Unit 1

Introduction and overview

Introduction

Statistical and machine learning

- Machine learning is an umbrella term for solving problems by machines “discovering” their “own” algorithms.
- Statistical learning theory is a framework for machine learning drawing from the fields of statistics and functional analysis.
- Statistical learning theory deals with the problem of finding a predictive function based on data.
- The goals of learning are understanding and prediction.

Terminology

- One distinguishes between:
  - Supervised learning:
    - Outcome measure available.
    - Regression, classification.
  - Unsupervised learning:
    - No outcome measure.
    - Clustering.
- The variables have different roles assigned:
  - Input: features, regressors, covariate, independent variable.
  - Output: outcome, dependent variable.
- Training set of data.
- The predictive model is a *learner*.

Overview

Overview of supervised learning

- One assumes that

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

- One aims at determining $\hat{f}$ which is the estimate of f to predict Y based on a training data set:

$$\hat{Y} = \hat{f}(X).$$

Overview of supervised learning / 2

- The accuracy of $\hat{Y}$ as a prediction of Y depends on two quantities:
  1. Reducible error.
  2. Irreducible error.

  $$\mathrm{E}[(Y - \hat{Y})^2] = \mathrm{E}[(f(X) + \epsilon - \hat{f}(X))^2] = (f(X) - \hat{f}(X))^2 + \mathrm{Var}(\epsilon),$$

  where $(f(X) - \hat{f}(X))^2$ is the reducible error and $\mathrm{Var}(\epsilon)$ is the irreducible error.
- The reducible error can be further split into
  1. Bias
  2. Variance

  depending on the mean and variance of $\hat{f}$ if it is repeatedly estimated using a large number of training data sets.

Overview of supervised learning / 3

- One differentiates between:
  - Regression: quantitative output.
  - Classification: qualitative output.
- Two simple approaches to prediction:
  - Least squares:
    - Huge assumptions.
    - Stable, but possibly inaccurate predictions.
  - Nearest neighbors:
    - Mild structural assumptions.
    - Accurate, but unstable predictions.

Linear models and least squares

- Given a vector of inputs $X^T = (X_1, X_2, \ldots, X_p)$ we predict the output Y via the model

$$\hat{Y} = \hat{\beta}_0 + \sum_{j=1}^{p} X_j \hat{\beta}_j.$$

- If the intercept / the constant variable 1 is included in X, then one can write

$$\hat{Y} = X^T \hat{\beta}.$$

- In the $(p+1)$-dimensional input-output space $(X, \hat{Y})$ represents a hyperplane. If the constant is included in X, the hyperplane goes through the origin and is a subspace. Otherwise it is an affine set.

Linear models and least squares / 2

- Viewed as a function over the p-dimensional input space

$$f(X) = X^T\beta$$

  is linear and the gradient

$$f'(X) = \beta$$

  is a vector in input space that points in the steepest uphill direction.

- The least squares fit is obtained by minimizing

$$\text{RSS}(\beta) = \sum_{i=1}^{N}(y_i - x_i^T\beta)^2 = (\boldsymbol{y} - \boldsymbol{X}\beta)^T(\boldsymbol{y} - \boldsymbol{X}\beta)$$

  with respect to β given N observations.

