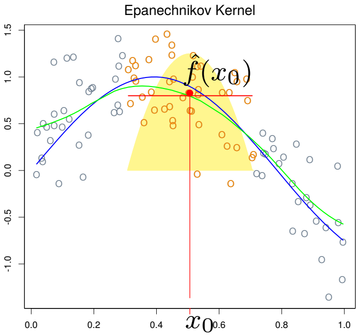

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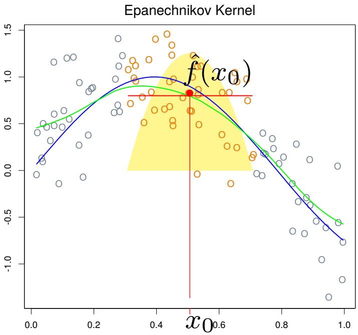

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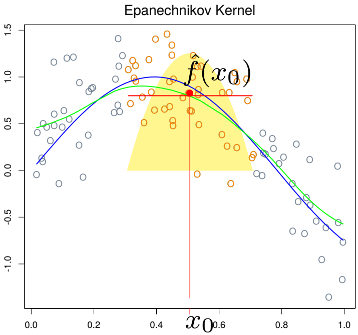

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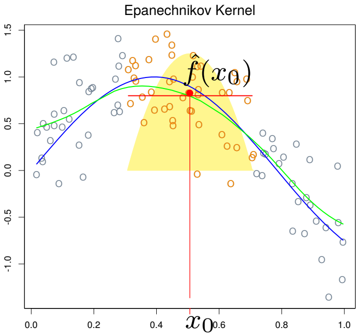

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2. **Parametric**: estimate a linear model for each point x_0

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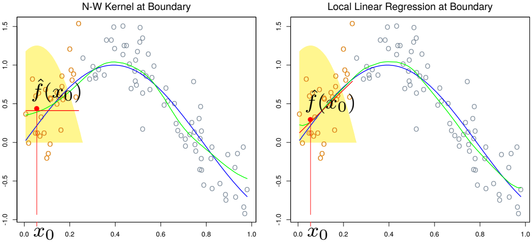

Figure: Locally weighted average (Nadaraya-Watson) versus local linear regression.

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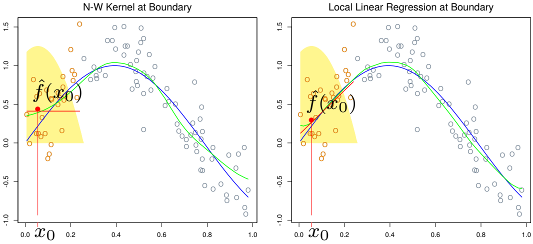

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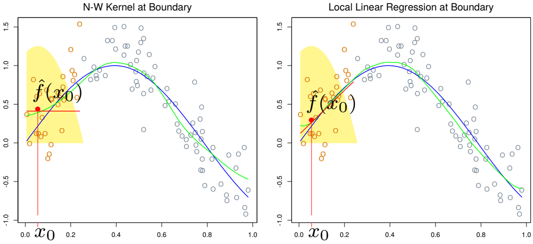

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$$\min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{n} K_\lambda(x_0, x_i)[y_i - \alpha(x_0) - \beta(x_0)x_i]^2 \tag{14}$$

Local linear regression estimates

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Let $b(x)^T = (1, x)$ and:

$$\boldsymbol{B} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \quad \boldsymbol{W}(x_0) = \begin{pmatrix} K_\lambda(x_0, x_1) & 0 & \cdots & 0 \\ 0 & K_\lambda(x_0, x_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & K_\lambda(x_0, x_n) \end{pmatrix} \tag{15}$$

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$$\hat{f}(x_0) = \sum_{i=1}^{n} \ell_i(x_0) y_i \tag{17}$$

The weights $\ell_i(x_0)$ are called the **equivalent kernel**

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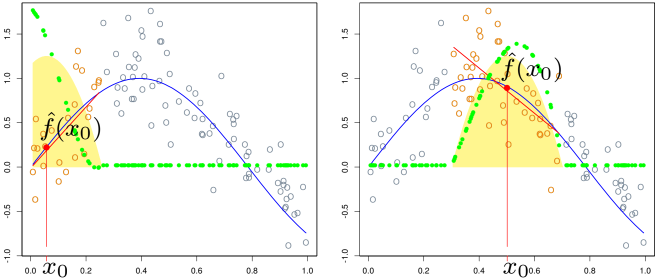

