ML Supervised Learning 7 by ambedkar@IISc

- Support Vector Machines
- Kernel Methods

Prelude to Support Vector Machines

Where are we? The story so far

- Gradient descent for logistic regression
- Bottleneck: each iteration required the whole data
- Approximation: just use a batch of data to calculate the gradient
- Batch size one leads to mistake driven learning which is nothing but Perceptron that was developed in 60s
- Perceptron is useful for only linearly seperable data

What if the data is not linearly separable?

Yes! In practice, most often the data is not linearly separable. Then

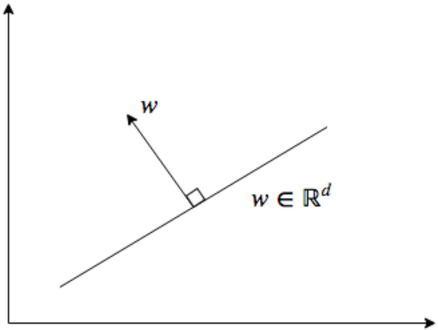
- Make linearly separable using kernel methods.
- (Or) Use multilayer perceptron.

What are all these?

- The first leads to Support Vector Machines, that rules machine learning for decades
- The second one leads to Deep Learning!

Hyperplanes

- Separates a D-dimensional space into two half spaces (positive and negative).
- $w \in \mathbb{R}^D$ is a normal vector pointing towards positive half.



- Equation of the hyperplane is $w^T x = 0$
- If hyperplane does not pass through origin, we add bias $b \in \mathbb{R}$

$$w^T x + b = 0$$

$b > 0$: moving it parallely along w

$b < 0$: opposite direction

Hyperplane based Classifiers

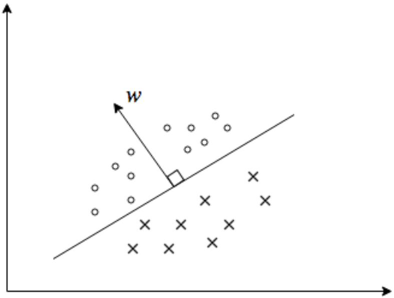
Classification rule

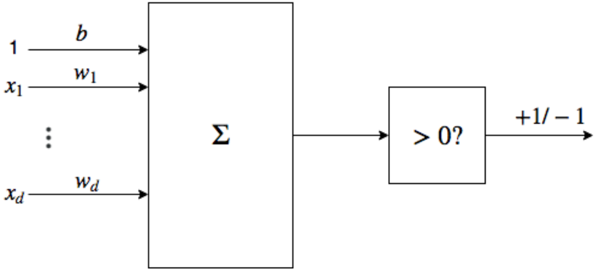
$$y = \mathrm{sign}(w^T x + b)$$

i.e.

$$w^T x + b > 0 \implies y = +1$$

$$w^T x + b < 0 \implies y = -1$$





What is the best hyperplane for a classification task

- Suppose we have several choices of classifiers, which is the most promising one?
  - promising. . . from the point view of learning
  - learning. . . means that has a better generalizing capacity
- Support vector machine provides an answer to this

Loss Function for Hyperplane based Classifiers

- The loss function for hyperplane based classifiers

$$\begin{aligned}\mathcal{L}(w, b) &= \sum_{n=1}^{N} l_n(w, b) \\ &= \sum_{n=1}^{N} \max\{0, -y_n(w^T x_n + b)\}\end{aligned}$$

  - If $y_n(w^T x_n + b) > 0$ then w, b predicts y_n correctly hence $l_n(w, b) = 0$
  - If $y_n(w^T x_n + b) < 0$ then w, b predicts y_n incorrectly hence $l_n(w, b) \neq 0$

Stochastic Gradients

- We are going to calculate gradients for l_n not $\mathcal{L}$. (Hence stochastic)

$$\frac{\partial l_n(w,b)}{\partial w} = \begin{cases} -y_n x_n \text{ when } w, b \text{ make a mistake} \\ 0 \text{ otherwise} \end{cases}$$

$$\frac{\partial l_n(w,b)}{\partial b} = \begin{cases} -y_n \text{ when } w, b \text{ make a mistake} \\ 0 \text{ otherwise} \end{cases}$$

- For every mistake, update rule is

$$w_{\text{new}} = w_{\text{old}} + y_n x_n$$
$$b_{\text{new}} = b_{\text{new}} + y_n$$

(Assuming the learning rate is 1.)