Linear models and least squares / 3

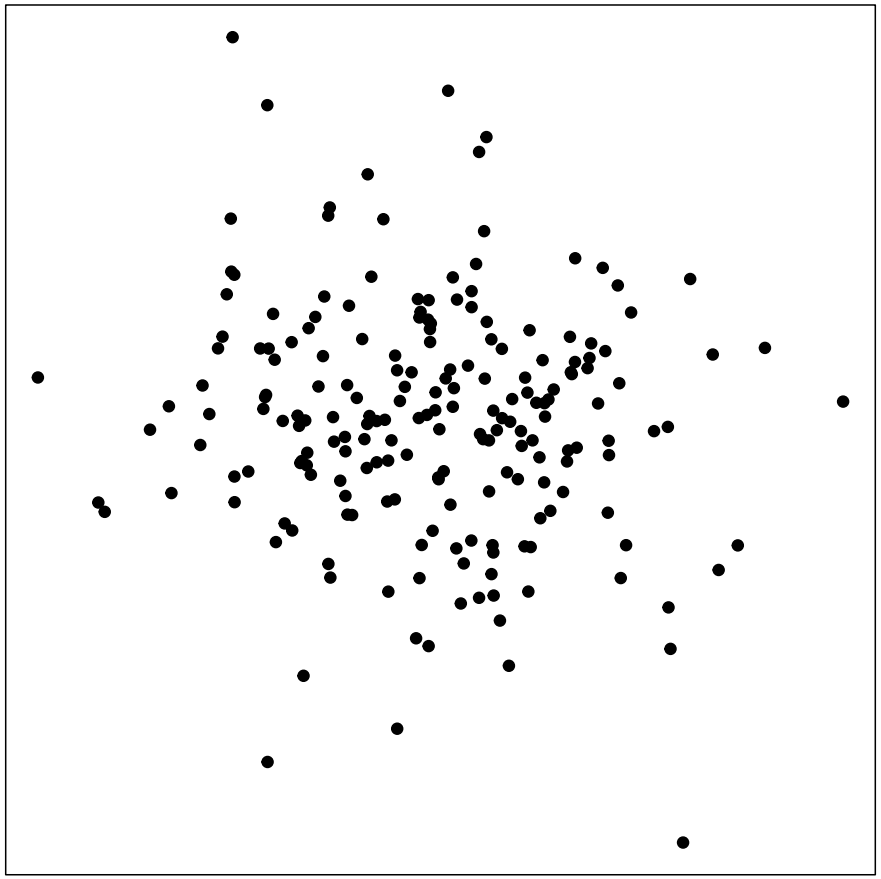
- RSS(β) is a quadratic function of the parameters:
  - There always exists a minimum.
  - The minimum might not be unique.
- If $\boldsymbol{X}^T\boldsymbol{X}$ is nonsingular, the unique solution is given by:

$$\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

- The fitted and predicted values are given by:

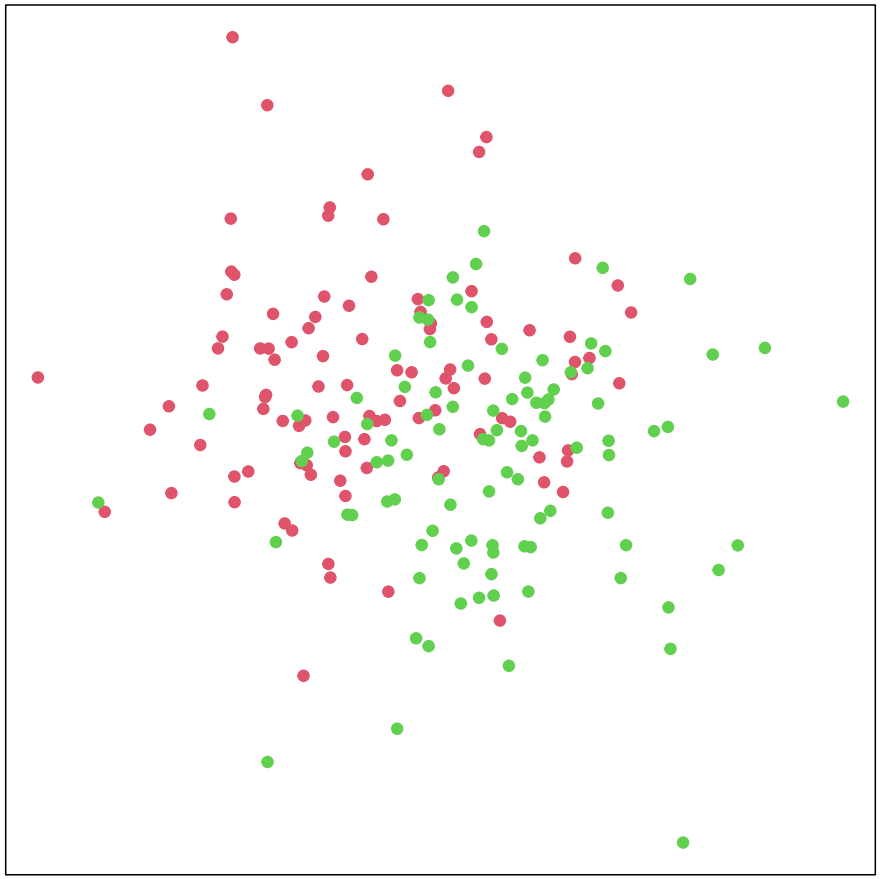
$$\hat{y}_i = x_i^T\hat{\beta}$$
$$\hat{y}(x_0) = x_0^T\hat{\beta}.$$