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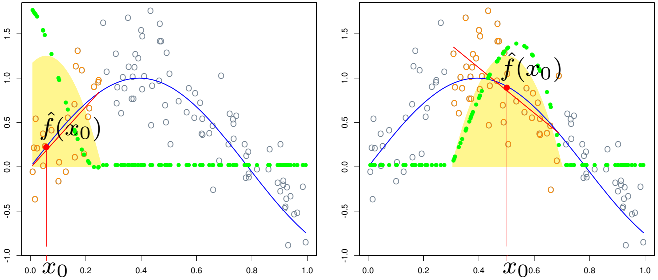

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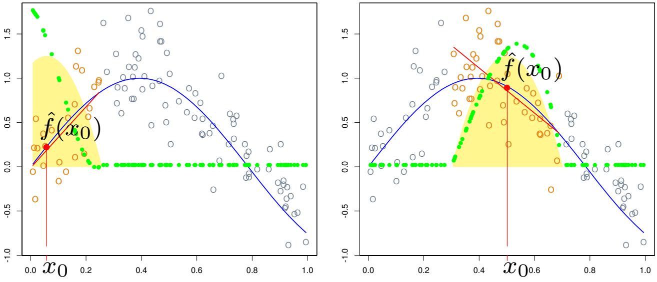

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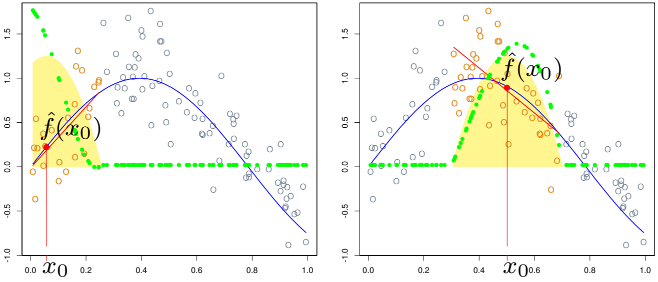

Figure: Green points show the weights $\ell_i(x_0)$ (rescaled for display purposes) along with those for the Nadaraya-Watson (N-W) local average (yellow shaded region; also rescaled).

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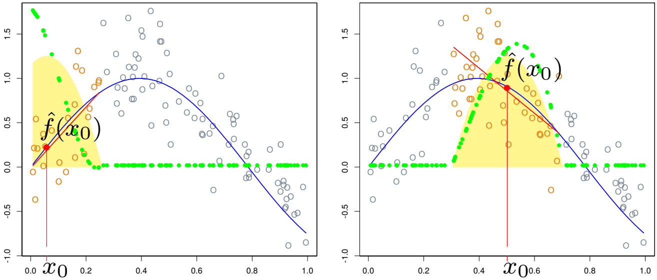

Figure: Green points show the weights $\ell_i(x_0)$ (rescaled for display purposes) along with those for the Nadaraya-Watson (N-W) local average (yellow shaded region; also rescaled). The correction effect of local regression can be observed.

Local polynomial regression

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$$\min_{\alpha(x_0),\beta(x_0),j=1,\ldots,d} \sum_{i=1}^{n} K_\lambda(x_0, x_i)\left[y_i - \alpha(x_0) - \sum_{j=1}^{d} \beta_j(x_0)x_i^j\right]^2 \tag{19}$$

Bias correction of local quadratic regression

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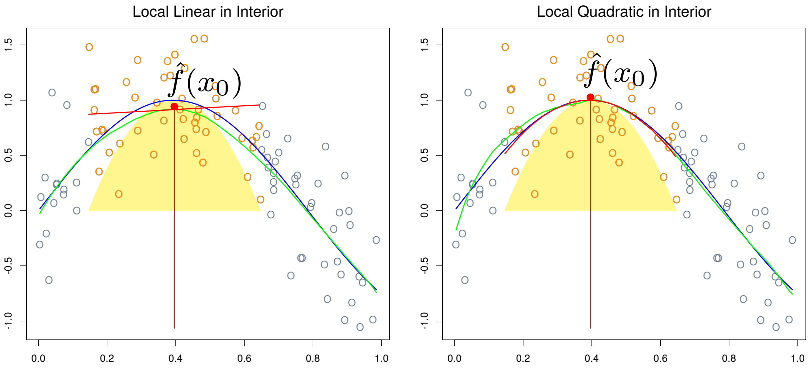

Figure: The local linear regression estimator is biased in curved regions. A higher-order local fit (in this case, quadratic) can eliminate this.

Local regression algorithms

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- LOESS: locally estimated scatterplot smoothing

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  - Identical approached earlier developed in 1964 by Savitzky and Golay for smoothing noisy data (known as the Savitzky-Golay filter)
  - "Rediscovered" by William Cleveland in 1979
- LOWESS: locally weighted scatterplot smoothing
  - Extension of LOESS by Cleveland and Susan Devlin (1988)
- LOESS can be considered a generalization of LOWESS, as it fits multivariate data, while LOWESS is for univariate cases

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- **ISLR 7.6:** Local Regression (pp. 280–282)