Perceptron Algorithm

Given training data: $\{(x_1, y_1), \ldots, (x_N, y_N)\}$
Initialize $w_{old} = \{0, \ldots, 0\}, b_{old} = 0$
Repeat until convergence

- For a random data sample (x_n, y_n)
- If $y_n(w^T x_n + b) \leq 0$ (or $sign(w^T x_n + b) \neq y_n$, i.e. mistake mode)

$$w_{new} = w_{old} + y_n x_n$$
$$b_{new} = b_{old} + y_n$$

Some Final Remarks

- If exists, perceptron finds one of many hyperplanes.
- Of many choices which is the best? : Hyperplane having maximum margin?
- Large margin leads to good generalization on the data.

Support Vector Machines

A bit of history[1]

- Pre 1980
  - Almost all learning methods learned linear decision surfaces
  - Linear learning methods have nice theoretical properties
- 1980's
  - Decision trees and Neural Networks allowed efficient learning of non linear decision surfaces
  - Little theoretical basis and all suffer from local minima
- 1990's
  - Efficient learning algorithms for nonlinear functions based on computational learning theory
  - Nice theoretical properties

[1] Slide credit R. Berwick

- SVM is a hyperplane based classifier
  - That means that our model is linear
  - Later we see how cleverly we can bring in nonlinearity
- Prediction rule $y = \mathrm{sign}(w^T x + b)$
- **Aim**: Given training data $\{(x_1, y_1), \ldots (x_n, y_n)\}$, build a "good" classifier
- **Trick**: Learn w and b such that *achieves maximum margin*

Distance from a point to a line

- Consider a two dimensional case
- For $a, b, c \in \mathbb{R}$, $ax + by + c = 0$ defines a line in two dimensional plane.
- Let (x_0, y_0) be any point then

$$\text{Distance}(ax + by + c = 0, (x_0, y_0)) = \frac{|ax_0 + by_0 + c|}{\sqrt{a^2 + b^2}}$$

Margins

- Let $w^T x + b = 0$ be a hyperplane in $\mathbb{R}^D$.
- Geometric margin is a distance

$$r_n = r_n(w^T x + b = 0, x_n) = \frac{|w^T x_n + b|}{\|w\|}$$

  Since margin is completely determined by w, we write

$$r_n = r_n(w, x_n) = \frac{|w^T x_n + b|}{\|w\|}$$

- Given a set of points $x_1, x_2, \ldots, x_N$, margin w.r.t. w is

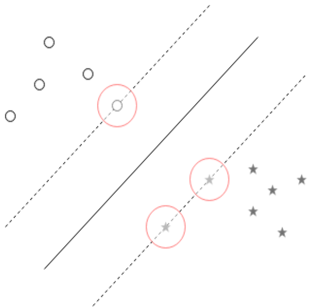
$$r = \min_{1 \leq n \leq N} |r_n| = \min_{1 \leq n \leq N} \frac{|w^T x + b|}{\|w\|}$$

Margins (contd. . .)

- Functional margin of w on a training sample (x_n, y_n) is defined as

$$f(w,(x_n,y_n)) = y_n(w^T x + b)$$
$$= \begin{cases} \text{positive if } w \text{ predicts } y_n \text{ correctly} \\ \text{negative if } w \text{ predicts } y_n \text{ incorrectly} \end{cases}$$

The points in the red circles are called support vectors.



Objective

- Let us consider two class classification problem with class labels $+1$ and -1
- We have the following perceptron objective

$$w^T x_n + b \geq 0 \implies y_n = +1$$

$$w^T x_n + b \leq 0 \implies y_n = -1$$

- We slightly modify our objective

$$w^T x_n + b \geq 1 \implies y_n = +1$$

$$w^T x_n + b \leq -1 \implies y_n = -1$$

Objective (cont. . .)

One can see that

$$w^T x_n + b \geq 1 \implies y_n = +1$$
$$w^T x_n + b \leq -1 \implies y_n = -1$$

$$\Downarrow$$

$$y_n(w^T x_n + b) \geq 1$$
$$\Rightarrow \min_{1 \leq n \leq N} |w^T x_n + b| = 1$$

Margin

- Given a set of points $x_1, x_2, \ldots, x_N$, margin w.r.t. w is

$$\gamma(w,b) = \min_{1 \le n \le N} |r_n| = \min_{1 \le n \le N} \frac{|w^T x + b|}{||w||}$$

- Now since we have

$$\min_{1 \le n \le N} |w^T x_n + b| = 1$$

- We get

$$\gamma(w,b) = \min_{1 \le n \le N} \frac{|w^T x_n + b|}{||w||} = \frac{1}{||w||}$$

Optimization Problem

Maximizing the margin

$$\gamma(w, b) = \frac{1}{||w||}$$

$$\Downarrow$$

Minimizing $||w||$

Optimization Problems:

$$\text{minimize } f(w, b) = \frac{||w||^2}{2}$$

$$\text{subject to } y_n(w^T x_n + b) \geq 1$$

which is a quadratic program with N linearity constraints.