Example



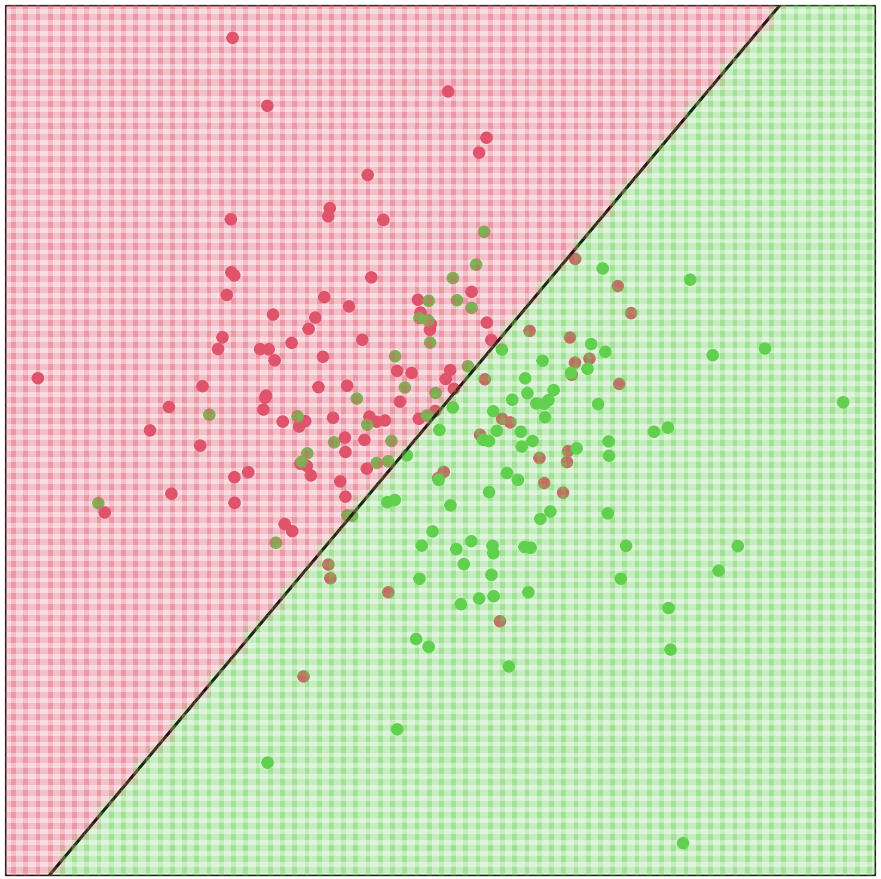
Example / 2

Data points with true class labels



Example / 3

Linear regression of 0/1 response



Nearest neighbor method

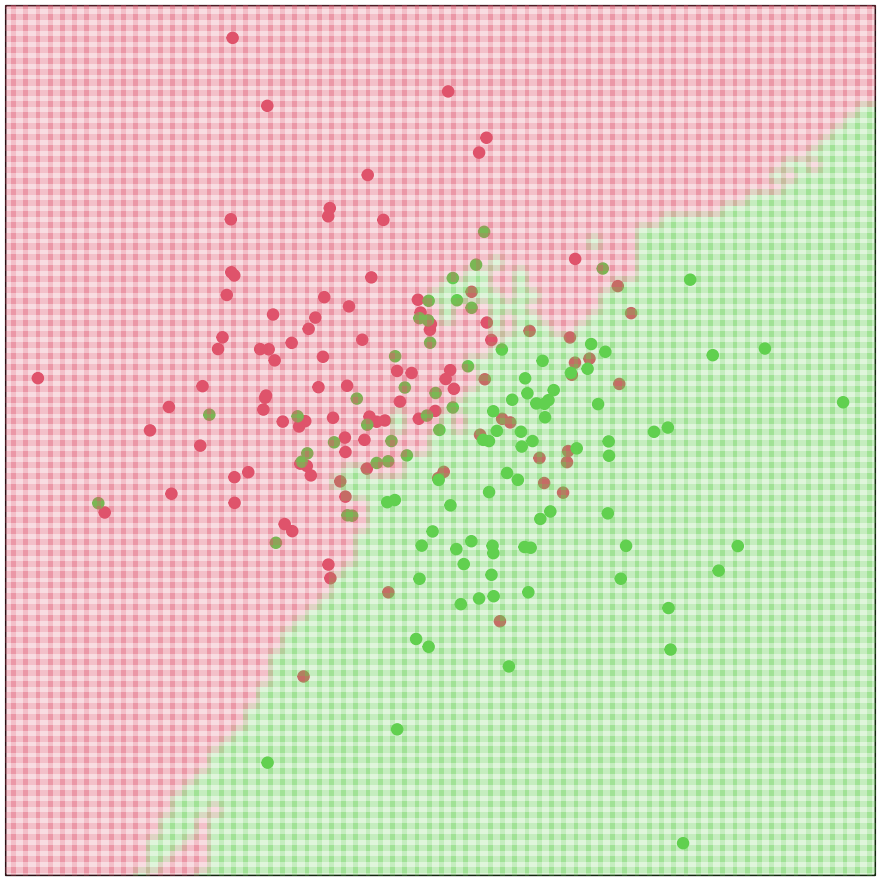
- The observations in the training set $\mathcal{T}$ closest in input space to x are used to form the prediction $\hat{Y}$ at position x.
- The k nearest neighbor fit for $\hat{Y}$ is defined as:

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

  where $N_k(x)$ is the neighborhood of x defined by the k closest points x_i in the training sample.
- Closeness implies a metric. For now, Euclidean distance.
- For k nearest neighbor fits the error on the training data should be approximately an increasing function of k, and will always be 0 for $k = 1$.
- In k nearest neighbors there is one parameter, k, to choose:
  - Effective number of parameters: $\frac{N}{k}$.
  - Minimizing the error in the training set would always choose $k = 1$.

