CEE 697M: Probabilistic Machine Learning

M4 Nonparametric Methods:
L4a: Exemplar-based methods

Jimi Oke

UMass Amherst

College of Engineering

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Outline

1. Introduction
2. KNN
3. Metric learning
4. Density kernels
5. Kernel smoothing
6. Local regression
7. Outlook

Nonparametric modeling

Parametric models seek to estimate $p(\boldsymbol{y}|\boldsymbol{\theta})$ (unconditional case) or $p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})$ (conditional case).

- $\boldsymbol{\theta}$ is a fixed-dimensinoal vector of **parameters**
- Estimation is performed using a dataset $\mathcal{D} = \{(\boldsymbol{x}_n, \boldsymbol{y}_n) : n = 1 : N\}$
- There is an assumed functional form: $\boldsymbol{y} \sim f_{\boldsymbol{\theta}}(\boldsymbol{x})$

Nonparametric models are defined based on similarity between a test input $\boldsymbol{x}$ at each training input $\boldsymbol{x}_n$: $d(\boldsymbol{x}, \boldsymbol{x}_n)$

- No assumption of functional form on model parameters
- Effective number of parameters can grow with size of dataset $|\mathcal{D}|$
- Known as **exemplar-based models** (as training samples are used to make each future prediction)
- Other names: instance-based learning, memory-based learning

Exemplar-based models

We will consider the following exemplar approaches:

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

K nearest neighbor classifier

Basic idea: classify new/test input $\boldsymbol{x}$ by assigning to most probable (majority) label in the neighborhood of $\boldsymbol{x}$ (closest examples) from the training set.
Thus, we estimate:

$$p(y = c|\boldsymbol{x}, \mathcal{D}) = \frac{1}{K} \sum_{n \in N_K(\boldsymbol{x}, \mathcal{D})} \mathbb{I}(y_n = c) \tag{1}$$

- c class label
- K: number of training samples in neighborhood
- $N_K(\boldsymbol{x}, \mathcal{D})$: neighborhood of $\boldsymbol{x}$ (size K) based on dataset $\mathcal{D}$

Illustration of KNN

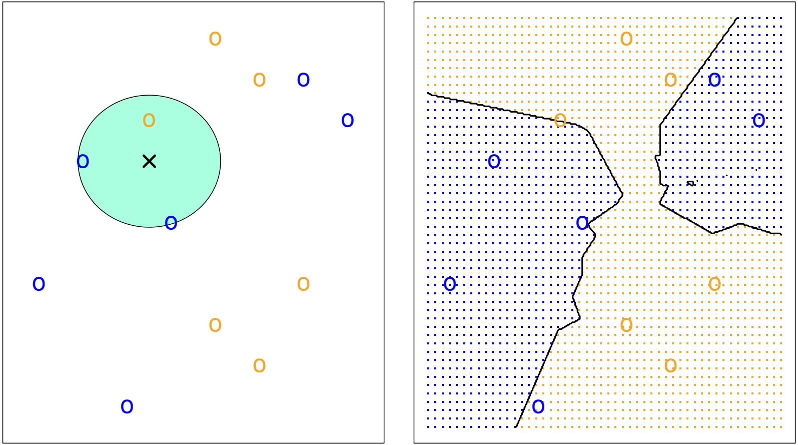


Figure: Illustration of the KNN approach on a training set of 12 observations and the resulting decision boundary. (ESL Fig 2.14)

Bias-variance trade-off in KNN

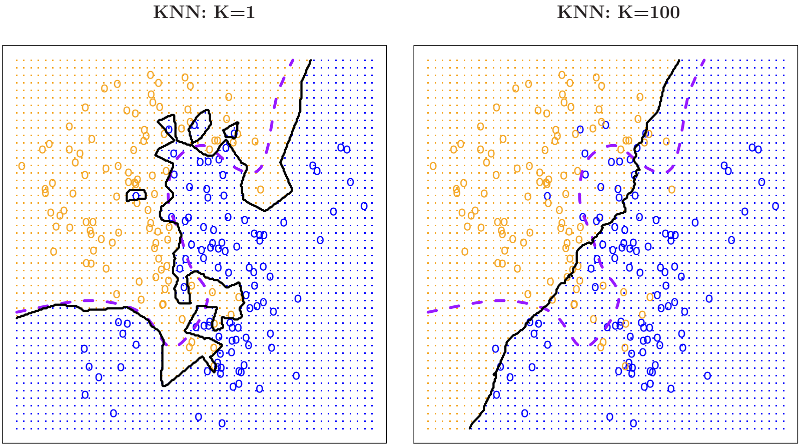


Figure: Comparing decision boundaries $K = 1$ and $K = 100$ for a dataset of 100 observations. Which model has lower bias? Which one gives a higher variance? The Bayes decision boundary is the purple dashed line (ESL Fig 2.16)

