Lecture 3: Statistical Learning (Textbook 2.2)

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- It is an important task to decide for any given dataset which method produces the best results.
- Selecting the best approach can be one of the most challenging parts of performing statistical learning in practice.

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  - We prefer the accuracy of the predictions on unseen test data.

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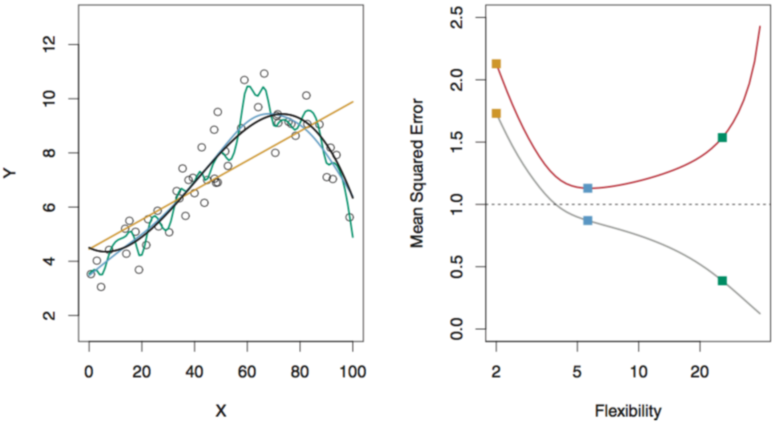
  - We'd like to select the model for which the test MSE is as small as possible.

Training MSE vs Test MSE

Left: Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two nonparametric fits (blue and green curves). Right: Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed line). Squares represent the training and test MSEs for the three fits shown in the left-hand panel.



Training MSE vs Test MSE: explanations

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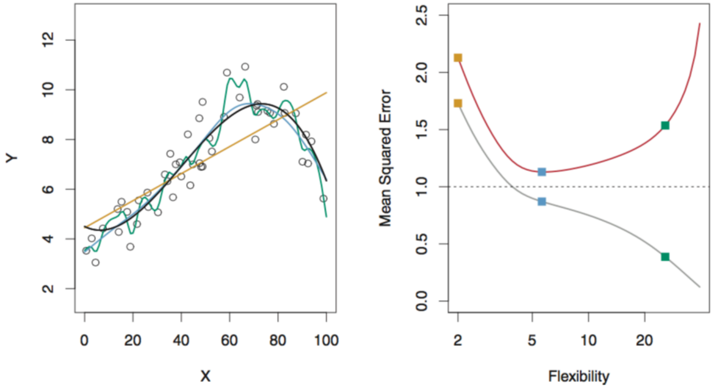

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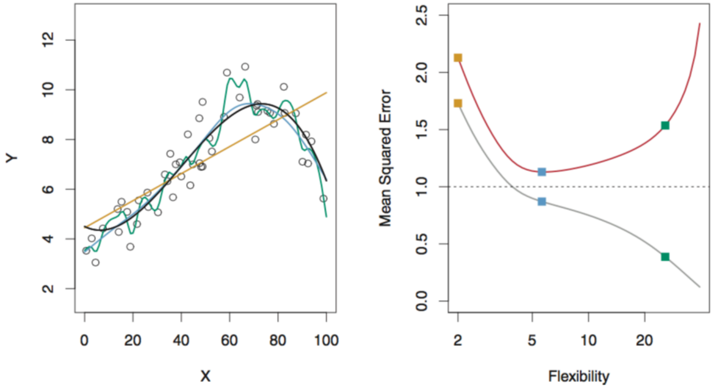

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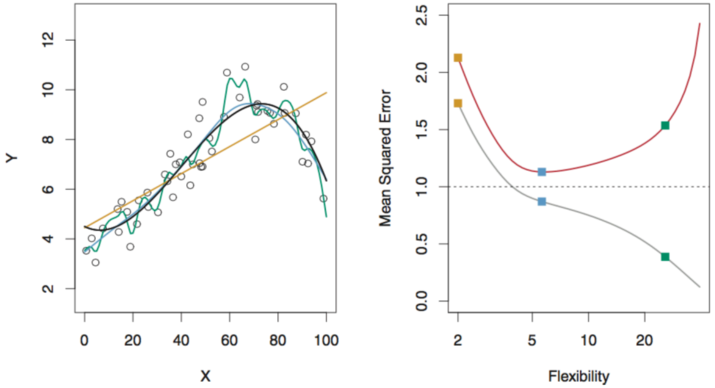

