Optimization

- Many more complex models in statistics and machine learning do not have analytic solutions to ML estimators.
- In most models parameters are learned by some numerical optimization technique.

$$\min_{\theta} F(\theta)$$

- How many minima are there?
- How do we find optimal θ?
- Are we guaranteed to find the global optimum θ^*, rather just a local one?
- How efficiently can we solve for θ?
- What if there are constraints?

Constrained Optimization

- Optimization problems with constraints, e.g.

$$\begin{aligned} \min_{\theta \in \mathbb{R}^d} \quad & F(\theta) \\ \text{subject to} \quad & g_i(\theta) \leq 0 \quad \text{for } i = 1, \ldots, I \\ & h_j(\theta) = 0 \quad \text{for } j = 1, \ldots, J \end{aligned}$$

  where g_i enforce inequality constraints and h_j equality constraints.
- Can write this succinctly:

$$\begin{aligned} \min_{\theta \in \mathbb{R}^d} \quad & F(\theta) \\ \text{subject to} \quad & g(\theta) \preceq 0 \\ & h(\theta) = 0 \end{aligned}$$

  where $g : \mathbb{R}^d \to \mathbb{R}^I$ is a vector-valued function with $g(\theta)_i = g_i(\theta)$. Similarly $h(\theta) : \mathbb{R}^d \to \mathbb{R}^J$. $x \preceq y$ iff $x_i \leq y_i \forall i$.
- These problems are called **programmes**.

Constrained Optimization

$$\begin{aligned} \min_{\theta \in \mathbb{R}^d} \quad & F(\theta) \\ \text{subject to} \quad & g(\theta) \preceq 0 \\ & h(\theta) = 0 \end{aligned}$$

- We can enforce constraints by using **Lagrange multipliers** or **dual variables** $\lambda \in \mathbb{R}^I$ and $\kappa \in \mathbb{R}^J$.
- The optimization problem can be written as a mini-max optimization of the Lagrangian:

$$\min_{\theta} \max_{\lambda \succeq 0, \kappa} \mathcal{L}(\theta, \lambda, \kappa) = \min_{\theta} \max_{\lambda \succeq 0, \kappa} F(\theta) + \lambda^\top g(\theta) + \kappa^\top h(\theta)$$

- Intuition: For any θ, we have:

$$\max_{\lambda \succeq 0, \kappa} \mathcal{L}(\theta, \lambda, \kappa) = \begin{cases} +\infty & \text{if there is some unsatisfied constraint,} \\ F(\theta) & \text{if all constraints are satisfied.} \end{cases}$$

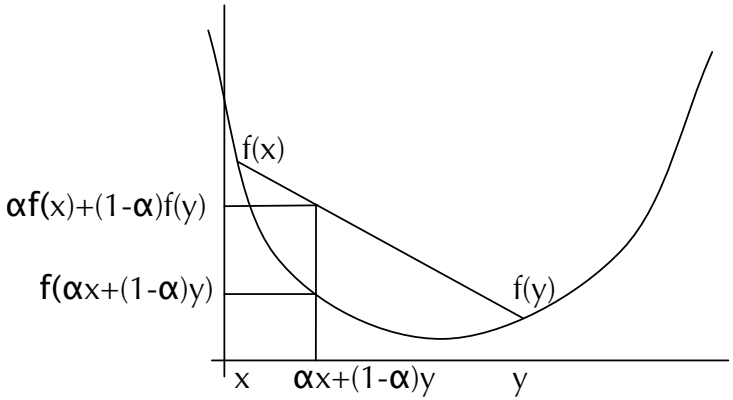
So the outer minimization over θ results in the same optimization problem.

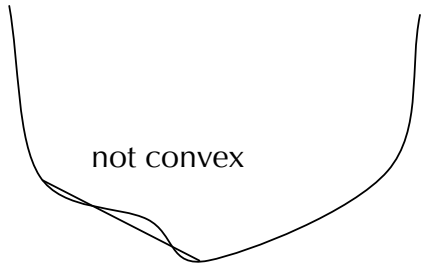
Convex Optimization

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y)$$

  for all $x, y \in \mathbb{R}^d$, $\alpha \in [0,1]$.
- For smooth functions: Equivalent to 2nd derivative (**Hessian**) being positive semidefinite.
- A programme is a **convex programme** if:
  - $F(\theta)$ is convex,
  - $g_i(\theta)$ is convex for each i,
  - $h(\theta) = A\theta + b$ is affine.
- Examples: linear, quadratic, semidefinite programming.
- Convex programmes have a unique minimum (typically), which can be efficiently found.





Boyd and Vandenberghe, Convex Optimization. 2004. MOOC right now.

Convex Duality

- Say the minimum is p^*, and occurred at θ^*.
- The **dual programme** inverts the order of max and min:

$$p^* = \min_{\theta} \max_{\lambda \succeq 0, \kappa} \mathcal{L}(\theta, \lambda, \kappa) \geq \max_{\lambda \succeq 0, \kappa} \min_{\theta} \mathcal{L}(\theta, \lambda, \kappa) = d^*$$

  where the dual optimum is d^*.
- **Karush-Kuhn-Tucker Theorem**: Subject to regularity conditions, a solution θ^* is the optimal solution of a convex programme, if and only if there are λ^* and κ^* (the dual optimal solution) such that:
  - **Primal feasible**: $g(\theta^*) \preceq 0$, $h(\theta^*) = 0$.
  - **Dual feasible**: $\lambda^* \succeq 0$.
  - $(\theta^*, \lambda^*, \kappa^*)$ is a **saddle point** of $\mathcal{L}$: For every $\theta, \lambda \succeq 0, \kappa$, we have

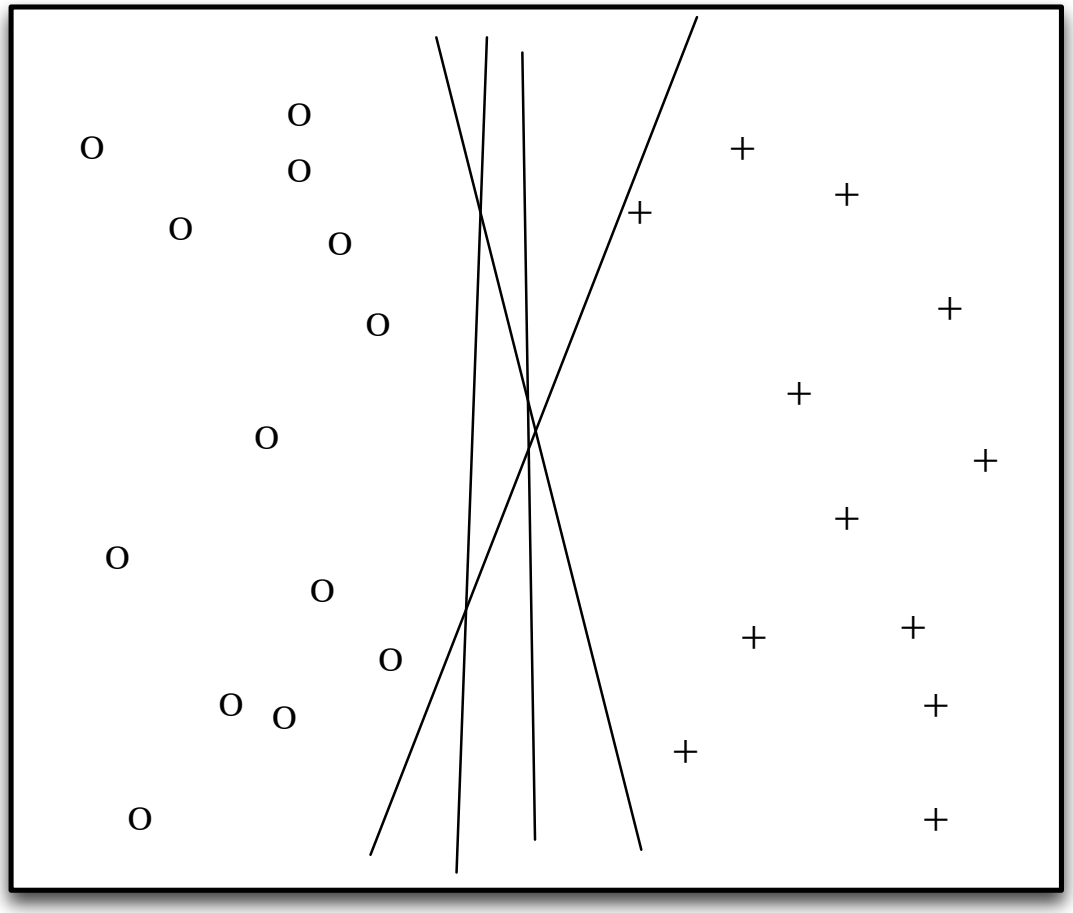
$$\mathcal{L}(\theta^*, \lambda, \kappa) \leq \mathcal{L}(\theta^*, \lambda^*, \kappa^*) \leq \mathcal{L}(\theta, \lambda^*, \kappa^*)$$

