STAT 542: Statistical Learning

K-Nearest Neighbor and the Bias-Variance Trade-Off

Ruoqing Zhu, Ph.D. <rqzhu@illinois.edu>

Course Website: https://teazrq.github.io/stat542/

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Department of Statistics
University of Illinois at Urbana-Champaign

K-Nearest Neighbour

An accurate prediction

- Let's consider a regression model,

$$Y = f(X) + \epsilon,$$

  where E$(\epsilon) = 0$ and Var$(\epsilon) = \sigma^2$.

- Suppose that we collect a set of training data $\mathcal{D}_n = \{x_i, y_i\}_{i=1}^n$
- from the training data, we are able to estimate the regression function as $\widehat{f}$ ("f-hat").
- Want to predict the value of Y at a target point x.

An accurate prediction

- Using squared-error loss, the error of the prediction is

$$
\begin{aligned}
&\mathsf{Err}(x) \\
&= \mathsf{E}_{\mathcal{D},Y}\left[\left(Y - \widehat{f}(x)\right)^2\right] \\
&= \mathsf{E}_{\mathcal{D},Y}\left[\left(Y - f(x) + f(x) - \mathsf{E}_{\mathcal{D}}\widehat{f}(x) + \mathsf{E}_{\mathcal{D}}\widehat{f}(x) - \widehat{f}(x)\right)^2\right] \\
&= \dots \\
&= \underbrace{\mathsf{E}_{Y}\left[\left(Y - f(x)\right)^2\right]}_{\text{Irreducible Error}} + \underbrace{\left(f(x) - \mathsf{E}_{\mathcal{D}}\widehat{f}(x)\right)^2}_{\text{Bias}^2} + \underbrace{\mathsf{E}_{\mathcal{D}}\left[\left(\widehat{f}(x) - \mathsf{E}_{\mathcal{D}}\widehat{f}(x)\right)^2\right]}_{\text{Variance}}
\end{aligned}
$$

- All the cross terms are zero

An accurate prediction

- $\mathsf{E}[(Y - f(x))^2] = \sigma^2$ is the irreducible error term that cannot be avoided, because we cannot predict ϵ
- $\mathsf{E}[(f(x) - \mathsf{E}\widehat{f}(x))^2]$ is the squared bias term that evaluates how the average of our estimator deviates from the truth
- $\mathsf{E}[(\widehat{f}(x) - \mathsf{E}\widehat{f}(x))^2]$ is the variance term that reflects the sensitivity of the function estimate $\widehat{f}(x)$ to the training sample

Of course we want to minimize both the Bias^2 and the Variance, however, this is not always possible...

An accurate prediction

- The first instinct is that one should minimize the bias^2 term $\mathsf{E}[(f(x) - \mathsf{E}\widehat{f}(x))^2]$
- Why would I produce a model that is asymptotically incorrect, i.e., $f(x) \neq \mathsf{E}\widehat{f}(x)$?
- This instinct is wrong! — This is usually at the expense of high variance, which eventually damages the prediction performance...
- To demonstrate this, lets start with a particular model, the k-Nearest Neighbour, in both classification and regression settings

k-Nearest Neighbour

- k-Nearest Neighbour (kNN) is a nonparametric method that predicts the target point $\mathbf{x}$ with averages of nearby observations in the training data
- For regression, the prediction at a given target point x is

$$\widehat{y} = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i,$$

  where $N_k(x)$ defines the k samples from the training data (in terms of their feature values) that are closest to x.
- For hard classification, the most prevalent class in $N_k(x)$ is used

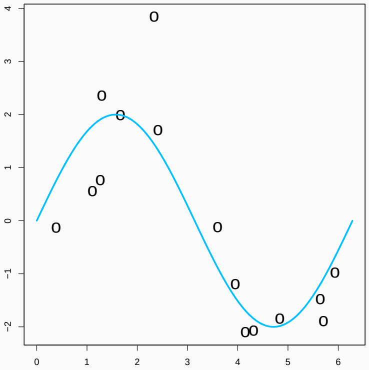
$$\widehat{y} = \arg\max_{c \in C} \sum_{x_i \in N_k(x)} \mathbf{1}\{y_i = c\},$$

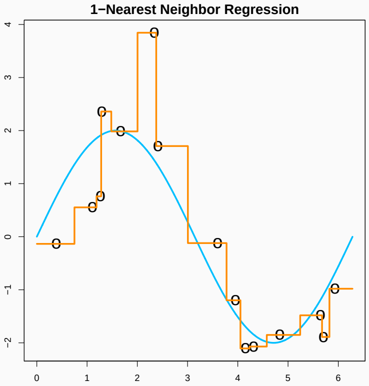
k-Nearest Neighbour in Regression

The the following data is observed, with only 1 feature, uniformly from $[0, 2\pi]$. The true model (blue line) is

$$Y = 2\sin(X) + \epsilon,$$

where ϵ is standard normal error. We fit the data with 1NN.