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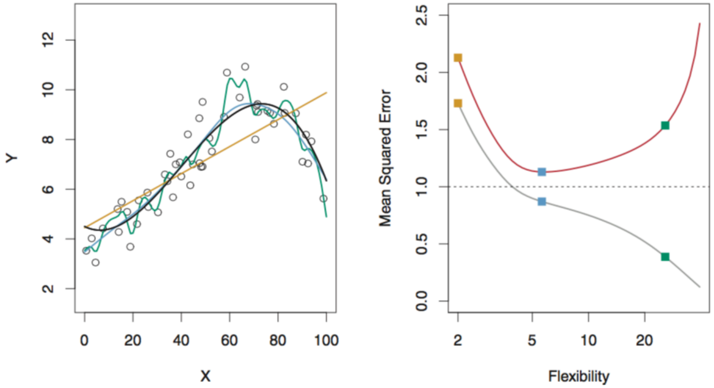
- The green curve, the most flexible, fits the observed data closely but poorly estimates the true f because it is too wiggly.



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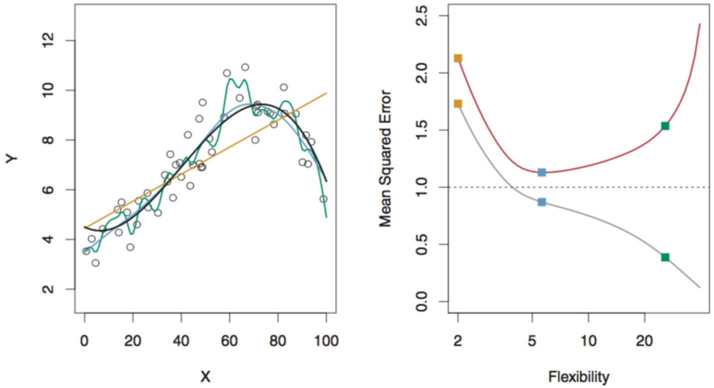

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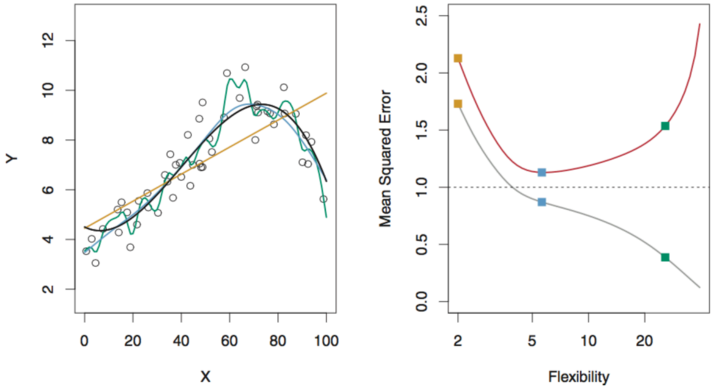

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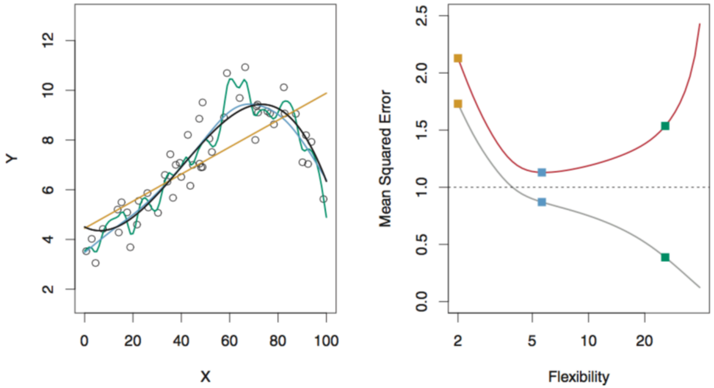