Approximating Bayes decision boundary with KNN

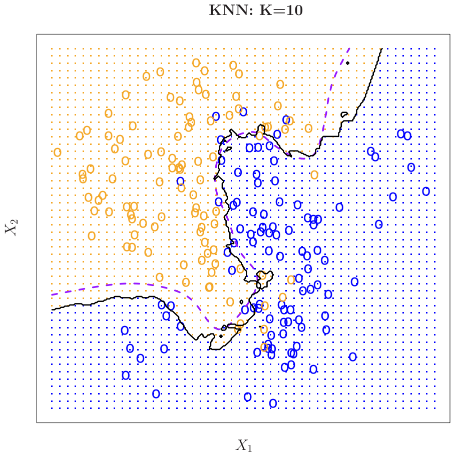


Figure: KNN decision boundary with $K = 10$ on the same training data set. (ESL Fig 2.15)

Training and test error rates for KNN

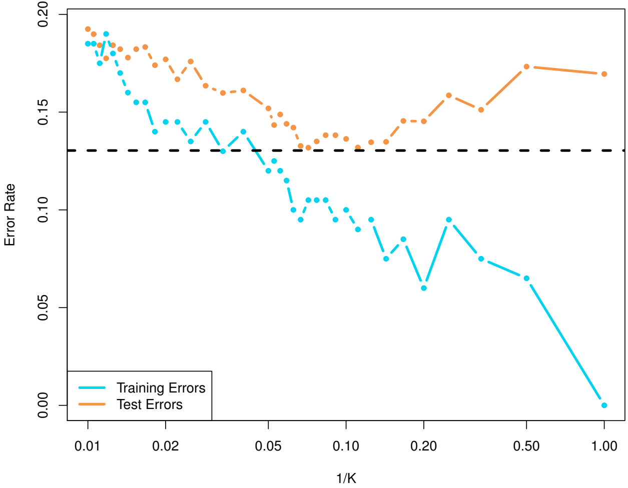
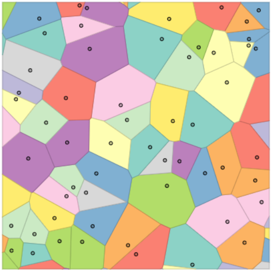


Figure: KNN training error rate (blue, 200 observations) and test error rate (orange, 5000 observations). Flexibility increases as K decreases. Which K should you choose? (ESL Fig 2.17)

KNN considerations

- To find the points in the neighborhood N_K, we need to determine the K-closest points to input $\boldsymbol{x}$. This is done via a specified distance metric:$d(\boldsymbol{x}, \boldsymbol{x}') \in \mathbb{R}^+$ (e.g. Euclidean, Mahalanobis)
- $K = 1$ induces a Voronoi tessellation: partitioning of input sapce such that all points $\boldsymbol{x} \in V(\boldsymbol{x}_n)$ are closer to $\boldsymbol{x}_n$ than to any other point (From a modeling perspective, this is overfitting)



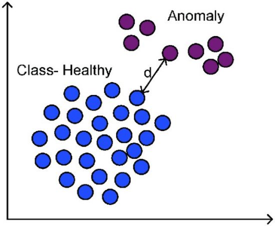
Source: https://package.elm-lang.org/packages/ianmackenzie/elm-geometry/latest/VoronoiDiagram2d

- Suffers under high dimensionality
- Memory intensive

KNN extension: open set recognition

KNN is readily applicable to open set recognition (set of classes $\mathcal{C}$ not fixed).

- Novelty/out-of-distribution/anomaly detection



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

- Incremental/online/life-long/continual learning: any potentially new label is added to new class C_{t+1}; dataset augmented
- Few-shot classification (for person re-identification or face verification)

Distance metrics

The [semantic] distance between points $\boldsymbol{x}$ and $\boldsymbol{x}'$ is specified by a distance metric $d(\boldsymbol{x}, \boldsymbol{x}') \in \mathbb{R}^+$.

- Alternately, the similarity $s(\boldsymbol{x}, \boldsymbol{x}')$ can be computed
- Distance/similarity required for KNN, unsupervised learning (e.g. clustering) among other tasks
- Common metrics:
  - Euclidean distance:

$$d_{\boldsymbol{E}}(\boldsymbol{x}, \boldsymbol{x}') = \sqrt{(\boldsymbol{x} - \boldsymbol{x}')^\top (\boldsymbol{x} - \boldsymbol{x}')} \qquad (2)$$

  - Mahalanobis distance:

$$d_{\boldsymbol{M}}(\boldsymbol{x}, \boldsymbol{x}') = \sqrt{(\boldsymbol{x} - \boldsymbol{x}')^\top \boldsymbol{M} (\boldsymbol{x} - \boldsymbol{x}')} \qquad (3)$$

  where $\boldsymbol{M}$ is the Mahalanobis distance matrix

Distance metrics

The process of finding the optimal $\boldsymbol{M}$ is called **metric learning**