  - $\nabla_\theta \mathcal{L}(\theta^*, \lambda^*, \kappa^*) = \nabla_\theta F(\theta^*) + (\lambda^*)^\top \nabla_\theta g(\theta^*) + (\kappa^*)^\top \nabla_\theta h(\theta^*) = 0$
  - **Complementary slackness**: For every i,

$$\lambda_i^* g_i(\theta^*) = 0$$

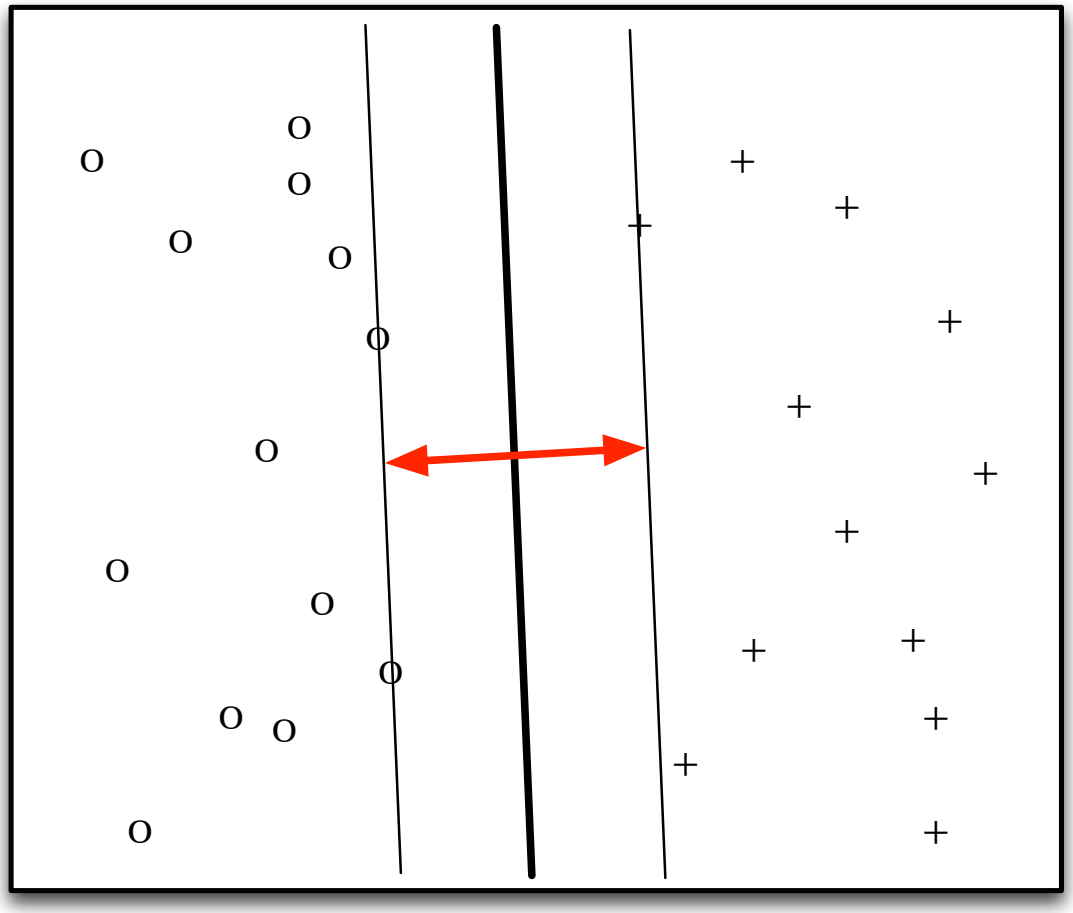
Linear Classification

- A dataset with $\{+1, -1\}$ labels is **linearly separable** if there is a hyperplane separating two classes.
- Typically there will be an infinite number of such **separating hyperplanes**.



Maximum Margin Classification

- Good choice of separating hyperplane: one with **large margin**.
- Such a hyperplane will be defined by a number of data vectors close to the boundary—the **support vectors**, leading to a method called **support vector machines**.



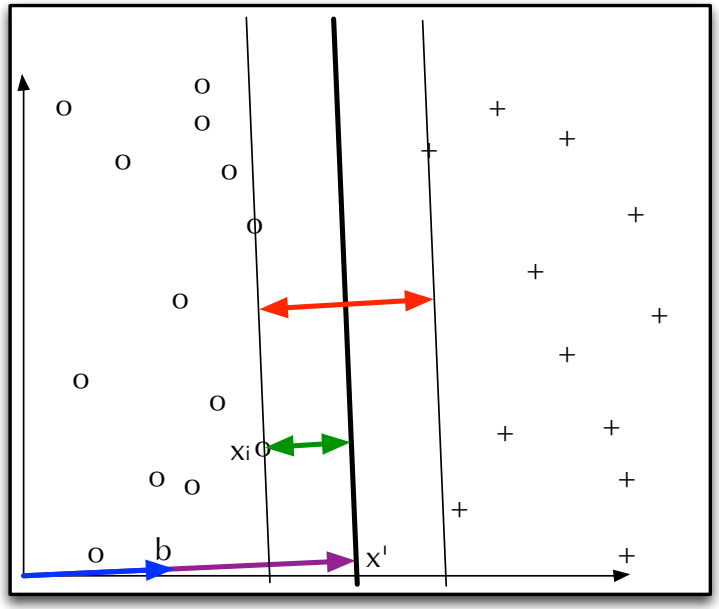
Support Vector Machines

- A hyperplane can be parametrized as:

$$g(x) = a + b^\top x = 0$$

  with the classification given by $\text{sign}(g(x))$.

- Distance and classification of a point x_i from hyperplane is $g(x_i)/\|b\|$.
- Multiplying a and b by $c > 0$ does not affect result. Rescale such that margin (closest distance of data vectors to hyperplane) is $1/\|b\|$.



$$y_i(a + b^\top x_i)/\|b\| \geq 1/\|b\|$$
$$y_i(a + b^\top x_i) \geq 1$$

- Constrained optimization problem to solve for a, b:

$$\max_{a,b} \quad 1/\|b\| \qquad \Leftrightarrow \qquad \min_{a,b} \quad \tfrac{1}{2}\|b\|^2$$
$$\text{subject to} \quad y_i(a + b^\top x_i) \geq 1 \qquad \text{subject to} \quad y_i(a + b^\top x_i) \geq 1 \quad \text{for all } i$$

Support Vector Machines

- Introduce Lagrange multipliers $\lambda_i \geq 0$ to enforce constraints:

$$\min_{a,b} \max_{\lambda \succeq 0} \mathcal{L}(a, b, \lambda) = \frac{1}{2}\|b\|^2 + \sum_{i=1}^{n} \lambda_i (1 - y_i(a + b^\top x_i))$$

- KKT optimality conditions:

Zero derivatives:

$$\nabla_a \mathcal{L}(a^*, b^*, \lambda^*) = -\sum_{i=1}^{n} \lambda_i^* y_i = 0$$

$$\nabla_b \mathcal{L}(a^*, b^*, \lambda^*) = b^* - \sum_{i=1}^{n} \lambda_i^* y_i x_i = 0$$

Primal feasibility:

$$y_i(a^* + (b^*)^\top x_i) \geq 1$$

Dual feasibility:

$$\lambda_i^* \geq 0$$

Complementary slackness:

$$\lambda_i^*(1 - y_i(a^* + (b^*)^\top x_i)) = 0$$

Support Vector Machines

- Substituting optimal a^* and b^* into Lagrangian leads to the **dual optimization problem**:

$$\max_{\lambda} \quad \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{n} \lambda_i \lambda_j y_i y_j (x_i)^\top (x_j)$$

$$\text{subject to} \quad \sum_{i=1}^{n} \lambda_i y_i = 0$$

$$\lambda \succeq 0$$

  A **quadratic programme**. Standard solvers can be used to find optimal λ^* in $O(n^3)$ cost.
- Those vectors with $\lambda_i > 0$ are called **support vectors**.
- Complementary slackness implies that if x_i does not lie on boundary, then $\lambda_i = 0$, i.e. not a support vector.
- Discriminant function is

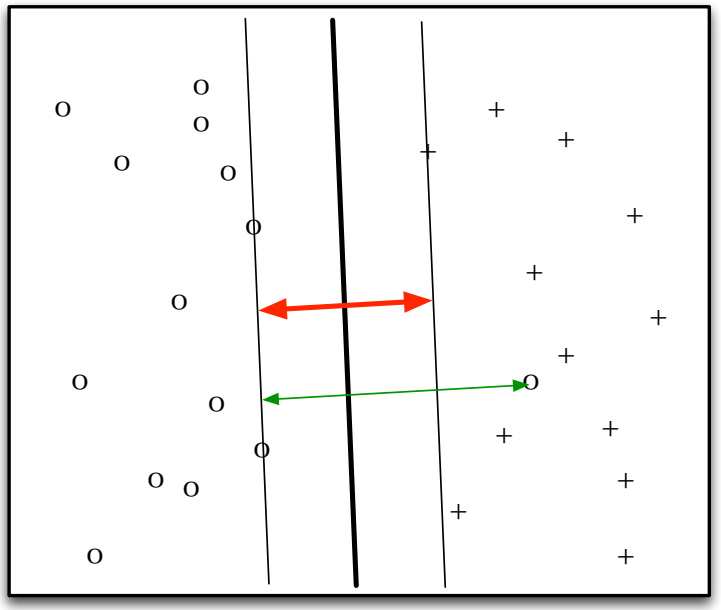
$$g(x) = a^* + \sum_{i=1}^{n} \lambda_i^* y_i x_i^\top x$$

  where a^* can be solved by noting that $y_j g(x_j) = 1$ for a support vector x_j.

Soft-Margin Support Vector Machines

- For **non-linearly separable** datasets, we can allow for **margin violations**

$$\xi_i = \begin{cases} 1 - y_i(a + b^\top x_i) & \text{if margin violated,} \\ 0 & \text{if not violated.} \end{cases}$$
$$= \max(0, 1 - y_i(a + b^\top x_i))$$



- Penalizing violations by their magnitude,

$$\begin{aligned} \min_{a,b,\xi} \quad & \frac{1}{2}\|b\|^2 + C\sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & y_i(a + b^\top x_i) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned}$$

where C is a tuning parameter.