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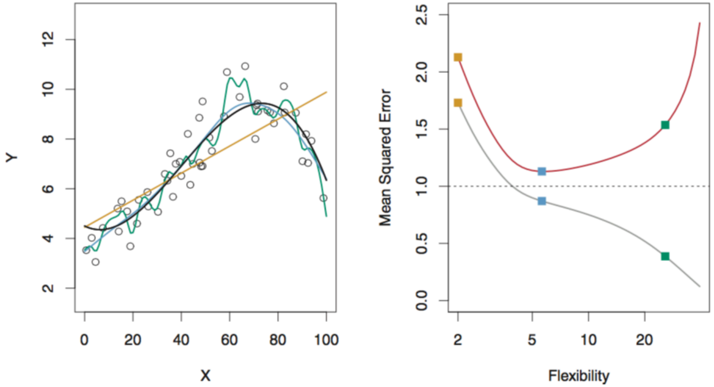

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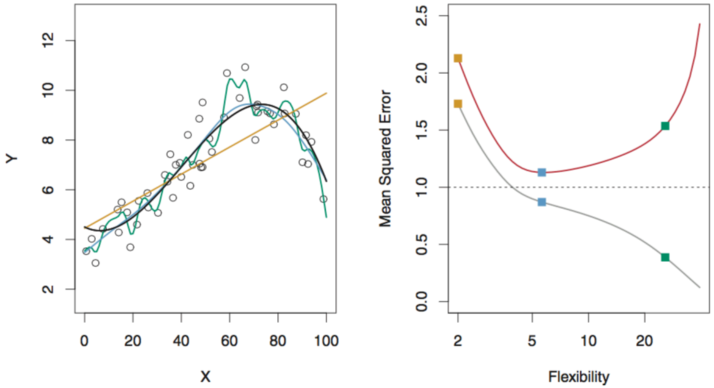
- Horizontal dashed line represents the irreducible error, Var(ϵ), the lowest achievable test MSE.



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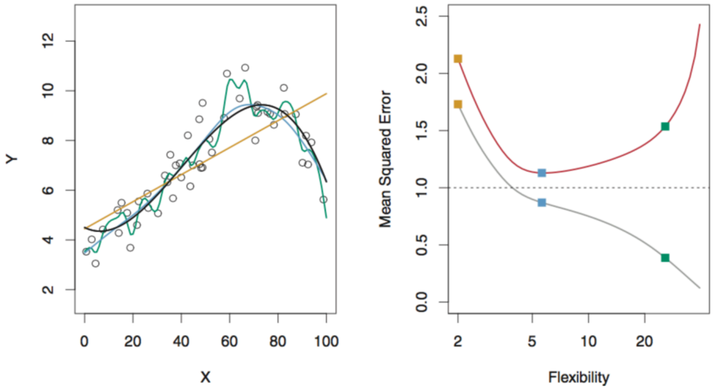

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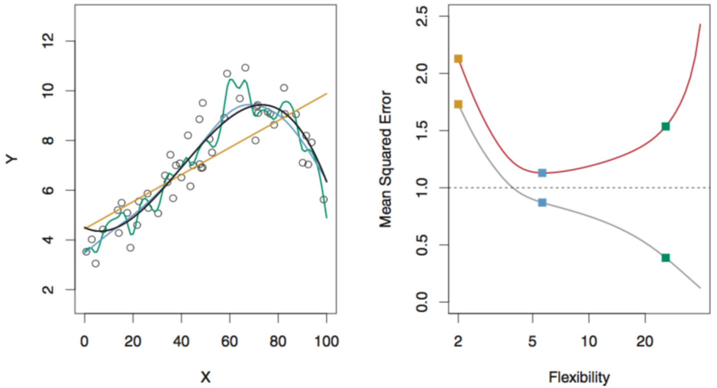

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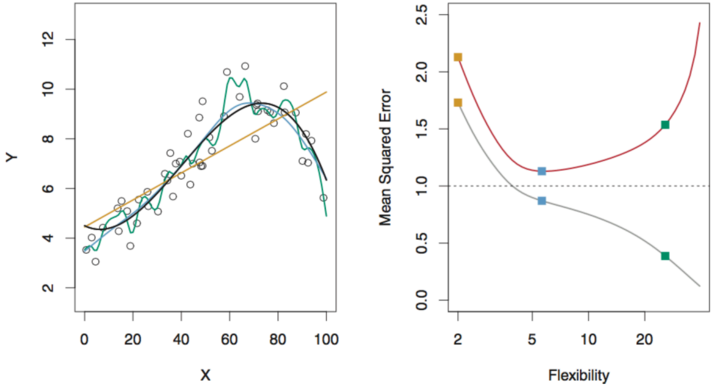