k-Nearest Neighbour in Regression

- The bias^2 term is minimized using 1NN, why?

$$\begin{aligned} \mathsf{E}\widehat{f}(x) &= \mathsf{E}\big[\sum Y_i \mathbf{1}\{X_i \in N_1(x)\}\big] \\ &= \mathsf{E}\big[\sum f(X_i)\mathbf{1}\{X_i \in N_1(x)\}\big] \end{aligned}$$

  which the closest we can get for approximating $f(x)$ (if we believe there is a certain continuity in f).

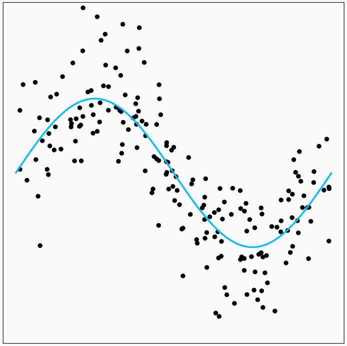
- However, the variance is large because the estimator only uses one observation

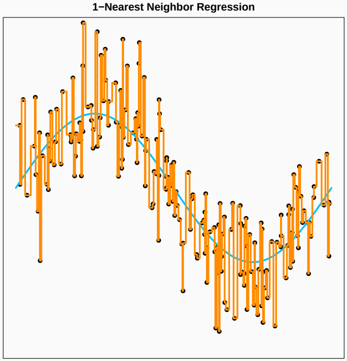
$$\mathsf{E}\left[(\widehat{f}(x) - \mathsf{E}\widehat{f}(x))^2\right] = \mathsf{E}\epsilon^2 = \sigma^2.$$

- If we use more “neighbouring” points, say k, the variance would reduce to σ^2/k. But the bias^2 will increase because as the neighbourhood expands, $f(X_i)$ is further away from $f(x)$.

k-Nearest Neighbour in Regression

Now we simulate 200 observations, and see how the model changes over k.





k-Nearest Neighbour in Regression

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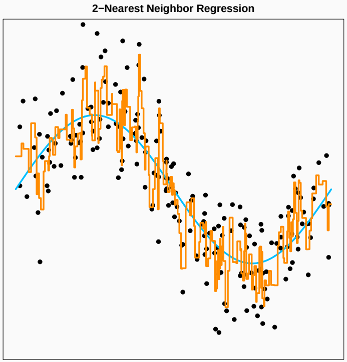
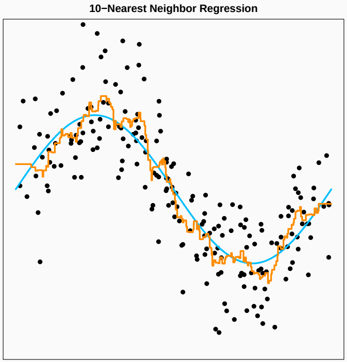
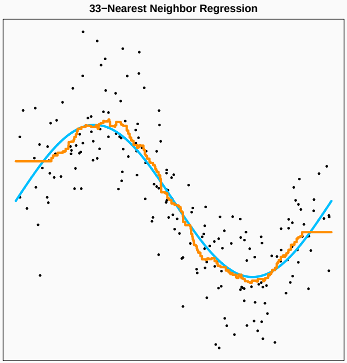
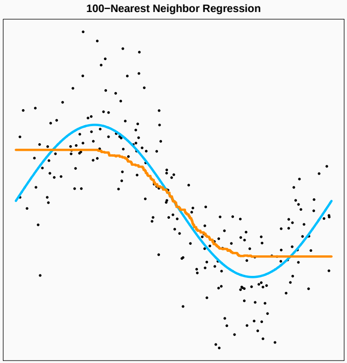




k-Nearest Neighbour in Regression

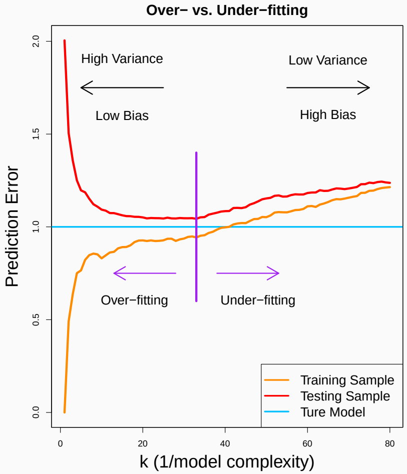
The model becomes “smoother” as k increases. However, this eventually introduces a significant bias.