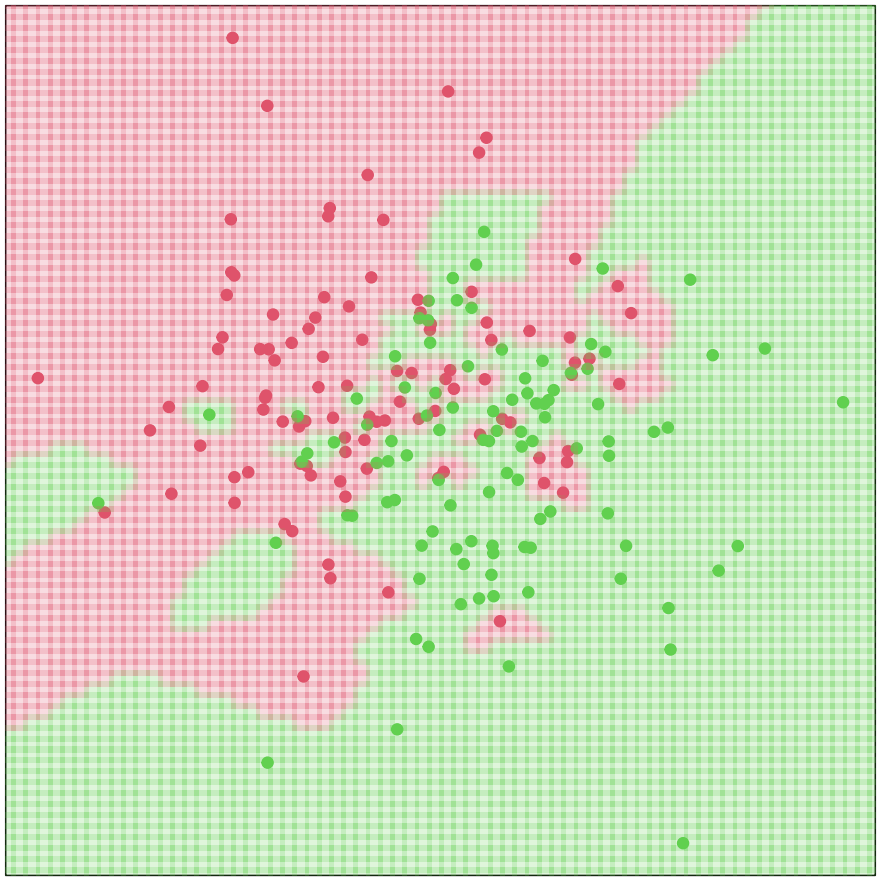
Example

20 nearest neighbor classifier



Example / 2

1 nearest neighbor classifier



From least squares to nearest neighbors

- Least squares leads to a linear decision boundary:
  - Smooth and apparently stable to fit.
  - Appears to heavily rely on the assumption that a linear decision boundary is appropriate.

  $\Rightarrow$ Low variance, potentially high bias.
- k nearest neighbors method
  - Relies on no stringent assumptions about the underlying data.
  - Any particular subregion of the decision boundary depends only on a handful of input points.

  $\Rightarrow$ High variance, low bias.

Statistical decision theory

- Given:
  - Assume we have a quantitative output.
  - Let $X \in \mathbb{R}^p$ denote a real valued random input vector.
  - Let $Y \in \mathbb{R}$ denote a real valued random output variable.
  - Denote the joint distribution by $\Pr(X, Y)$.
- Target:
  - Determine a function $f(X)$ for predicting Y which minimizes a loss function

    $$L(Y, f(X)),$$

    which penalizes prediction errors.

Statistical decision theory / 2

- Possible loss functions are for example the *squared error loss*

$$L(Y, f(X)) = (Y - f(X))^2.$$

- This leads to the expected squared prediction error as criterion for choosing f:

$$\mathrm{EPE}(f) = \mathrm{E}(Y - f(X))^2 = \int [y - f(x)]^2 \mathrm{Pr}(dx, dy).$$

- By conditioning on X we obtain

$$\mathrm{EPE}(f) = \mathrm{E}_X \mathrm{E}_{Y|X}([Y - f(X)]^2 | X),$$

using $\mathrm{Pr}(X, Y) = \mathrm{Pr}(Y|X)\mathrm{Pr}(X)$.

Statistical decision theory / 3

- This implies that it suffices to minimize EPE pointwise:

$$f(x) = \arg\min_c \mathrm{E}_{Y|X}([Y - c]^2 | X = x),$$

with the solution

$$f(x) = \mathrm{E}_{Y|X}(Y|X = x).$$

This is the conditional expectation, also known as *regression* function.

Statistical decision theory: k nearest neighbors

- Nearest neighbor methods attempt to estimate this conditional mean using

$$\hat{f}(x) = \text{Ave}(y_i | x_i \in N_k(x)),$$

where $\text{Ave}(\cdot)$ denotes average and two approximations are exploited:

1. Expectation is approximated by averaging over the sample data.
2. Conditioning at a point is relaxed to conditioning on some region “close” to the target point.

Statistical decision theory: k nearest neighbors / 2

- Thus, under mild regularity conditions on the joint probability distribution $\Pr(X, Y)$, one can show that as $N, k \to \infty$ such that $k/N \to 0$,

$$\hat{f}(x) \to \mathrm{E}(Y|X = x).$$

- Problems:
  - If only a small sample size is available, exploiting structure in the data could lead to more stable estimators.
  - The *rate* of convergence depends on the dimension of the feature space. The rate decreases if the dimension increases.