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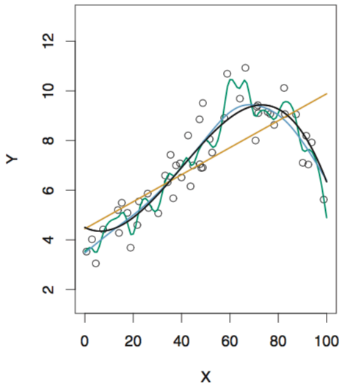
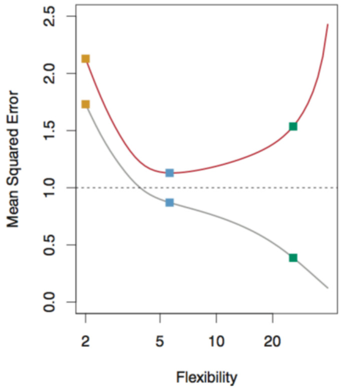
- Overfitting occurs when the method finds patterns in the training data that are due to random chance, leading to a high test MSE.
- Even without overfitting, training MSE is usually smaller than test MSE because most methods aim to minimize the training MSE.





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Then the **expected test MSE** at x_0 is:

$$\mathbb{E}[(y_0 - \hat{f}(x_0))^2] = \underbrace{\mathbb{V}(\hat{f}(x_0))}_{\textit{Variance}} + \underbrace{[\mathbb{E}[\hat{f}(x_0)] - f(x_0)]^2}_{\textit{Bias}} + \underbrace{\mathbb{V}(\epsilon)}_{\textit{Irreducible error}} .$$

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Note: the expected test MSE can never lie below $\mathbb{V}(\epsilon)$.

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Generally, more flexible methods have higher variance.

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- The challenge lies in finding a method for which both the variance and the squared bias are low.

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We will explore very flexible methods that can eliminate bias. This does not guarantee that they will outperform a much simpler method such as linear regression.

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Setup: Observe $\{(x_1, y_1), \ldots, (x_n, y_n)(x_{n+1}, y_{n+1}), \ldots, (x_{n+T}, y_{n+T})\}$ where for $i = 1, \ldots, n$: $y_i = f(x_i) + \epsilon_i$.

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TER computes the fraction of incorrect classifications.
As in the regression setting, we are most interested in the error rates that result from applying our classifier to test observations that were not used in training.

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In this case, the Bayes classifier corresponds to predicting class one if $\mathbb{P}[Y = 1|X = x_{n+1}] > 0.5$.

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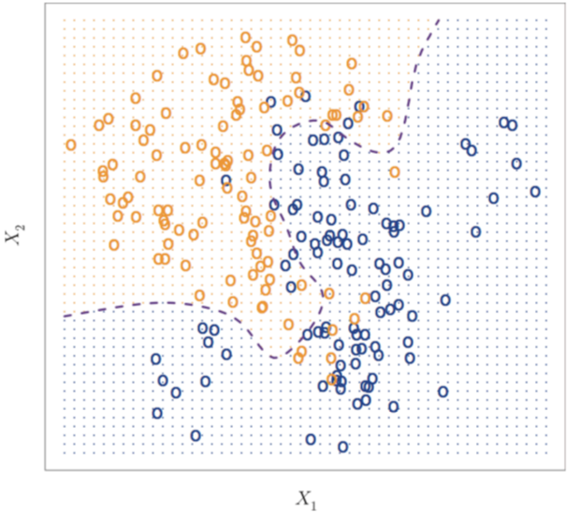
Numerical Example: Simulated data set in a two-dimensional space consisting of predictors X_1 and X_2.