Soft-Margin Support Vector Machines

- Introduce Lagrange multipliers $\lambda_i \geq 0$, $\gamma_i \geq 0$ to enforce constraints:

$$\mathcal{L}(a, b, \xi, \lambda, \gamma) = \frac{1}{2}\|b\|^2 + C\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\lambda_i(1 - \xi_i - y_i(a + b^\top x_i)) - \sum_{i=1}^{n}\gamma_i\xi_i$$

- KKT optimality conditions:

Zero derivatives:

$$\nabla_a \mathcal{L}(a^*, b^*, \xi^*, \lambda^*, \gamma^*) = -\sum_{i=1}^{n}\lambda_i^* y_i = 0$$

$$\nabla_b \mathcal{L}(a^*, b^*, \xi^*, \lambda^*, \gamma^*) = b^* - \sum_{i=1}^{n}\lambda_i^* y_i x_i = 0$$

$$\nabla_{\xi_i} \mathcal{L}(a^*, b^*, \xi^*, \lambda^*, \gamma^*) = C - \lambda_i^* - \gamma_i^* = 0$$

Primal feasibility:

$$y_i(a^* + (b^*)^\top x_i) \geq 1 - \xi_i^*$$

$$\xi_i^* \geq 0$$

Dual feasibility:

$$\lambda_i^* \geq 0$$

$$\gamma_i^* \geq 0$$

Complementary slackness:

$$\lambda_i^*(1 - \xi_i^* - y_i(a^* + (b^*)^\top x_i)) = 0$$

$$\gamma_i^*\xi_i^* = 0$$

Soft-Margin Support Vector Machines

- Setting derivatives of primal variables to zero leads to the dual programme:

$$\begin{aligned} \max_{\lambda} \quad & \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{n} \lambda_i \lambda_j y_i y_j (x_i)^\top (x_j) \\ \text{subject to} \quad & \sum_{i=1}^{n} \lambda_i y_i = 0 \\ & 0 \preceq \lambda \preceq C \end{aligned}$$

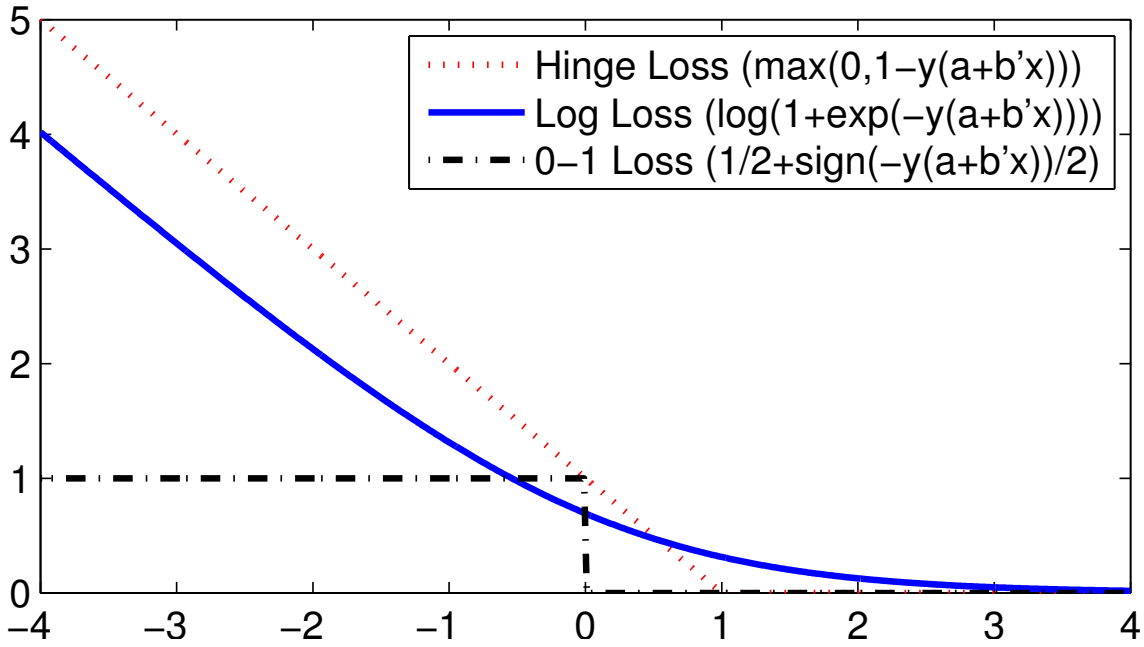
Only difference is the **box constraint** on $\lambda_i \in [0, C]$.

Soft-Margin Support Vector Machines

- From primal programme, we can first minimize over ξ_i's, leading to an unconstrained convex programme:

$$\min_{a,b} \quad \frac{1}{2}\|b\|^2 + C\sum_{i=1}^{n} \max(0, 1 - y_i(a + b^\top x_i))$$

- Interpretation: regularized empirical risk minimization with the **hinge loss**.

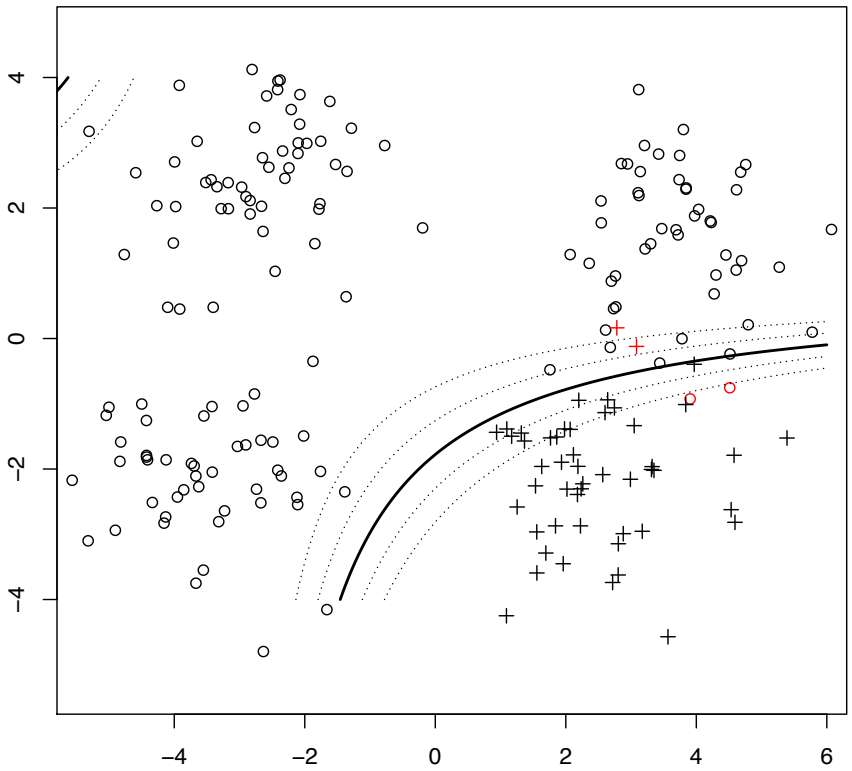


Support Vector Machines – Discussion

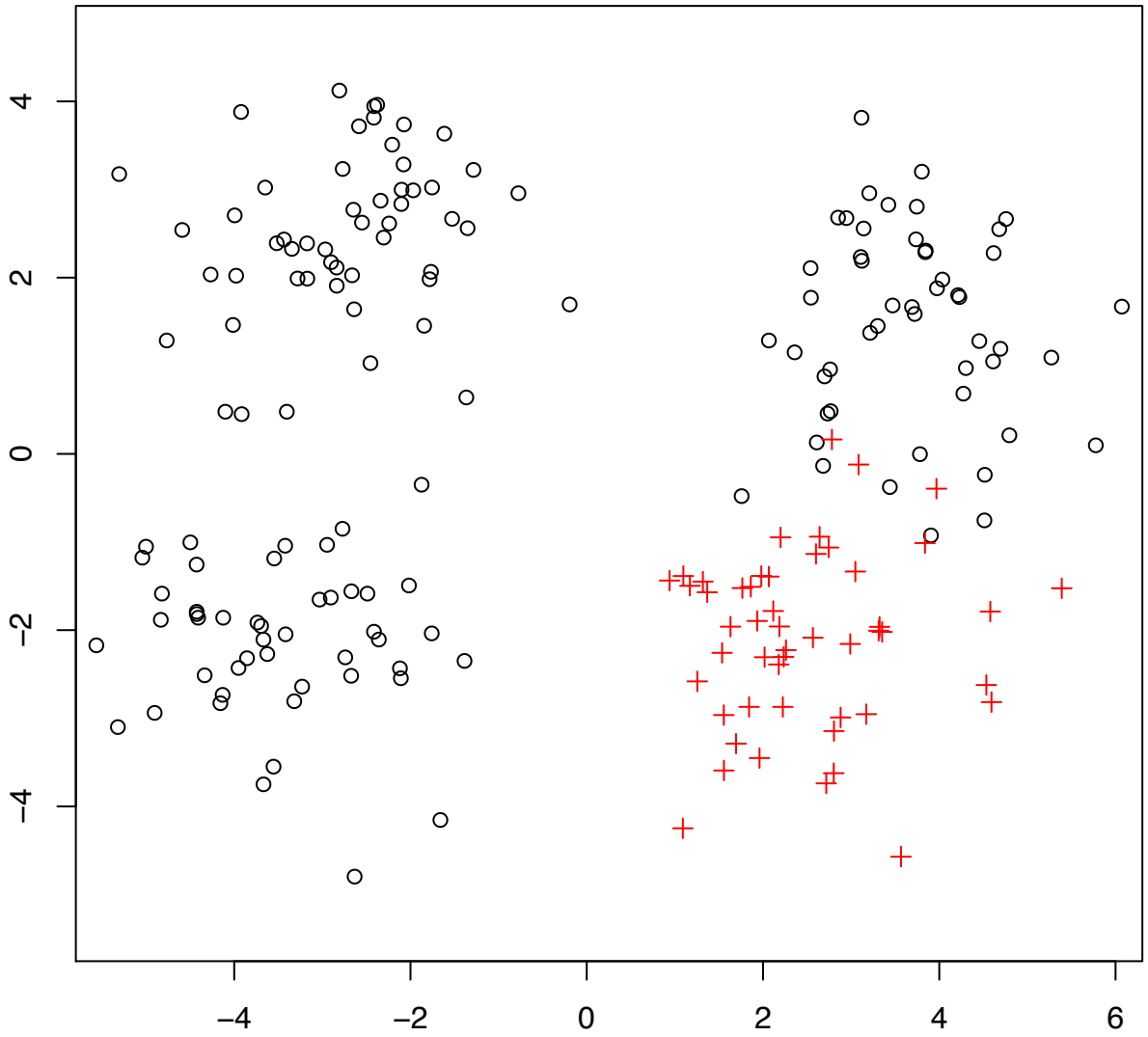
- **Multiclass classification**: If there are more than two classes, there are multiclass generalizations of the SVM.
- A simple practical idea: treat a multiclass problem as multiple binary classification problems.
  - One-vs-one: train $K(K-1)$ binary SVMs, for each pair of classes. At test time, predict class that got the most votes.
  - One-vs-rest: train K binary SVMs, one for each class vs all other classes. At test time, predict class with largest discriminant value $a_k + b_k^\top x$.
- Optimization for large scale problems:
  - Standard quadratic programme solvers not scalable.
  - Sequential minimal optimization (SMO): iterative solve pairs of λ_i's.
  - Pegasos : stochastic gradient descent on regularized hinge loss objective.
- L_2 regularization controls overfitting.
- Not probabilistic and cannot produce uncertainty estimates.
- Statistical learning theory foundations.
- Further readings:
  - Bishop, Chapter 6.
  - Christopher Burgess, A Tutorial on Support Vector Machines for Pattern Recognition. 1998.