- When D is large, we typically learn an embedding (mapping): $\boldsymbol{e} = f(\boldsymbol{x})$ and then compute $d_{\boldsymbol{M}}(\boldsymbol{e}, \boldsymbol{e}')$ instead.
- When f is a deep neural network, this process is termed **deep metric learning**

Methods for estimating *M*

- Large margin nearest neighbors (LMNN)
- Neighborhood component analysis (NCA)
- Latent coincidence analysis (LCA)
- Minimization of classification and ranking losses (with mining techniques and proxy methods):
  - Pairwise/contrastive loss
  - Triplet loss
  - N-pairs loss

Density kernel

A density kernel $\mathcal{K}(x)$ is a weighting function that specifies a mapping or transformation of an input x: $\mathcal{K} : \mathbb{R} \rightarrow \mathbb{R}_+$.
Density kernels have two important properties:

- **Normalization**:

$$\int x\mathcal{K}(x)dx = 0 \tag{4}$$

- **Symmetry**:

$$\mathcal{K}(-x) = \mathcal{K}x \tag{5}$$

Kernels have several uses, e.g.

- density function estimation
- local regression (our focus)
- smoothing time series

Kernel functions

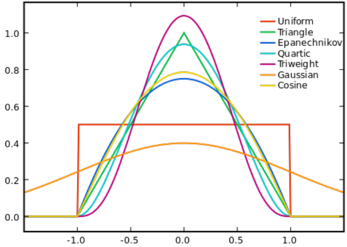


Figure: Popular kernel functions

- 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: $\mathcal{K}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$

Radial basis function

The radial basis function (RBF) kernel is a generalization of a density kernel to an input vector $\boldsymbol{x}$:

$$\mathcal{K}_h(\boldsymbol{x}) \propto \mathcal{K}_h(||\boldsymbol{x}||) \tag{6}$$

where h is the bandwidth parameter:
The RBF Gaussian kernel is thus given by:

$$\mathcal{K}_h(\boldsymbol{x}) = \frac{1}{h^D(2\pi)^{D/2}} \prod_{d=1}^{D} \exp\left[-\frac{1}{2h^2} x_d^2\right] \tag{7}$$

Bandwidth parameter

Specifies the width of the kernel:

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

K-nearest neighbor smoother

In the simple case of the KNN kernel, we use the neighborhood average:

$$\hat{f}(x_0) = \frac{1}{k} \sum_{i \in N_K(x_0)} y_i \tag{9}$$

where $N_K(x_0)$ is the K-nearest neighborhood of x_0.

- All points in the neighborhood are equally weighted
- The resulting $\hat{f}(x)$ is not smooth
- To achieve smoothness, we weight observations by distance to the target point

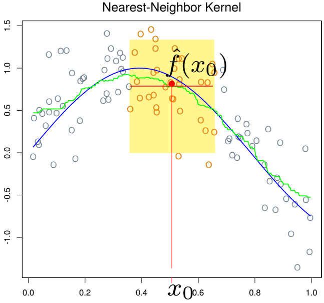


Figure: KNN equally-weighted kernel

Nadaraya-Watson smoother

Nadaraya-Watson kernel-weighted average implements distance-based weighting:

$$\mathbb{E}[y|\boldsymbol{x}, \mathcal{D}] = \hat{f}(x_0) = \frac{\sum_{i=1}^{n} K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{n} K_\lambda(x_0, x_i)} \tag{10}$$

where K_λ can be any kernel function.

If we use the popular **Epanechnikov** (quadratic) kernel, then:

$$K_\lambda(x_o, x_i) = D\left(\frac{|x_i - x_0|}{\lambda}\right) \tag{11}$$

where

$$D(t) = \begin{cases} \frac{3}{4}\left(1 - t^2\right) & |t| \leq 1 \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

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

Nadaraya-Watson smoother (Epanechnikov kernel)

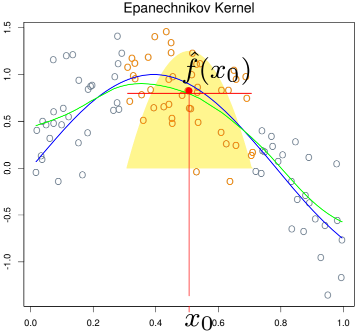


Figure: Nadaraya-Watson estimate of $\hat{f}(x)$ using the Epanechnikov kernel. Half-width is fixed at $\lambda = 0.2$

The half-width can be generalized as any function h_λ of the target point x_0:

$$K_\lambda(x_0, x_i) = D\left(\frac{|x_i - x_0|}{h_\lambda(x_0)}\right) \tag{13}$$