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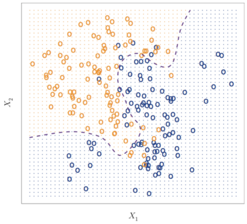

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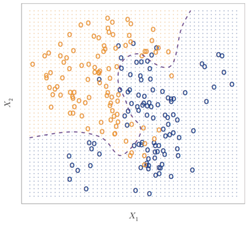

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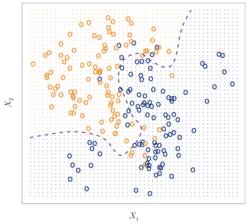

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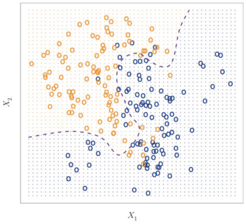

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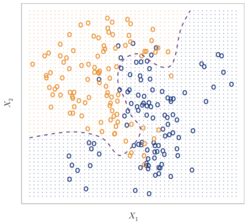

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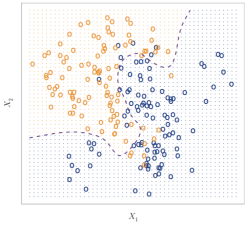

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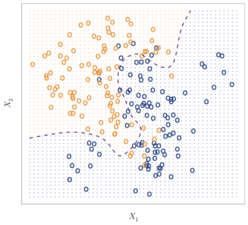

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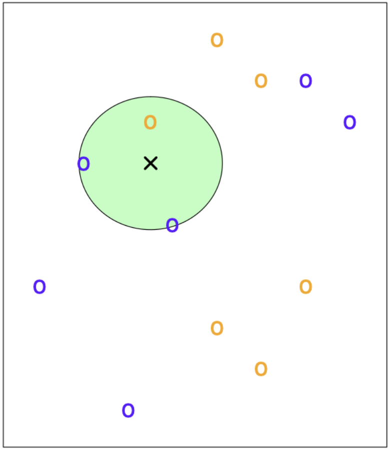
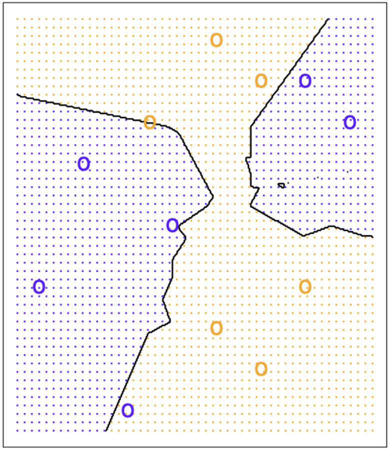
Finally, KNN classifies the test observation x_{n+1} to the class with the largest probability.

KNN

The KNN approach, using K = 3, is illustrated in a simple situation with six blue observations and six orange observations.





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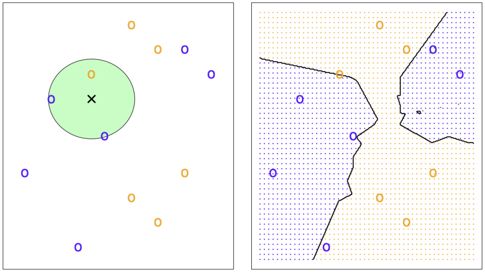

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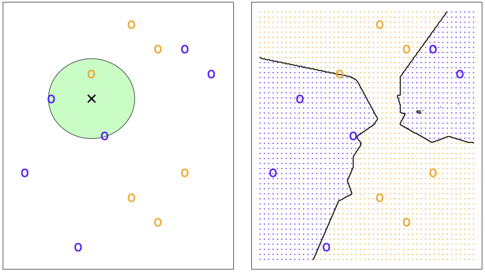
Right: The KNN decision boundary for this example is shown in black. The blue grid indicates the region in which a test observation will be assigned to the blue class, and the orange grid indicates the region in which it will be assigned to the orange class.



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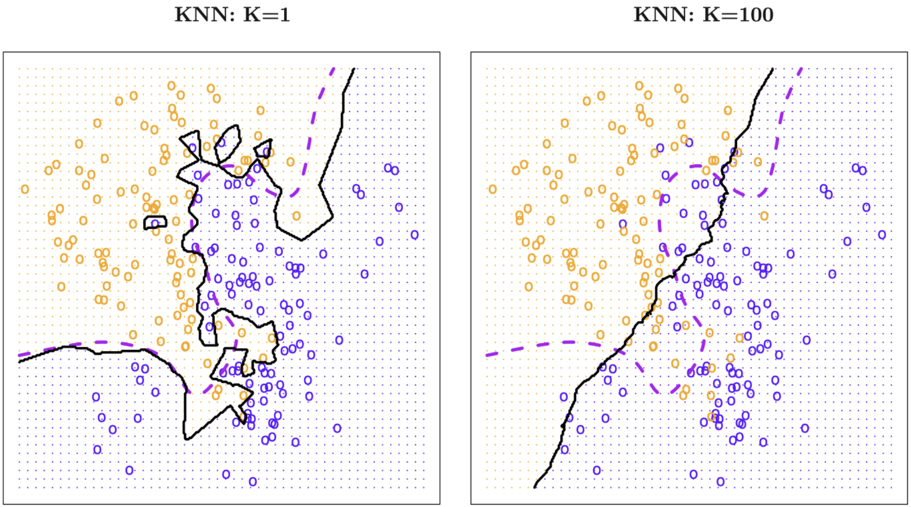