Nonlinear Methods

- Decision boundaries and regression functions often need to be nonlinear.
- One general approach: transform data $x \mapsto \phi(x)$.
- A **global** approach. Decisions and optimal parameters depend on **whole** training dataset.
- Alternative approach: $p(Y = 1|X = x)$ or $f(x)$ depends only on data cases in **local neighbourhood** of x.



Local Methods



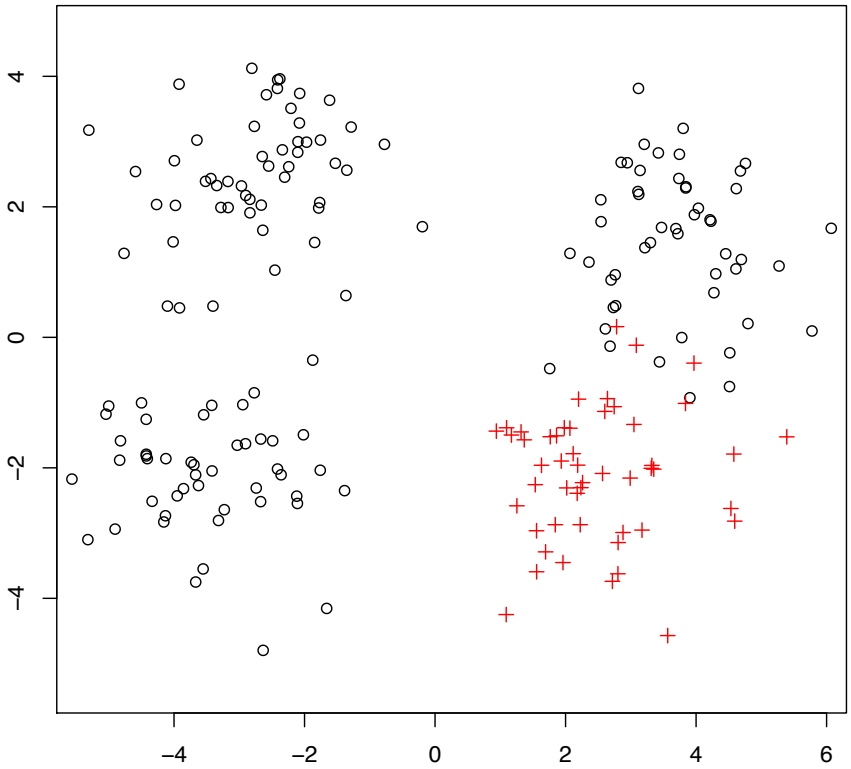
k-Nearest Neighbours

- A simple, local, nonlinear, non-model-based, method.
- Prediction at a data vector x is simply determined by the k nearest neighbours $ne_k(x)$ of x among the training set.
- Classification: predict the **majority vote** of the neighbours:

$$f^{\text{kNN}}(x) = \underset{l}{\text{argmax}} \quad |\{j \in ne_k(x) : y_j = l\}|.$$

- Regression: predict the average among the neighbours:

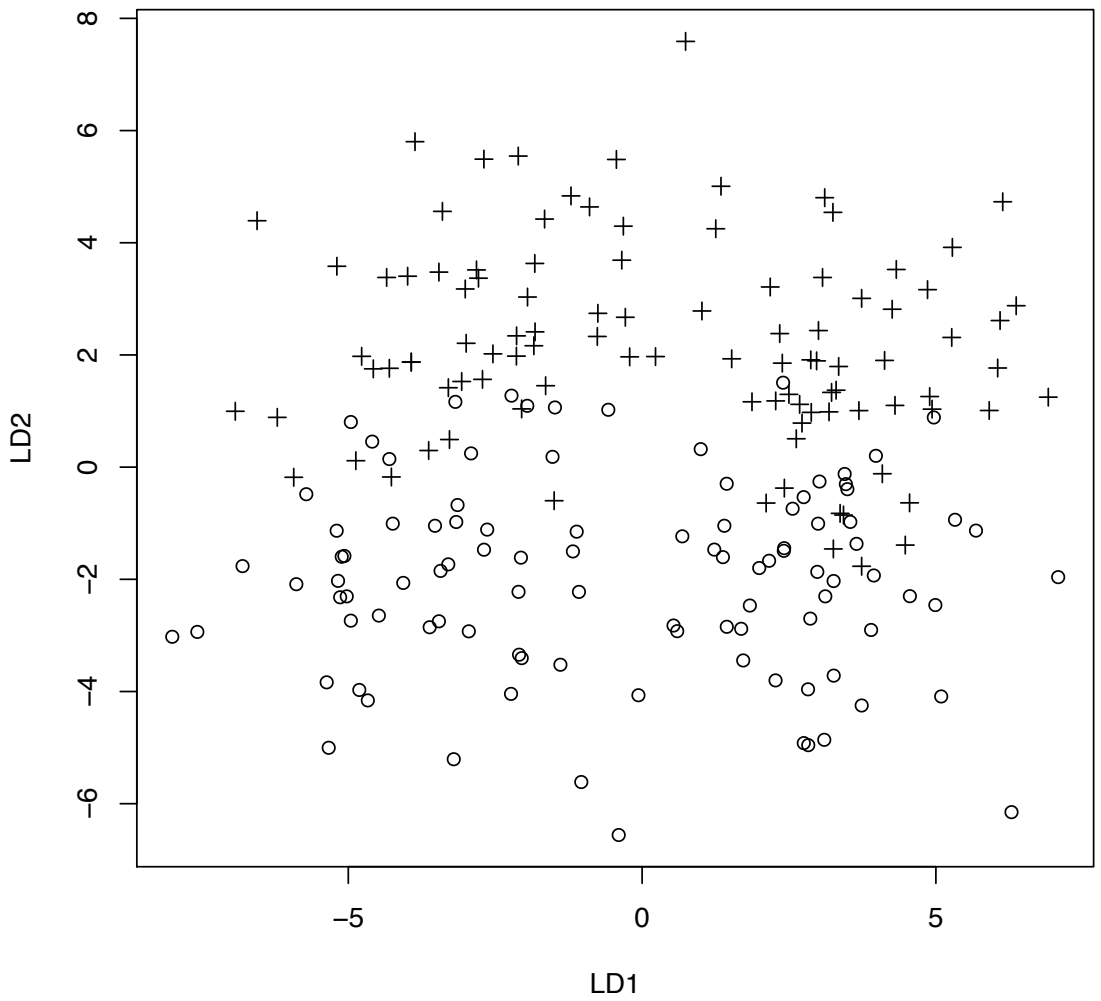
$$f^{\text{kNN}}(x) = \frac{\sum_{j \in ne_k(x)} y_j}{\sum_{j \in ne_k(x)} 1}.$$