Model Complexity, over- and under-fitting

- Model complexity $\uparrow$ (small k) $\longrightarrow$ Bias^2 $\downarrow$ and Variance $\uparrow$
- Model complexity $\downarrow$ (large k) $\longrightarrow$ Bias^2 $\uparrow$ and Variance $\downarrow$



Prevent over-fitting

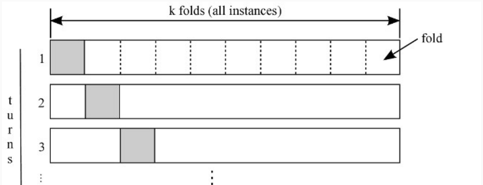
- As we can see, model complexity, bias-variance trade-off and over- and under-fitting are usually related concepts
- Over-fitting happens when the model performs well on the training sample, but not on the testing sample
- Controlling complexity can prevent overfitting. Complexity can be measured in different ways. In statistics, we often use degrees of freedom (number of parameters is a model)
- The degrees of freedom of a kNN model is roughly n/k
  - intuition: if neighborhoods don't overlap, there would be n/k neighborhoods, with one parameter for each

Prevent over-fitting

- To control complexity, one approach is to "penalize" it (we will see this a lot later on):

$$\arg\min_{f} \ \text{loss}(f) + \lambda\, \text{complexity}(f)$$

- Another common approach is to use cross-validation (CV). A 10-fold CV is carried out as follows
  - Randomly split the data into 10 equal sized subsamples
  - Fit the model using 9 out of 10 subsamples as training data and calculate the testing error using the remaining one.
  - Alternate the testing sample, and average the total of 10 experiments



Remark on the degrees of freedom

A rigorous definition for the degrees of freedom is

$$\text{df}(\widehat{f}) = \frac{1}{\sigma^2} \sum_{i=1}^{n} \text{Cov}(\widehat{Y}_i, Y_i)$$

- The amount of covariance between outcome Y_i and its fitted values $\widehat{Y}_i$, at the same target point x_i.
- Treat $X_i = x_i$ as fixed value, but not random.
- $1/\sigma^2$ takes care of the variance of the random error term.
- In many situations, it is more convenient to define it in the matrix form, noticing that we are just adding up the diagonal elements of the covariance matrix of $\widehat{\mathbf{Y}} = (\widehat{Y}_1, \ldots, \widehat{Y}_n)$ and $\mathbf{Y} = (Y_1, \ldots, Y_n)$

$$\text{df}(\widehat{f}) = \frac{1}{\sigma^2} \text{Trace}\Big(\text{Cov}(\widehat{\mathbf{Y}}, \mathbf{Y})\Big)$$

Remark on the degrees of freedom

Based on this definition, we can easily verify several cases:

- For 1NN, df $= n$
- If $\widehat{y}_i = \overline{y}$, i.e., nNN, then df = 1
- For linear regression, df $= p$
- For kNN, df $= n/k$

The formula works for kernel methods too, we shall see that later on.

Bias-Variance Trade-off in Classification

- Classification problems have the same bias-variance trade-off, although the formulation is slightly different due to their loss functions (0-1 loss for "hard" classification)
- A very nice paper about this issue by Friedman (1997)

  — "On bias, variance, 0/1—loss, and the curse-of-dimensionality"

  Try example 7.2 in HTF.
- The optimal classifier is call the Bayes classifier:

$$f_B(x) = \mathbf{1}\{\mathsf{P}(Y|X = x) > 1/2\}$$

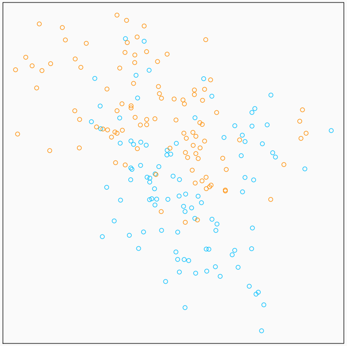
- Error produced by Bayes classifier

$$\min\left\{\mathsf{P}(Y|X = x), 1 - \mathsf{P}(Y|X = x)\right\}$$

  is analog to the irreducible error σ^2 in a regression setting

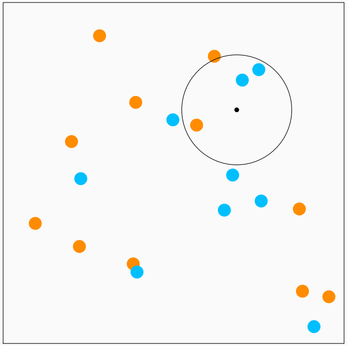
k-Nearest Neighbour in Classification

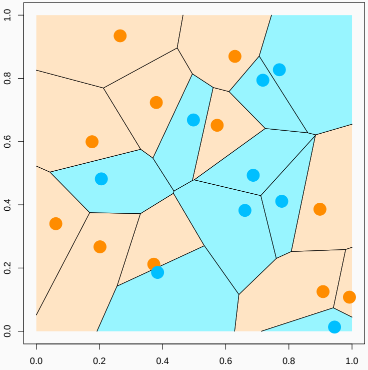
Let's look at a classification example from the HTF text book.
(BLUE = 0, ORANGE = 1)



k-Nearest Neighbour in Classification

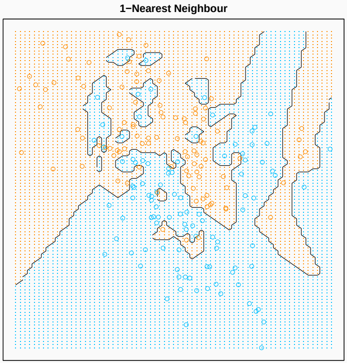
Similar to the regression case, the k-NN classification model does majority vote (the most prevalent class) within the neighborhood of a target point x. 1NN plot is a Voronoi tessellation

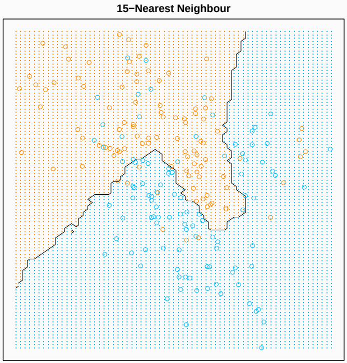




k-Nearest Neighbour in Classification

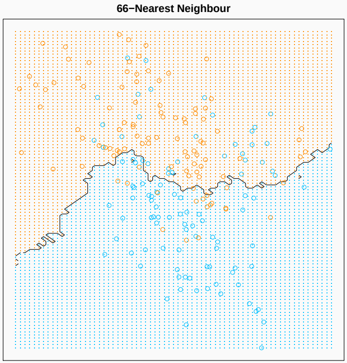
We fit k-NN classification model to the example. Of course, we would not expect 1NN to perform well...

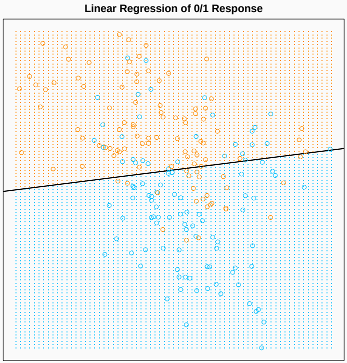




k-Nearest Neighbour in Classification

As we further increase k, the model tends to be less complex. Compare 66NN with a linear model that uses only 3 parameters.



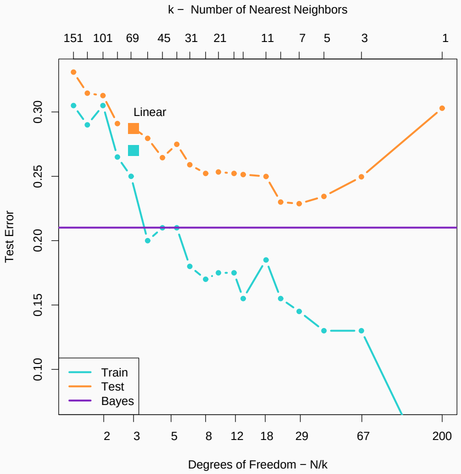


k-Nearest Neighbour vs. Linear Regression

- The goal is to approximate $f(x) = \mathsf{E}(Y|X = x)$
- Linear regression makes a structural assumption: f is linear.
  - low variance: Number of parameters is p (fixed); we know that when sample size n grows, the variance of $\widehat{\boldsymbol{\beta}}$ is $\propto 1/n$.
  - high bias (underfit): linear assumption is very restrictive
- kNN makes on assumption on f, except some smoothness.
  - low bias (overfit): flexible and adaptive. It can be shown that as if $k \to \infty$ and $n/k \to 0$, kNN is consistent.
  - high variance: number of parameters for kNN is roughly n/k;

k-Nearest Neighbour in Classification

An “U” shaped prediction error curve is again observed for the testing sample (Figure from HTF):



Distance measures

- Closeness between two points needs to be defined based on some distance measures
- By default, we use Euclidean distance (ℓ_2 norm) for continuous variables

$$d^2(\boldsymbol{u}, \boldsymbol{v}) = \|\boldsymbol{u} - \boldsymbol{v}\|_2^2 = \sum_{i=1}^{p} (u_i - v_i)^2$$

Hence the neighbourhood is not invariant to the scaling of the variables.