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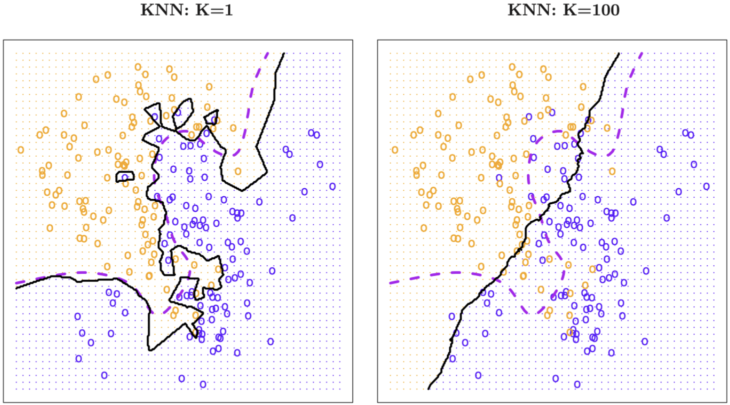
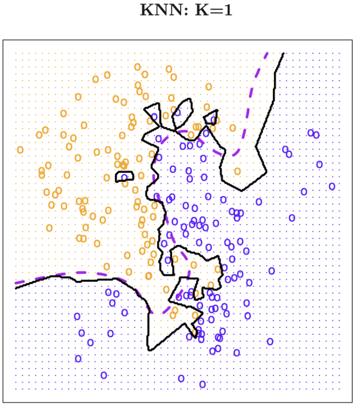
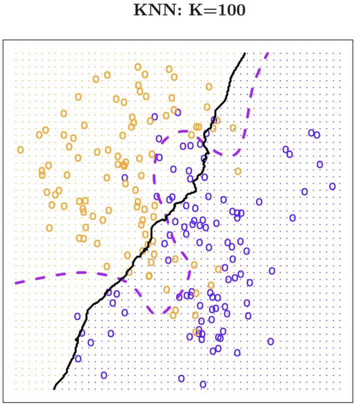
Bias-variance trade-off: As K diminishes, the method becomes more flexible ! When K $= 1$, the decision boundary is overly flexible and finds patterns in the data that don't correspond to the Bayes decision boundary. This corresponds to a classifier that has **low bias** but very **high variance**.



KNN

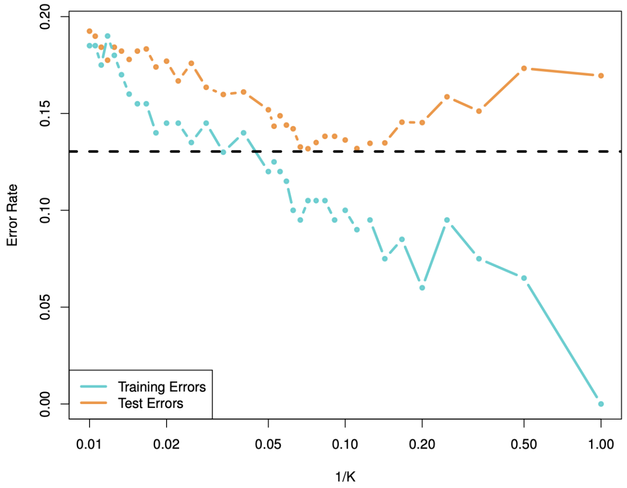
Bias-variance trade-off: As *K* diminishes, the method becomes more flexible ! When K = 100, the method becomes less flexible and produces a decision boundary that is close to linear. This corresponds to a **low-variance** but **high-bias classifier**.