k-Nearest Neighbours

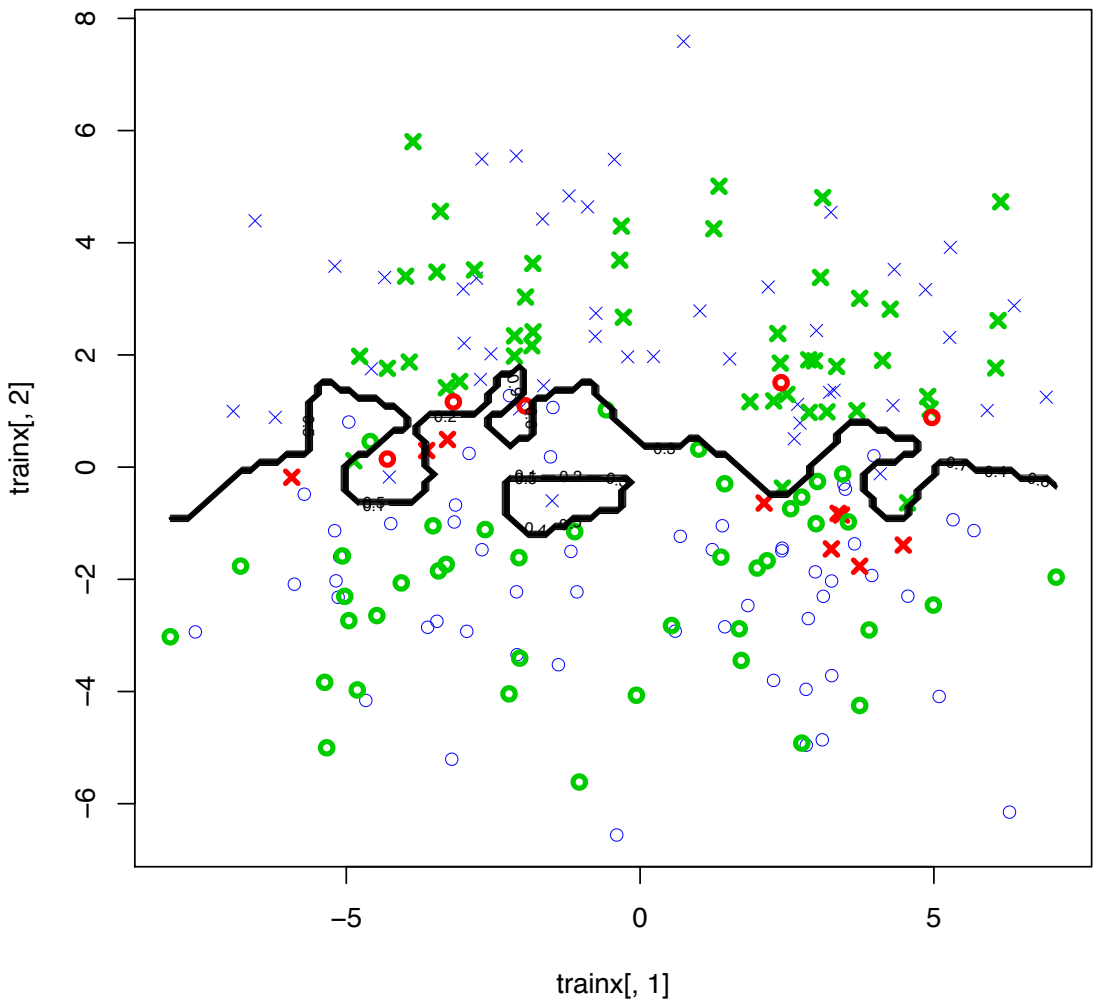
- Nearest neighbours are simple and essentially model-free methods for classification.
- Weaker modelling assumptions than e.g. LDA, Naïve Bayes and logistic regression.
- These methods are not very useful for understanding relationships between attributes and class predictions.
- As **black box** classification methods however, they are often perform reasonably on real life problems and provide a good benchmark.
- Can break down in high-dimensional data:
  - Effectively, partitions input space into regions each containing k data points, and prediction in each region estimated separately.
  - In a space of dimension $p \gg 0$, number of regions needed is $R = m^p$, so size of dataset needed is km^p.