Statistical decision theory: linear regression

- Assumes that the regression function $f(x)$ is approximately linear in its arguments:

$$f(x) \approx x^T \beta.$$

- Thus, we specify a model for the regression function and minimize the EPE. This gives

$$\beta = [\mathrm{E}(XX^T)]^{-1}\mathrm{E}[XY].$$

- Linear regression does not condition on X, but pools over all values of X using the knowledge of the functional relationship.
- Estimating β consists of replacing the expectation by taking the average over the training data.

Statistical decision theory: comparison

- Model assumptions:
  - Least squares assumes $f(x)$ is well approximated by a globally linear function.
  - k nearest neighbors assumes $f(x)$ is well approximated by a locally constant function.

Statistical decision theory: loss functions

- So far we considered the squared error loss, also referred to as L_2 loss.
- Alternatives are for example the L_1 loss:

$$L(Y, f(X)) = |Y - f(X)|,$$

  which if this expected loss is minimized gives the conditional median as estimate:

$$\hat{f}(x) = \text{median}(Y|X = x).$$

- L_1 criteria have discontinuities in their derivatives, which have hindered their widespread use.

Loss functions: categorical outcome

- The categorical outcome G takes values in $\mathcal{G}$, the set of possible classes.
- The estimate $\hat{G}$ also takes values in $\mathcal{G}$.
- The loss can be represented by a $K \times K$ matrix $\mathbf{L}$, where $K = \text{card}(\mathcal{G})$.
- The matrix $\mathbf{L}$ has
  - zero values on the diagonal,
  - nonnegative values elsewhere,

  where $L(k, l)$ denotes the price to pay for classifying an observation belonging to the kth class $\mathcal{G}_k$ into the lth class $\mathcal{G}_l$.
- The EPE can be written as

$$\text{EPE}(\hat{G}) = \text{E}(L(G, \hat{G}(X))) = \text{E}_X \left[\sum_{k=1}^{K} L(\mathcal{G}_k, \hat{G}(X)) \text{Pr}(\mathcal{G}_k | X) \right].$$

Loss functions: categorical outcome / 2

- The pointwise minimization is again sufficient:

$$\hat{G}(x) = \arg\min_{g \in \mathcal{G}} \sum_{k=1}^{K} L(\mathcal{G}_k, g) \Pr(\mathcal{G}_k | X = x).$$

- Examples for loss functions:
  - Zero-one loss function:

$$L(k, l) = \begin{cases} 0 & l = k, \\ 1 & l \neq k. \end{cases}$$

The EPE is minimized for the zero-one loss by

$$\hat{G}(x) = \arg\min_{g \in \mathcal{G}} [1 - \Pr(g | X = x)] = \max_{g \in \mathcal{G}} \Pr(g | X = x).$$