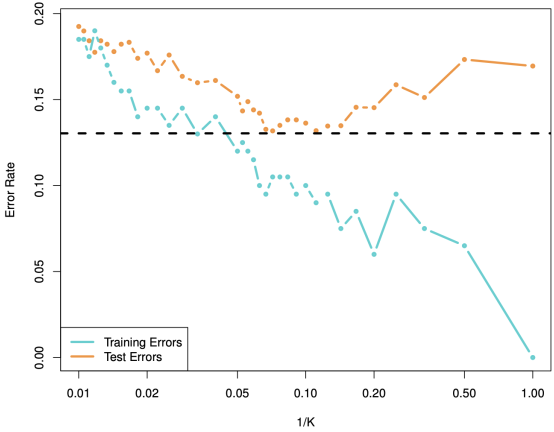
KNN

The KNN training error rate (blue, 200 observations) and test error rate (orange, 5,000 observations) on the data set, as the level of flexibility (assessed using 1/K on the log scale) increases.



KNN

As 1/K increases, the method becomes more flexible. As in the regression setting, the training error rate consistently declines as the flexibility increases. However, the test error exhibits a characteristic U-shape, declining at first (minimum at $\approx K = 10$) before increasing again when the method becomes excessively flexible and overfits.



Curse of dimensionality

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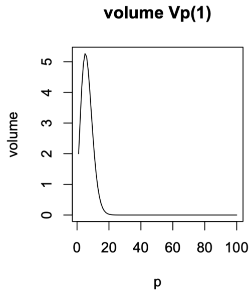
- As the number of features (dimensions) increases, the volume of the data space grows exponentially. The volume $V_p(r)$ of a p-dimensional ball of radius $r > 0$ is equal to

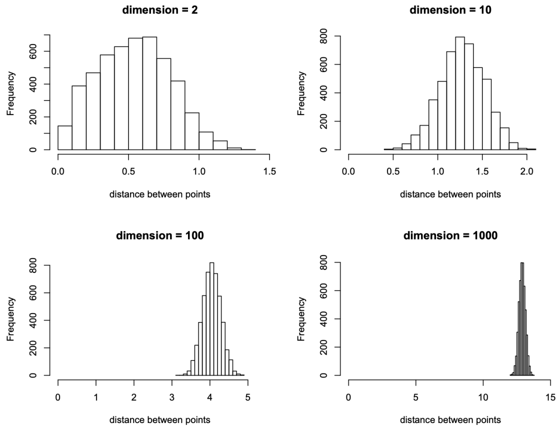
$$V_p(r) = r^p \frac{\pi^{p/2}}{\Gamma(p/2+1)} \sim_{p\to\infty} \left(\frac{2e\pi r^2}{p}\right)^{p/2} (p\pi){-}1/2).$$

The volume $V_p(r)$ of a ball of radius r goes to zero more than exponentially fast with the dimension p !!



Curse of dimensionality

- Histograms of the pairwise-distances between $n = 100$ points sampled uniformly in the hypercube $[0, 1]^p$ for $p = 2,10,100,$ and 1000.



Curse of dimensionality

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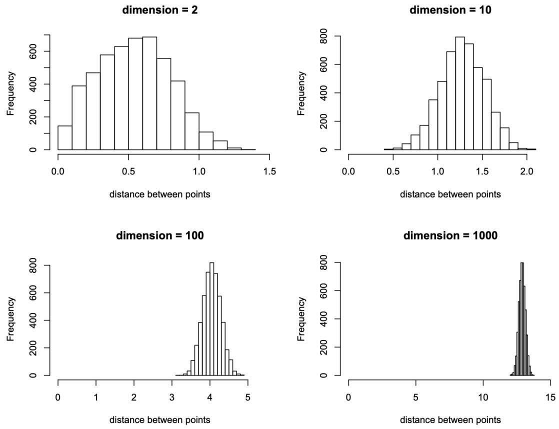
- We observe that, when the dimension p increases, the minimal distance between two points increases and all the points are at a similar distance from the others, so the notion of "nearest points" vanishes.



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- The algorithm struggles to find the k nearest neighbors and makes less accurate predictions.
- As the number of dimensions increases, the distance between data points increases exponentially.
- This makes it harder for KNN to find the k nearest neighbors, leading to decreased accuracy.

References

- Introduction to Statistical Learning with applications in R, Gareth James, Daniela Witten, Trevor Hastie & Robert Tibshirani, Springer
- Introduction to high-dimensional statistics, Christophe Giraud, Chapman and Hall/CRC.