Scaling issues

- We often scale the variables marginally when using kNN, so that the distance is

$$d^2(\boldsymbol{u}, \boldsymbol{v}) = \sum_{j=1}^{p} \frac{(u_i - v_i)^2}{\sigma_j^2}$$

  where σ_j^2 is the variance of variable j.

- Mahalanobis distance is also scale-invariant and takes care of correlation

$$d^2(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u} - \boldsymbol{v})^{\mathsf{T}} \Sigma^{-1} (\boldsymbol{u} - \boldsymbol{v}),$$

  where Σ is a covariance matrix.

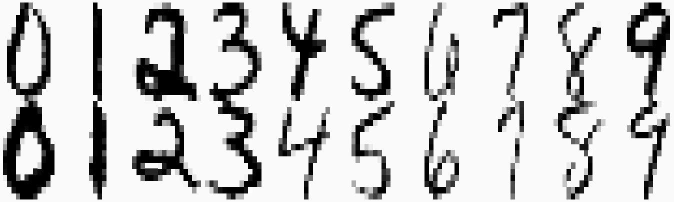
- Hamming distance is usually used for categorical variables

Drawbacks of kNN

- Need to score the entire training data for future prediction
- Calculating the prediction can be slow. To find the nearest neighbor of x, one needs to calculate the distance from x to all training sample and compare them. This is computationally expansive especially in high-dimensional setting
- There are some fast nearest neighbor search algorithms such as kd-tree
- A distance measure needs to be specified — it may affect accuracy

Example: Handwritten Digit Recognition Data

- Digits 1-9 scanned from envelopes by the U.S. Postal Service
- 7291 training samples, 2007 testing samples
- Apply kNN and calculate the errors
- 1NN with Euclidean distance gives 5.6% error rate
- 1NN with tangent distance (Simard et al., 1993) gives 2.6% error



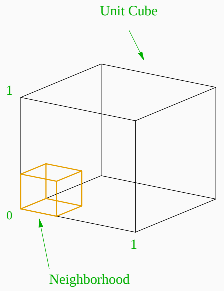
New Challenges

New Challenge

- High-dimension low sample size ($p \gg n$)
  - The resolution of the handwritten digit example is $16 \times 16 = 256$
  - Some common imaging data in medical are 1024×1024 while only a few hundred samples are available
  - Strategy games (Go, StarCraft, etc.) may have a huge number of variables
- Curse of Dimensionality
  - For fixed n, as p increases, the data become sparse
  - As p increases, the number of possible models explodes (computation burden, variable selection necessary)

Curse of Dimensionality

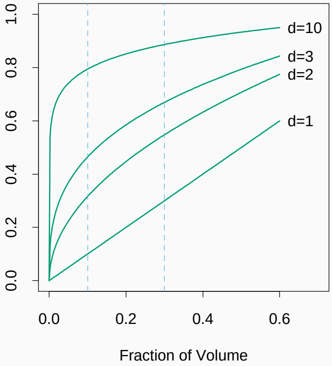
- The curse of dimensionality is well illustrated by a subcubical neighborhood for uniform data in a unit cube.
- Suppose the sample points are evenly spread out on $[0, 1]^p$, and we want to capture 10% of the data by constructing a hypercube neighborhood of x. What is the edge length l of this cube? Since the volume of the cube is $l^p = 10\%$, we need $l = 0.1^{1/p}$,



- When $p = 1$, l = 0.1
- When $p = 2$, l = 0.32
- When $p = 10$, l = 0.79

Curse of Dimensionality

- Suppose we have sample points evenly spread out on $[0, 1]$
- In ten dimensions we need to cover 80% of the range of each coordinate to capture 10% of the data.



Curse of Dimensionality

- In linear regression, the curse of dimensionality is easy to see from the normal equation:

$$\widehat{\beta} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

  where $\mathbf{X}_{n\times p}$ is the design matrix, $\mathbf{y}_{n\times 1}$ is the response vector.
- $\mathbf{X}^\mathsf{T}\mathbf{X}$ is not invertible when $p > n$, hence $\widehat{\beta}$ is not unique
- In fact, since $\mathbf{X}$ is of rank n, we can always find some $\widehat{\beta}$ such that $\mathbf{y} = \mathbf{X}\widehat{\beta}$, this means we are modeling the error term ϵ!
- Some penalized methods can deal with this problem