Optimization Problem (cont. . .)

Data: $\{(x_1, y_1), \ldots (x_N, y_N)\}$

Modal: $w^T x + b = 0$

Parameters: w a D-dimensional vector and b a number

Optimization Problem:

$$\text{minimize } f(w, b) = \frac{||w||^2}{2}$$

$$\text{subject to } y_n(w^T x_n + b) \geq 1$$

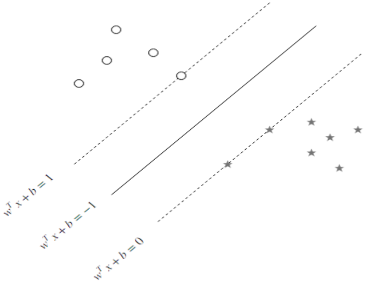
which is a quadratic program with N linearity constraints.

Why a large margin implies good generalization?

- In SVM we have $\gamma \propto \frac{1}{||w||}$. That is margin is proportional to $\frac{1}{||w||}$
- Large margin $\Rightarrow$ small $||w||$ $i.e$ small ℓ_2 norm.
- Small $||w|| \Rightarrow$ regularized solution i.e w_i does not become too big anumber
- Generalizes very well on the test data.

Hard SVM

Assumption: Every training example need to fulfill the margin condition i.e $y_n(w^T x_n + b) \geq 1$



Objective:

$$\min_{w,b} f(w,b) = \frac{||w||^2}{2}$$

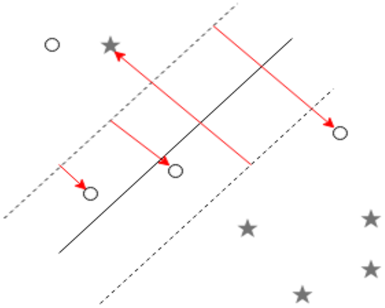
subject to $y_n(w^T x_n + b) \geq 1, \qquad n = 1, 2, \ldots N$

Soft Margin

Allow some training examples

- fall within the margin
- misclassified (i.e fall on the wrong side)

ζ (slack) : distance by which it violates the margin



Case 1 : $\zeta_n < 1$: x_n violates the margin but on the right side.
Case 2: $\zeta_n > 0$: x_n not only violates the margin but totally on the wrong side.

In the case data satisfies

$$y_n(w^T x_n + b) \geq 1 - \zeta_n, \qquad \zeta_n > 0$$

Goal: Not only maximize margins but also minimize the sum of slacks.

Objective: The principle objective is

$$\min_{w,b,\zeta} f(w, b, \zeta) = \frac{||w||^2}{2} + c \sum_{n=1}^{N} \zeta_n$$

subject to $y_n(w^T x_n + b) \geq 1 - \zeta_n, \qquad \zeta_n \geq 0$

This is also convex objective function which is a quadratic program (QP) with $2N$ inequality constraints.

Diversion: Solving constrained optimization problems

Consider the following optimization problem

$$\min_w f(w)$$

subject to

$$\begin{aligned} g_n(w) &\leq 0, \qquad & n = 1, 2, \ldots, N \\ h_m(w) &= 0, \qquad & m = 1, 2, \ldots, M \end{aligned}$$

- Constrained optimization problems are difficult to solve
- So we will introduce non-negative lagrange multipliers

  $$\alpha = \{\alpha_n\}_{n=1}^{N} \text{and } \beta = \{\beta_n\}_{n=1}^{M}$$

  one for each constraints
- Lagrangian:
  $\mathscr{L}(w, \alpha, \beta) = f(w) + \sum_{n=1}^{N} \alpha_n g_n(x) + \sum_{m=1}^{M} \beta_m h_m(x)$

Diversion: Solving constrained optimization problem (contd. . .