k-Nearest Neighbour Demo



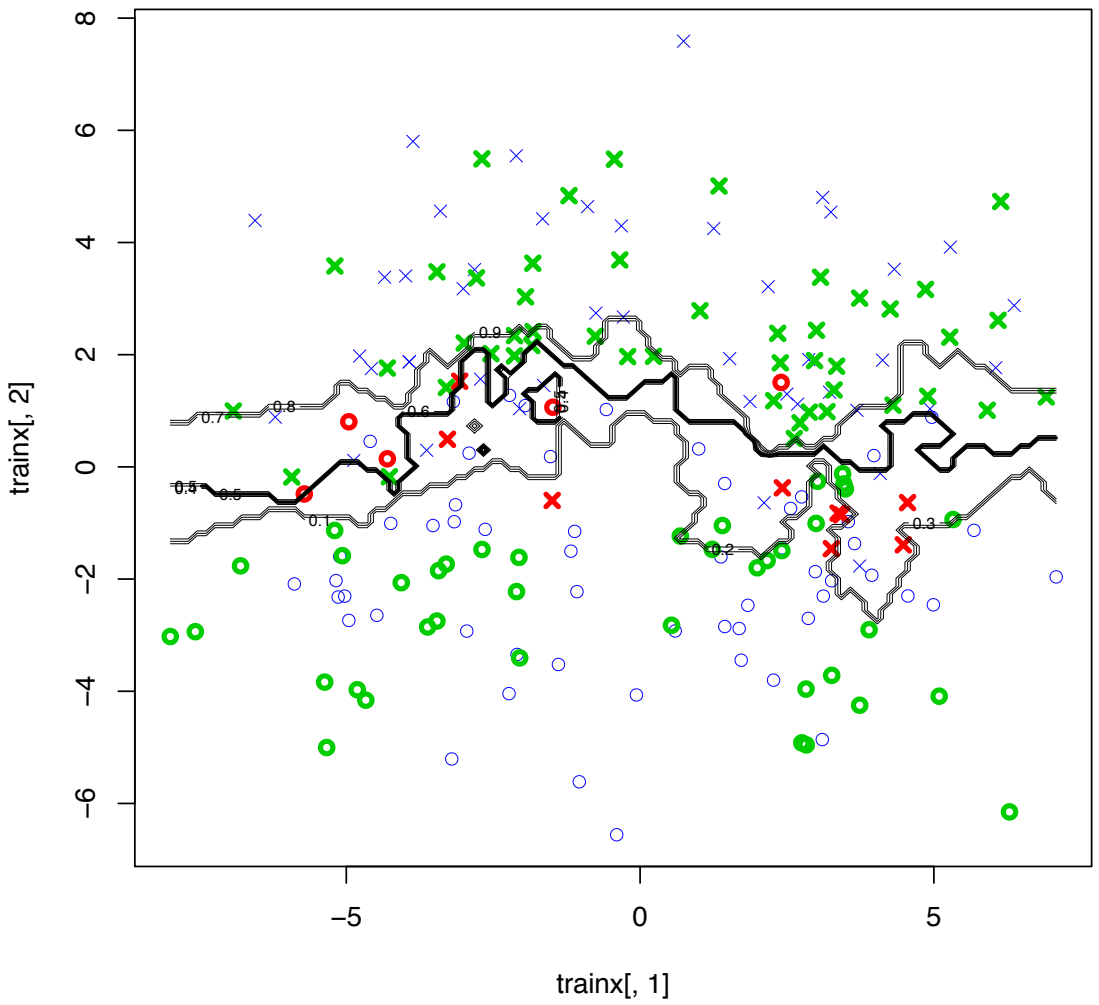
Data

k-Nearest Neighbour Demo



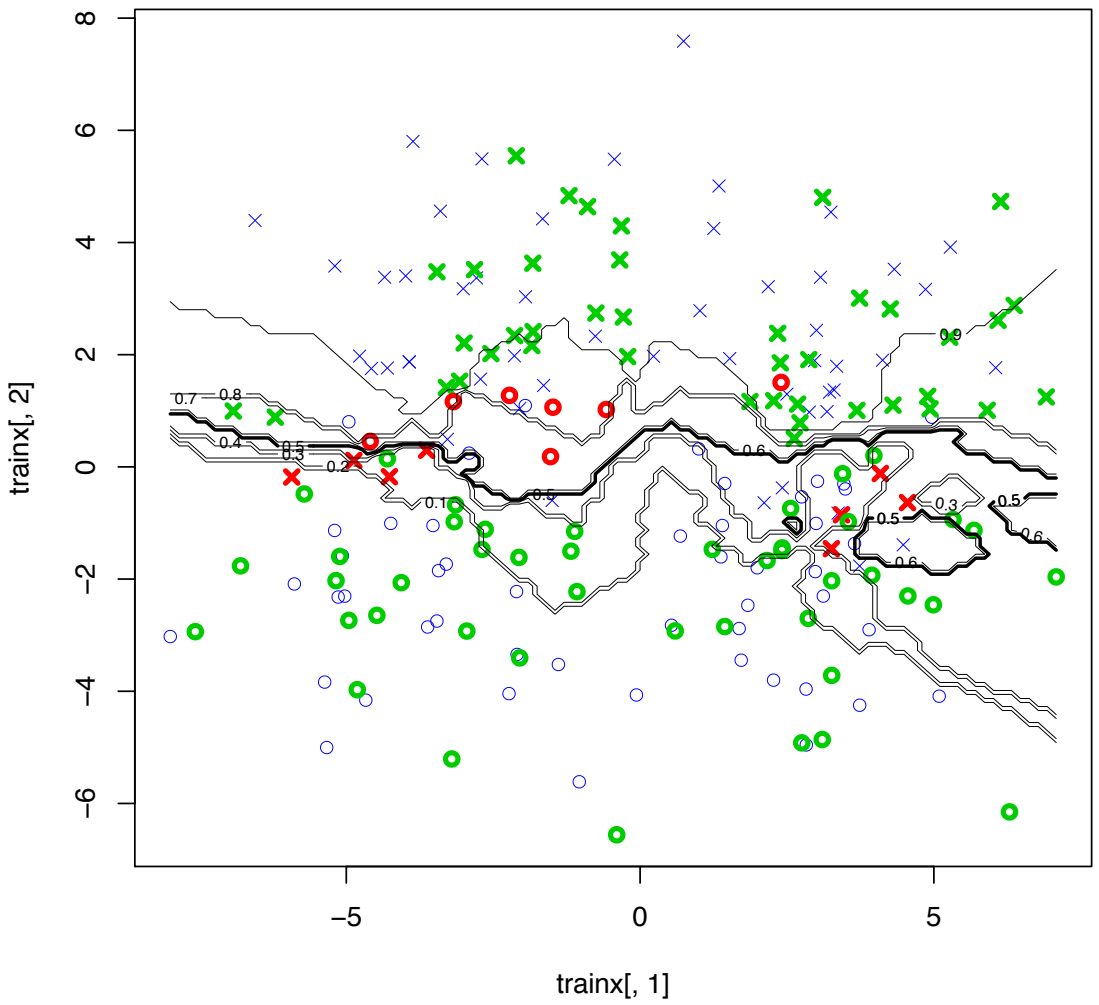
Result of 1NN

k-Nearest Neighbour Demo



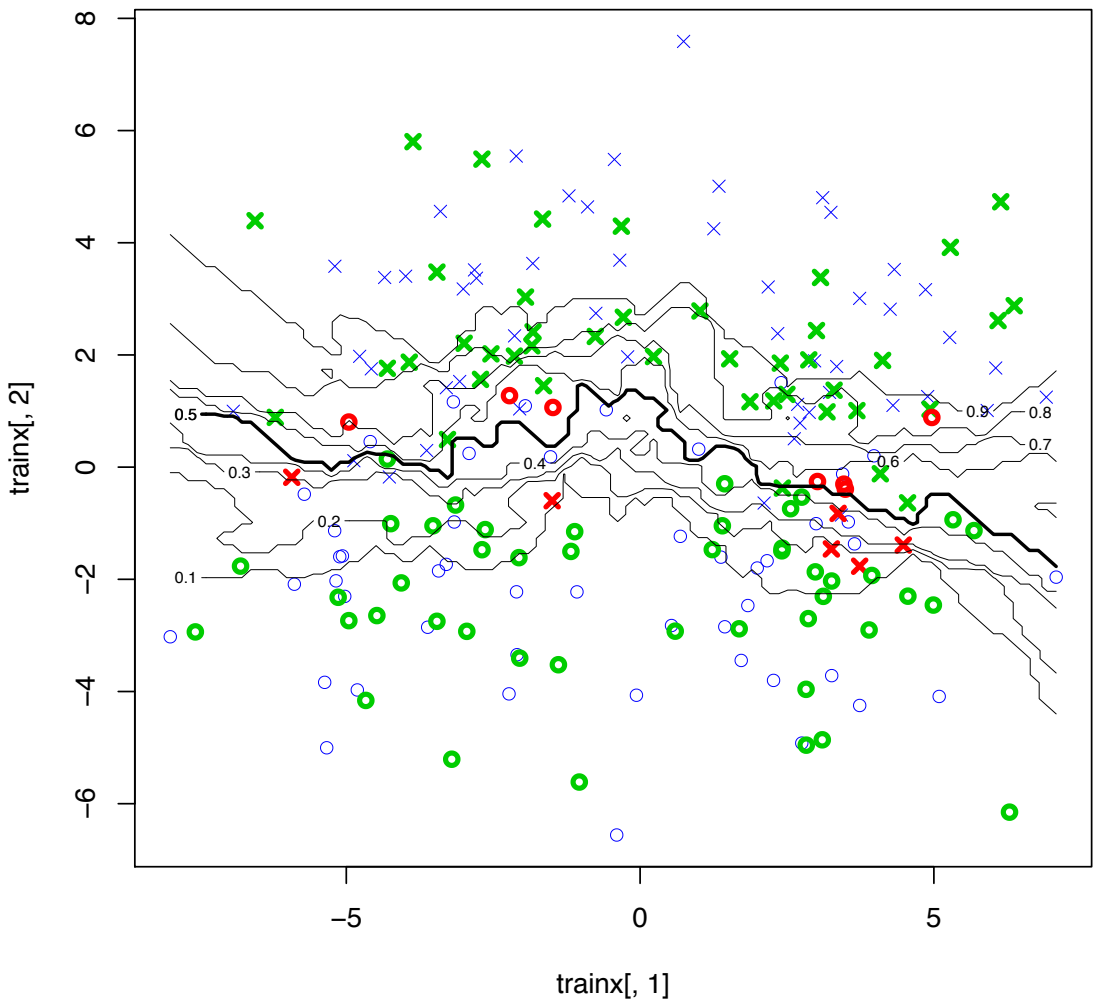
Result of 3NN

k-Nearest Neighbour Demo



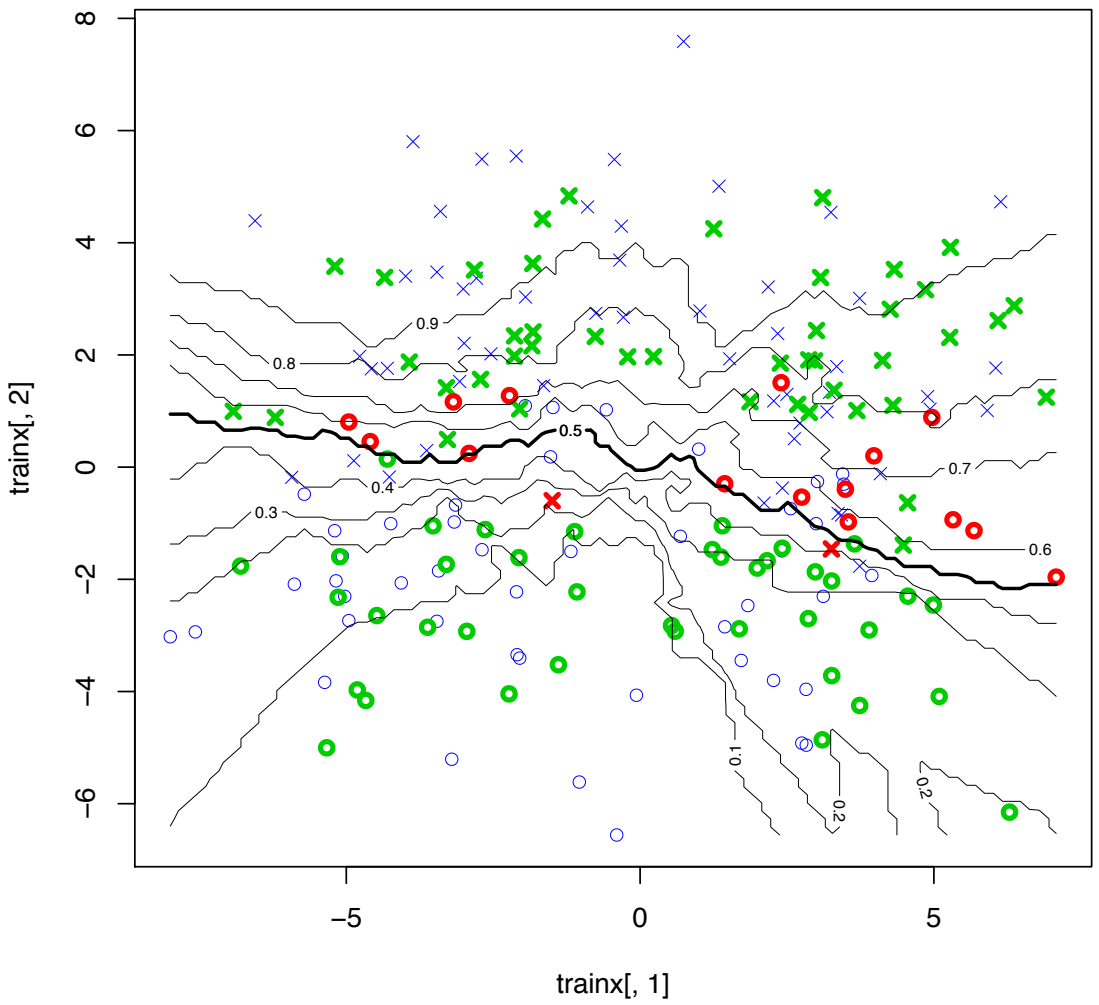
Result of 5NN

k-Nearest Neighbour Demo



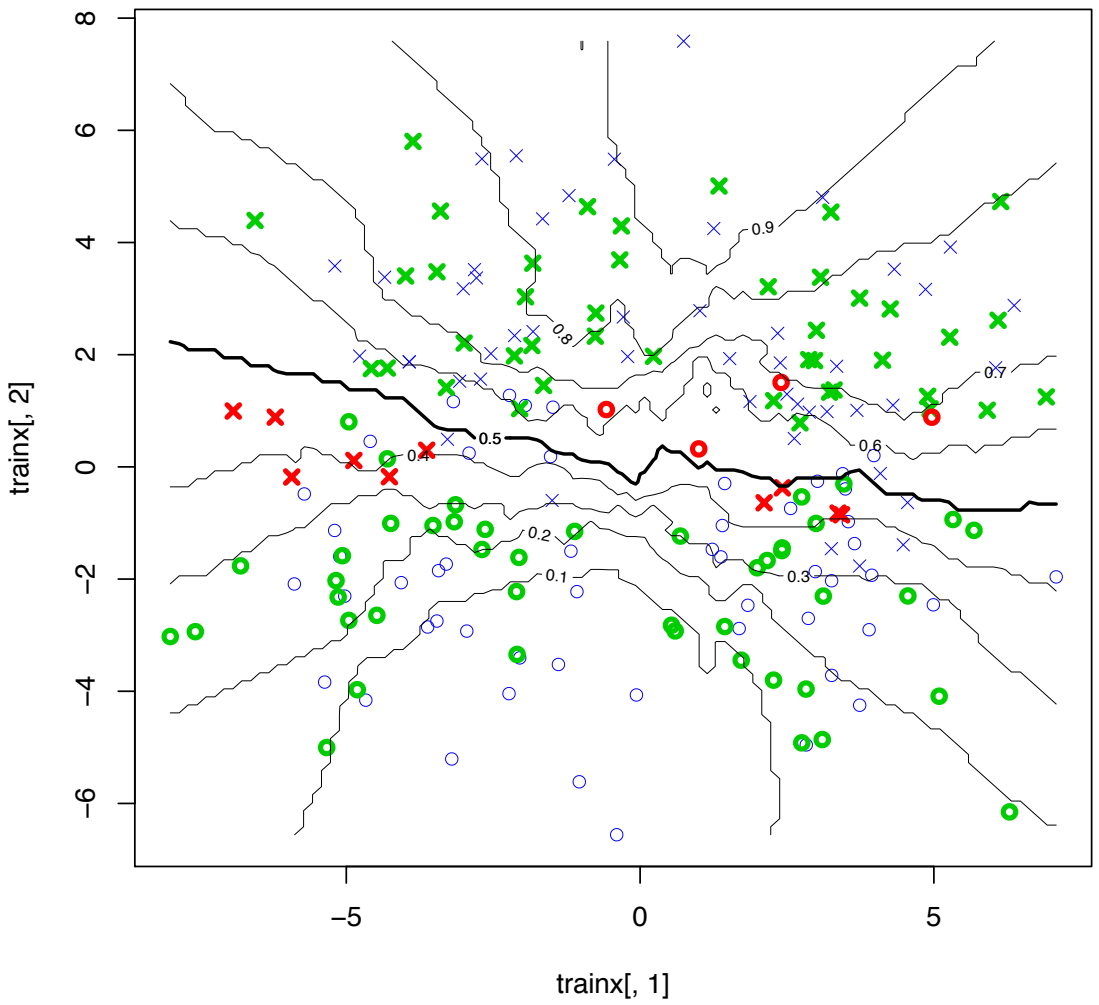
Result of 11NN

k-Nearest Neighbour Demo



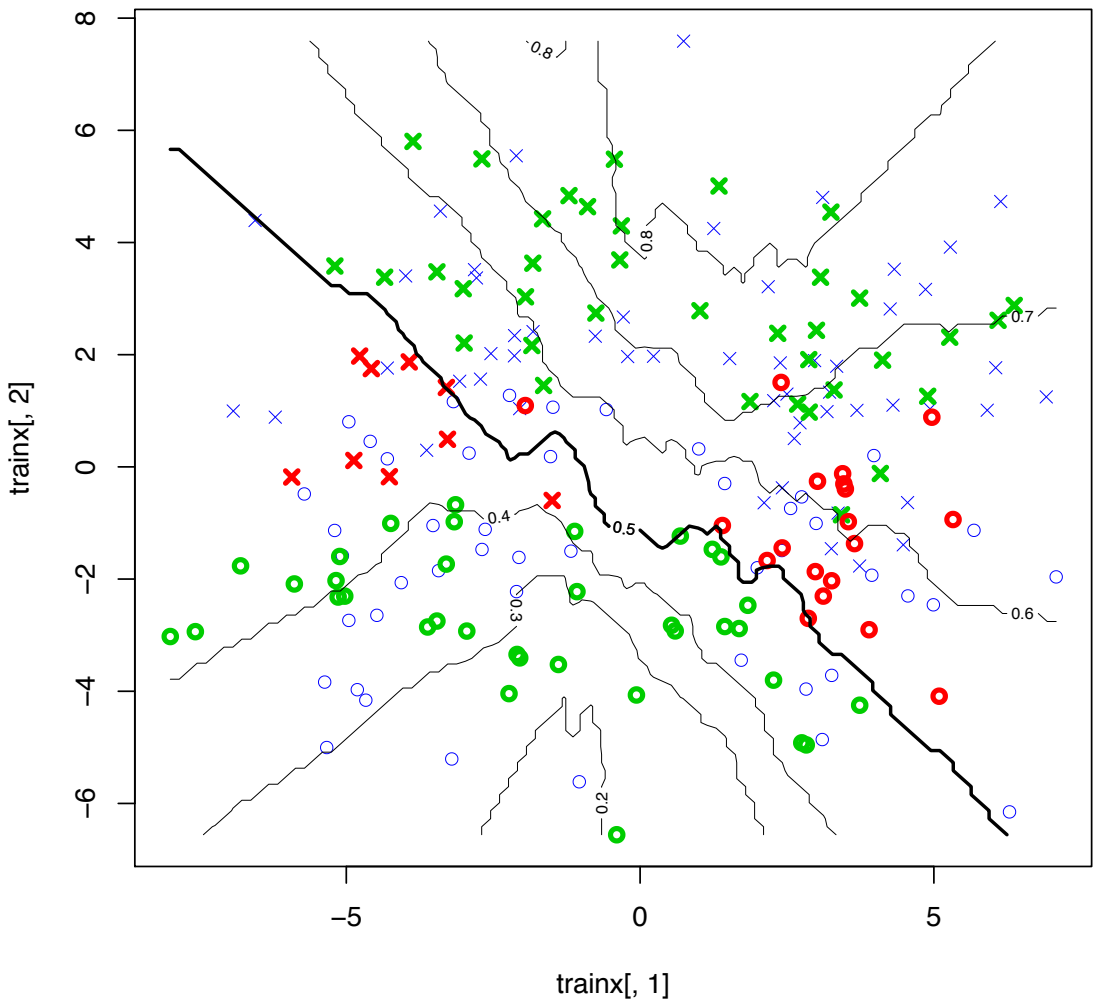
Result of 21NN

k-Nearest Neighbour Demo



Result of 31NN

k-Nearest Neighbour Demo



Result of 51NN

k-Nearest Neighbour Demo – R Code I

```
library(MASS)
## load crabs data data(crabs)
ct <- as.numeric(crabs[,1])-1+2*(as.numeric(crabs[,2])-1)
## project into first two LD
cb.lda <- lda(log(crabs[,4:8]),ct)
cb.ldp <- predict(cb.lda)
x <- as.matrix(cb.ldp$x[,1:2])
y <- as.numeric(crabs[,2])-1
x <- x + rnorm(dim(x)[1]*dim(x)[2])*1.5
eqscplot(x,pch=2*y+1,col=1)

k <- 3

kNN <- function(k,x,y,gridsize=100) {

  n      <- length(y)
  p      <- dim(x)[2]
  i      <- sample(rep(c(TRUE,FALSE),each=n/2),n,replace=FALSE)
  train  <- (1:n)[i]
  test   <- (1:n)[!i]
  trainx <- x[train,]
  trainy <- y[train]
  testx  <- x[test,]
  testy  <- y[test]


  trainn <- dim(trainx)[1]
  testn  <- dim(testx)[1]

  gridx1 <- seq(min(x[,1]),max(x[,2]),length=gridsize)
  gridx2 <- seq(min(x[,2]),max(x[,2]),length=gridsize)
  gridx  <- as.matrix(expand.grid(gridx1,gridx2))
  gridn  <- dim(gridx)[1]

  # calculate distances, smart and intelligently.
  trainxx <- t((trainx*trainx) %*% matrix(1,p,1))
```

k-Nearest Neighbour Demo – R Code II

```
  testxx  <- (testx*testx)   %*% matrix(1,p,1)