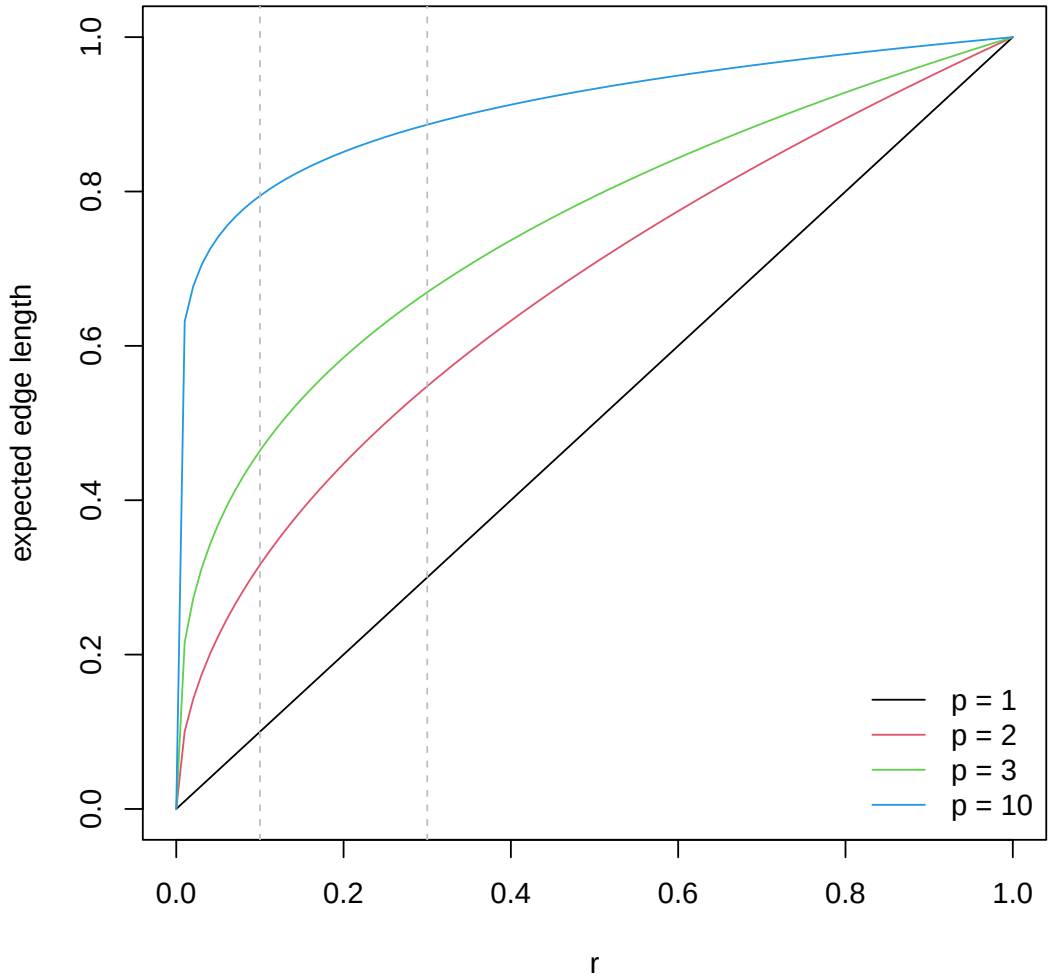
This solution is called *Bayes classifier*. The error rate of the Bayes classifier is called *Bayes rate*.

Local methods in high dimensions

- High dimensional problems suffer from the *curse of dimensionality* (Bellman, 1961).
  - Observations tend to have no “close” neighbors.
  - Observations are closer to the boundary than to any other data point.
- Example: Assume uniformly distributed data in the p-dimensional unit cube. If the fraction r of observations to be contained in a hypercubical neighborhood is fixed, the expected edge length of this cube is given by

$$e_p(r) = r^{1/p}.$$

Local methods in high dimensions / 2



Model selection and the bias-variance tradeoff

- Many statistical learning models contain a *smoothing* or *complexity* parameter.
- More complex models will in general have a better performance on the training data, but this will not translate to a better performance on new test data.
- The expected squared prediction error at point x_0 for a fixed procedure to estimate f by $\hat{f}$ based on the training set $\mathcal{T}$ is given by

$$\begin{aligned}
\mathrm{EPE}_{\hat{f}_{\mathcal{T}}}(x_0) &= \mathrm{E}[(Y - \hat{f}_{\mathcal{T}}(x_0))^2 | X = x_0] \\
&= \mathrm{Var}(Y|X = x_0) + \mathrm{E}_{\mathcal{T}}[(\mathrm{E}(Y|X = x_0) - \hat{f}_{\mathcal{T}}(x_0))^2 | X = x_0] \\
&= \mathrm{Var}(Y|X = x_0) + [\mathrm{Bias}^2_{\mathcal{T}}(\hat{f}_{\mathcal{T}}(x_0)) + \mathrm{Var}_{\mathcal{T}}(\hat{f}_{\mathcal{T}}(x_0))]
\end{aligned}$$

Model selection and the bias-variance tradeoff / 2

- This decomposition indicates:
  - The first term is the *irreducible* error.
  - The second and third terms are the *mean squared error* of $\hat{f}_{\mathcal{T}}(x_0)$ in estimating $f(x_0)$ decomposed into *bias* and *variance*.
- In general one has:
  - If the model complexity is increased, the bias is reduced.
  - If the model complexity is increased, the variance is increased.

Model selection and the bias-variance tradeoff / 3