Let $\mathscr{L}_p(w) = \max_{\alpha,\beta} \mathscr{L}(w, \alpha, \beta)$

- $\mathscr{L}_p(w) = \infty$ if w violates any of the constraints
- $\mathscr{L}_p(w) = f(w)$ if w satisfies all the constraints

$$\Rightarrow \min_w \mathscr{L}_p(w) = \min_w \max_{\alpha,\beta} \mathscr{L}(w, \alpha, \beta)$$

Further if f, g, h are convex then

$$\min_w \max_{\alpha,\beta} \mathscr{L}(w, \alpha, \beta) = \max_{\alpha,\beta} \min_w \mathscr{L}(w, \alpha, \beta)$$

KKT Condition: At optimal solution

$$\alpha_n g_n(w) = 0 \text{ and } \beta_m h_m(w) = 0$$

Solving hard margin SVM

- We have the following hard margin SVM

$$\min_{w,b} f(w,b) = \frac{||w||^2}{2}$$

$$\text{subject to } 1 - y_n(w^T x_n + b) \le 0, n = 1, 2, \ldots, N$$

- Lagrangian can be written as

$$\min_{w,b} \max_{\alpha \ge 0} \mathscr{L}(w, b, \alpha)$$

$$= \frac{||w||^2}{2} + \sum_{n=1}^{N} \alpha_n (1 - y_n(w^T x_n + b))$$

- We can solve this by solving the dual problem (Eliminate w and b and solve for dual variables)

Solving hard margin SVM (contd...)

- Derivative of lagragian w.r.t w

$$\frac{\delta \mathscr{L}}{\delta w} = w - \sum_{n=1}^{N} \alpha_n y_n x_n = 0$$

$$\Rightarrow w = \sum_{n=1}^{N} \alpha_n y_n x_n$$

- Derivative of lagragian w.r.t b

$$\frac{\delta \mathscr{L}}{\delta b} = \sum_{n=1}^{N} \alpha_n y_n = 0$$

- Now we substitute $w = \sum_{n=1}^{N} \alpha_n y_n x_n$ in lagragian and also we use $\sum_{n=1}^{N} \alpha_n y_n = 0$

Solving hard margin SVM (contd. . .)

$$
\begin{aligned}
\max_{\alpha \geq 0} \mathscr{L}_D(\alpha) &= \frac{1}{2}(\sum_{n=1}^{N} \alpha_n y_n x_n)^T (\sum_{n=1}^{N} \alpha_n y_n x_n) \\
&\quad + \sum_{n=1}^{N} \alpha_n [1 - y_n(\sum_{m=1}^{N} \alpha_m y_m x_m)^T x_n + b y_n] \\
&= \frac{1}{2}(\sum_{n=1}^{N} \alpha_n y_n x_n^T)(\sum_{m=1}^{N} \alpha_m y_m x_m) \\
&\quad + \sum_{n=1}^{N} \alpha_n - \sum_{n=1}^{N} \alpha_n y_n (\sum_{m=1}^{N} \alpha_m y_m x_m^T) x_n \\
&\quad + b \sum_{n=1}^{N} \alpha_n y_n
\end{aligned}
$$

$$\max_{\alpha \geq 0} \mathscr{L}_D(\alpha) = \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m x_n^T x_m + \sum_{n=1}^{N} \alpha_n$$

$$- \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m x_n^T x_m$$

$$= \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m x_n^T x_m$$

$$\text{such that } \sum_{n=1}^{N} \alpha_n y_n = 0$$

Let $G_{mn} = y_m y_n x_m^T x_n$ a $n \times n$ matrix
Then the optimization problem is :

$$\max_{\alpha \geq 0} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2}\alpha^T G \alpha \qquad s.t \sum_{n=1}^{N} \alpha_n y_n = 0$$

Solving hard margin SVM (contd...)

- We have a maximization of a concave function. (because Hessian of G is p.s.d)
- Note that the original primal SVM objective is also convex
- The input x appear as inner product have one can apply something called "kernel trick".
- On solving dual optimization problem We can treat the objective on a quadratic program and by running QP solver like quadprog, CPLE etc.

Solving hard margin SVM (contd...)

- once we solve for α_n, w and b can be computed :

$$w = \sum_{n=1}^{N} \alpha_n y_n x_n$$

$$b = -\frac{1}{2}(\min_{x:y_n=\pm 1} w^T x_n + \max_{x:y_n=-1} w^T x_n)$$

- most $\alpha_n{}'s$ will be zero.
  - $\alpha_n \neq 0$ only if x_n lies on one of the two margin boundaries

    i.e $y_n(w^T x_n + b) = 1$

  - These one called support vectors.