  gridxx  <- (gridx*gridx)   %*% matrix(1,p,1)
  testtraindist <- matrix(1,testn,1) %*% trainxx +
                   testxx %*% matrix(1,1,trainn) -
                   2*(testx %*% t(trainx))
  gridtraindist <- matrix(1,gridn,1) %*% trainxx +
                   gridxx %*% matrix(1,1,trainn) -
                   2*(gridx %*% t(trainx))

  # predict
  testp <- numeric(testn)
  gridp <- numeric(gridn)
  for (j in 1:testn) {
    nearestneighbors <- order(testtraindist[j,])[1:k]
    testp[j] <- mean(trainy[nearestneighbors])
  }
  for (j in 1:gridn) {
    nearestneighbors <- order(gridtraindist[j,])[1:k]
    gridp[j] <- mean(trainy[nearestneighbors])
  }
  predy <- as.numeric(testp>.5)

  plot(trainx[,1],trainx[,2],pch=trainy*3+1,col=4,lwd=.5)
  points(testx[,1],testx[,2],pch=testy*3+1,col=2+(predy==testy),lwd=3)
  contour(gridx1,gridx2,matrix(gridp,gridsize,gridsize),
        levels=seq(.1,.9,.1),lwd=.5,add=TRUE)
  contour(gridx1,gridx2,matrix(gridp,gridsize,gridsize),
        levels=c(.5),lwd=2,add=TRUE)
}
```

Asymptotic Performance of 1NN

- Let $(x_i, y_i)_{i=1}^n$ be training data where $x_i \in \mathbb{R}^p$ and $y_i \in \{1, 2, ..., K\}$.
- We define

$$\widehat{y}_{\text{Bayes}}(x) = \underset{l \in \{1,\ldots,K\}}{\arg\max}\ \pi_l f_l(x)$$

and

$$\widehat{y}_{\text{1NN}}(x) = y\,(\text{nearest neigbour of } x)\,.$$

- The (optimal) Bayes risk and 1NN risk are:

$$\begin{aligned} R_{\text{Bayes}} &= \mathbb{E}\left[\mathbb{I}\left(Y \neq \widehat{y}_{\text{Bayes}}(X)\right)\right] \\ R_{\text{1NN}} &= \mathbb{E}\left[\mathbb{I}\left(Y \neq \widehat{Y}_{\text{1NN}}(X)\right)\right] \end{aligned}$$