Kernels as a localization device

Rather than estimate a regression function $f(X)$ over the entire $\mathbb{R}^D$, we can estimate the response at each training point using a weighted average:

- only observations close a target point x_0 are used in estimating f at that point
- the function defining how the points in the neighborhood of x_0 are weighted is called a **kernel**: $K_\lambda(x_0, x_i)$ where λ controls the width of the neighborhood
- this is a localized/memory-based approach
- the resulting $\hat{f}(X)$ is smooth in $\mathbb{R}^D$

Using kernel functions, we can estimate $\hat{f}(X)$ in two ways:

1. **Nonparametric**: define an averaging function (kernel) to estimate y_0 for each point x_0
2. **Parametric**: estimate a linear model for each point x_0

Local linear regression

Using a nonparametric average function produces biased estimates at the boundaries.

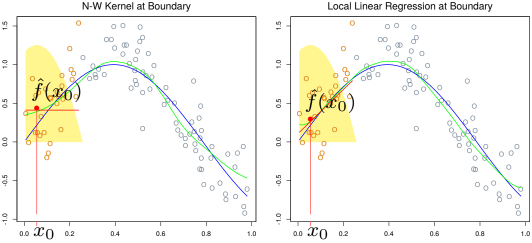


Figure: Locally weighted average (Nadaraya-Watson) versus local linear regression.

To correct this, we can estimate a linear model at each point x_0 by solving a weighted least squares:

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

Local linear regression estimates

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

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

Then the solution to the locally weighted regression problem is:

$$\hat{f}(x_0) = b(x_0)^T(\boldsymbol{B}^T\boldsymbol{W}(x_0)\boldsymbol{B})^{-1}\boldsymbol{B}^T\boldsymbol{W}(x_0)\boldsymbol{y} \tag{16}$$

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

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

Effect of equivalent kernel

The equivalent kernel (local regression) corrects the bias from local average kernel methods to the first order.

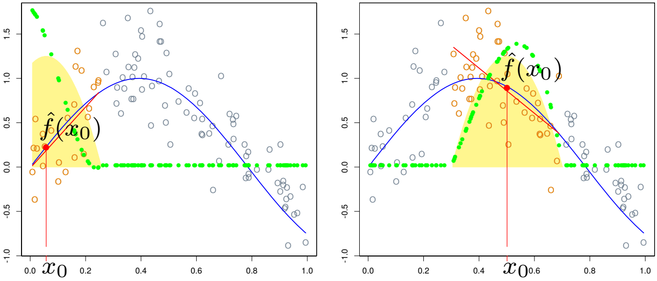


Figure: Green points show the weights $\ell_i(x_0)$ (rescaled for display purposes) along with those for the Nadaraya-Watson (N-W) local average (yellow shaded region; also rescaled). The correction effect of local regression can be observed.

Local polynomial regression

- Higher-order terms in $\hat{f}(x)$ are required to reduce bias in curved regions
- Local polynomial regression can correct this at the cost of higher variance
- Given by:

$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \sum_{j=1}^{d} \hat{\beta}_j(x_0) x_0^j \tag{18}$$

where $\hat{f}(x_0)$ is the solution to:

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

Bias correction of local quadratic regression

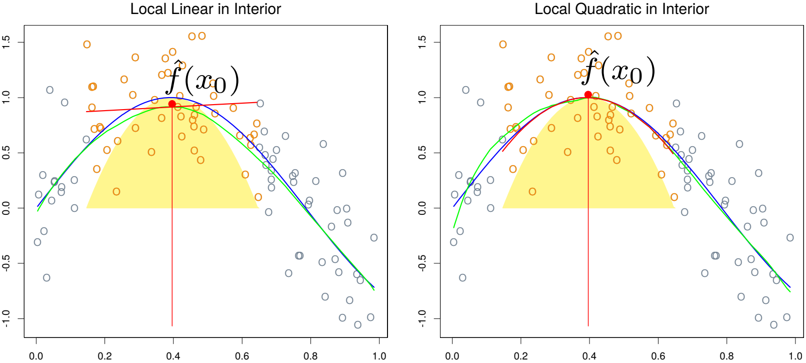


Figure: The local linear regression estimator is biased in curved regions. A higher-order local fit (in this case, quadratic) can eliminate this.

Local regression algorithms

- LOESS: locally estimated scatterplot smoothing
  - 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

Summary

- Kernel smoothing methods can be used for flexible functional fitting
- Local regression generates a linear/polynomial fit at each target point using a kernel weighted loss function

Reading:

- **PMLI** 16
- **ESL 6.1** One-dimensional Kernel Smoothers (pp. 191–199)
- **ISLR 7.6:** Local Regression (pp. 280–282)