- As $n \to \infty$, we have the following powerful result

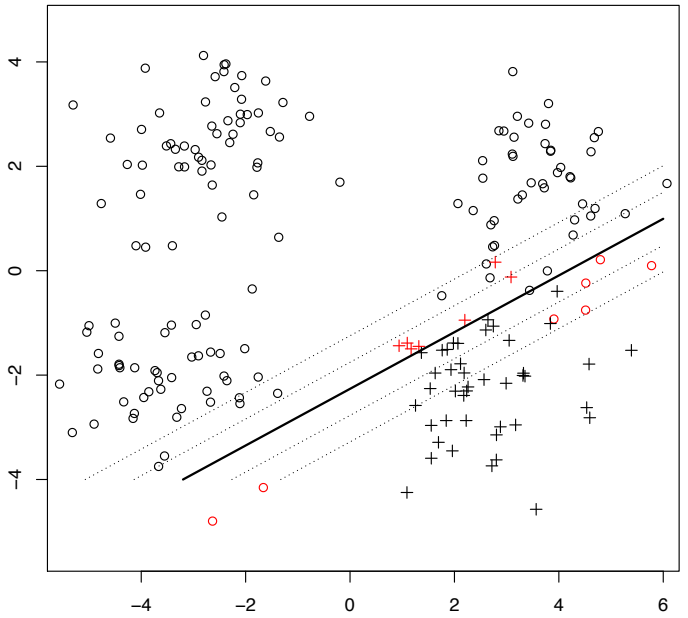
$$R_{\text{Bayes}} \leq R_{\text{1NN}} \leq 2R_{\text{Bayes}} - \frac{K}{K-1} R_{\text{Bayes}}^2.$$

K-Nearest Neighbours – Discussion

- kNN is sensitive to distances: normalize data and find suitable metric.
- Choice of k important: controls flexibility of model.
- Computational cost of kNN is very high.
  - Need to store **all** training data.
  - Need to compare each test data vector to **all** training data.
  - Need **a lot of data** in high dimensions.
- Mitigation techniques:
  - Compute approximate nearest neighbours, using kd-trees, cover trees, random forests.
  - Apply K-means to data in each class, to reduce size of data (need to use large K).

Non-linear Problems

- Linear methods (PCA, LDA, linear and logistic regression) are simple and effective techniques to learn from data “to first order”.
- To capture more intricate information from data, flexible, non-linear methods are often needed.
  - Explicit non-linear transformations $x \mapsto \phi(x)$.
  - Local methods like kNN.
- **Kernel methods**: introduce non-linearities through **implicit** non-linear transforms, often local in nature.



The Kernel Method

- Back to the soft-margin SVM. The dual objective is:

$$\max_{\lambda} \quad \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{n} \lambda_i \lambda_j y_i y_j \phi(x_i)^\top \phi(x_j) \quad \text{subject to} \quad \begin{cases} \sum_{i=1}^{n} \lambda_i y_i = 0 \\ 0 \preceq \lambda \preceq C \end{cases}$$

- Suppose $p = 2$, and we would like to introduce quadratic non-linearities,

$$\phi(x_i) = (1, \sqrt{2}x_{i1}, \sqrt{2}x_{i2}, x_{i1}^2, x_{i2}^2, x_{i1}x_{i2})^\top$$

  Then

$$\begin{aligned} \phi(x_i)^\top \phi(x_j) &= 1 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} + x_{i1}^2 x_{j1}^2 + x_{i2}^2 x_{j2}^2 + x_{i1}x_{i2}x_{j1}x_{j2} \\ &= (1 + x_i^\top x_j)^2 \end{aligned}$$

- Since only dot-products are needed in the objective function, non-linear transform need not be computed explicitly!
- Generally, m-order interactions can be implemented simply by $\phi(x_i)^\top \phi(x_j) = (1 + x_i^\top x_j)^m$. This is called a **polynomial kernel**.

The Kernel Method

- The **Gram matrix** is the matrix of dot-products, $B_{ij} = \phi(x_i)^\top \phi(x_j)$.

$$B = \begin{pmatrix} — \ \phi(x_1)^\top \ — \\ \vdots \\ — \ \phi(x_i)^\top \ — \\ \vdots \\ — \ \phi(x_n)^\top \ — \end{pmatrix} \times \begin{pmatrix} | & & | & & | \\ \phi(x_1) & \cdots & \phi(x_j) & \cdots & \phi(x_n) \\ | & & | & & | \end{pmatrix}$$

- Since $B = \Phi\Phi^\top$, it is symmetric and positive semidefinite.
- The Gram matrix is sufficient for training the soft-margin SVM.

$$\max_{\lambda} \quad \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{n} \lambda_i \lambda_j y_i y_j B_{ij} \qquad \text{subject to} \quad \begin{cases} \sum_{i=1}^{n} \lambda_i y_i = 0 \\ 0 \preceq \lambda \preceq C \end{cases}$$

The Kernel Method

- A **kernel** is a function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that:
  - Symmetric: $\kappa(x, x') = \kappa(x', x)$.
  - Positive semidefinite: given any finite set $\{x_i\}_{i=1}^n \subset \mathcal{X}$, the matrix $B \in \mathbb{R}^{n \times n}$ with entries $B_{ij} = \kappa(x_i, x_j)$ is positive definite. Equivalently, for any $c \in \mathbb{R}^n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \kappa(x_i, x_j) \geq 0$$

- **Mercer's Theorem**: if κ is continuous, symmetric and positive semidefinite, then there is a function $\phi : \mathcal{X} \to \mathcal{H}$ into a Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot, \rangle$ such that

$$\kappa(x, x') = \langle \phi(x), \phi(x') \rangle$$

The Kernel Method

$$\kappa(x, x') = \langle \phi(x), \phi(x') \rangle$$

- We do not need to compute the features ever—the Gram matrix is sufficient for learning and prediction. The discriminant function (absorbing a into b) is

$$g(x) = \sum_{i=1}^{n} \lambda_i^* y_i \phi(x_i)^\top \phi(x) = \sum_{i=1}^{n} \lambda_i^* y_i \kappa(x_i, x)$$

- The function ϕ can be interpreted as non-linear **features** of our data vectors $x \in \mathcal{X}$.
- Generally, the Hilbert space can be **infinite-dimensional**, so we are effectively computing an infinite number of features of our data, and learning a SVM based on all features.
- There are an infinite number of parameters in the SVM—a **nonparametric** method.
- The L_2 regularization of SVMs is very important to prevent overfitting.

Examples of Kernels

- Polynomial kernel:

$$\kappa(x, x') = (1 + x^\top x')^m$$

- **Gaussian, radial-basis function (RBF), or squared-exponential kernel**:

$$\kappa(x, x') = \exp\left(-\frac{1}{2}\|x - x'\|_M^2\right)$$

  This leads to a discriminant function of form

$$g(x) = \sum_{i=1}^{n} \lambda_i^* y_i \exp\left(-\frac{1}{2}\|x_i - x\|_M^2\right)$$

  A local method very similar to kNN.

- If κ_1 and κ_2 are both kernels, then so are kernels defined by

$$\kappa_3(x, x') = \kappa_1(x, x') + \kappa_2(x, x')$$
$$\kappa_4(x, x') = \kappa_1(x, x') \times \kappa_2(x, x')$$

Kernel SVM Demo

```
library(MASS)
library(e1071)
## load crabs data, project onto LD space, add noise.
data(crabs)
ct <- as.numeric(crabs[,1])-1+2*(as.numeric(crabs[,2])-1)
cb.lda <- lda(log(crabs[,4:8]),ct)
cb.ldp <- predict(cb.lda)
x <- as.matrix(cb.ldp$x[,1:2])
y <- as.numeric(crabs[,2])-1
x <- x + rnorm(dim(x)[1]*dim(x)[2])*1.5
gridsize <- 100
xlim   <- c(min(x[,1]),max(x[,1]))
ylim   <- c(min(x[,2]),max(x[,2]))
gridx1 <- seq(xlim[1],xlim[2],length=gridsize)
gridx2 <- seq(ylim[1],ylim[2],length=gridsize)
gridx  <- as.matrix(expand.grid(gridx1,gridx2))
gridn  <- dim(gridx)[1]
plot(x,pch=2*y+1,col=1,xlim=xlim,ylim=ylim)

n      <- length(y)
p      <- dim(x)[2]
i      <- sample(rep(c(TRUE,FALSE),each=n/2),n,replace=FALSE)
train  <- (1:n)[i]
test   <- (1:n)[!i]
trainx <- x[train,]
trainy <- y[train]
testx  <- x[test,]
testy  <- y[test]

svmdemo <- function(kernel,gamma=1,coef0=0,cost=1,degree=3) {
  model <- svm(trainx,trainy,kernel=kernel,gamma=gamma,coef0=coef0,degree=degree,cost=cost)
  gridp <- predict(model,gridx)
  predy <- as.numeric(predict(model,testx)>.5)

  plot(trainx[,1],trainx[,2],pch=trainy*3+1,col=4,lwd=.5,xlim=xlim,ylim=ylim)
  points(testx[,1],testx[,2],pch=testy*3+1,col=2+(predy==testy),lwd=3)
  contour(gridx1,gridx2,matrix(gridp,gridsize,gridsize),levels=seq(.1,.9,.1),lwd=.5,add=TRUE)
  contour(gridx1,gridx2,matrix(gridp,gridsize,gridsize),levels=c(.5),lwd=2,add=TRUE)
}
```

Kernel Methods – Discussion

- The kernel method allows for very flexible and powerful machine learning models.
- Kernels can be defined over much more complex structures than vectors, e.g. graphs, strings.
- Can be hard to interpret.
- $O(n^3)$ computation and $O(n^2)$ memory cost can be prohibitive.
- Further readings:
  - Bishop, Chapter 6.
  - Christopher Burgess, A Tutorial on Support Vector Machines for Pattern Recognition. 1998.
  - Rasmussen and Williams, Gaussian Processes for Machine Learning. 2006.