Solving soft margin SVM

- Optimization problems:

$$\min_{w,b,\zeta} f(w,b,\zeta) = \frac{||w||^2}{2} + c\sum_{n=1}^{N} \zeta_n$$

$$\text{subject to } 1 \le y_n(w^T x_n + b) + \zeta_n, \qquad \zeta_n \ge 0$$

$$n = 1, 2, \ldots, N$$

- By introducing lagrange multiplier

$$\min_{w,b,\zeta} \max_{\alpha\ge 0,\beta\ge 0} \mathscr{L}(w,b,\zeta,\alpha,\beta)$$

$$= \frac{||w||^2}{2} + c\sum_{n=1}^{N} \zeta_n + \sum_{n=1}^{N} \alpha_n(1 - y_n(w^T x_n + b) - \zeta_n) - \sum_{n=1}^{N} \beta_n \zeta_n$$

Solving soft margin SVM (contd. . .)

- Next step is to eliminate the primal variables w, b, ζ to get dual problem containing dual variable

$$\frac{\delta \mathscr{L}}{\delta w} = 0 \Rightarrow w = \sum_{n=1}^{N} \alpha_n y_n x_n$$

$$\frac{\delta \mathscr{L}}{\delta b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\frac{\delta \mathscr{L}}{\delta \zeta_n} = 0 \Rightarrow c - \alpha_n - \beta_n = 0$$

Solving soft margin SVM (contd . . .)

- This gives

$$\max_{\alpha \le C, \beta \ge 0} \mathscr{L}_D(\alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (x_m^T x_n)$$

$$\text{such that} \sum_{n=1}^{N} \alpha_n y_n = 0$$

(Note dual variable β does not appear)

$$\Rightarrow \max_{\alpha \le C} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2} \alpha^T G \alpha \qquad s.t \sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\text{where } G_{mn} = y_m y_n x_m^T x_n \text{ a NxN matrix}$$

- **Note:**
  - $\alpha' s$ are again sparse
  - Nonzero $\alpha_n' s$ corresponds to the support vector.

The Nature of support vectors

- Hard Margin SVM : It has only one type of support vectors.
  - Lying on the margin boundaries

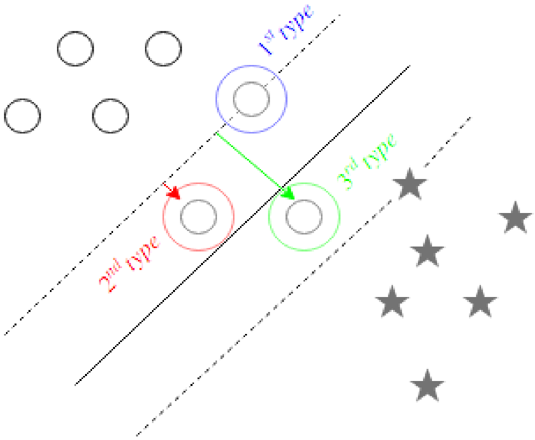
$$w^T x + b = -1 \text{and } w^T x + b = +1$$

- Soft Margin SVM : Three types of support vectors
  - Lying on the margin boundaries

$$w^T x + b = -1 \text{ and } w^T x + b = +1 (\zeta = 0)$$

  - Lying within the margin region $(0 < \zeta_n < 1)$ but still on the correct side.
  - Lying on the wrong side of the hyperplane $(\zeta_n \geq 1)$

The nature of support types



The nature of support types

SVM via Dual Formulation

Hard Margin SVM

$$\max_{\alpha \geq 0} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2}\alpha^T G \alpha \qquad \text{s.t } \sum_{n=1}^{N} \alpha_n y_n = 0$$

Soft margin SVM

$$\max_{\alpha \leq C} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2}\alpha^T G \alpha \qquad \text{s.t } \sum_{n=1}^{N} \alpha_n y_n = 0$$

Advantages of Dual Formulation:

- The dual problem has only one constraint that is non trivial $(\sum_{n=1}^{N} \alpha_n y_n = 0)$
  The original primal formulation of SVM has many more (N-number of training examples)
- Allow non linear separator by replacing the linear product by kernalized similarities.

Drawbacks of Dual Formulation

- Dual formulation can be expensive if N (The size of the data) is very large $\Rightarrow$ Have to solve for N variables $\alpha = [\alpha_1, \ldots, \alpha_N]$
- Need to store an $N \times N$ matrix G

Loss functions in hyperplane based classifier

- Perceptron Loss: $l(w,b) = \sum_{n=1}^{N} l_n(w,b)$

$$= \sum_{n=1}^{N} \max\{0, -y_n(w^T x_n + b)\}$$

- SVM Loss: For each training sample we need

$$y_n(w^T x_n + b) \geq 1 - \zeta_n$$

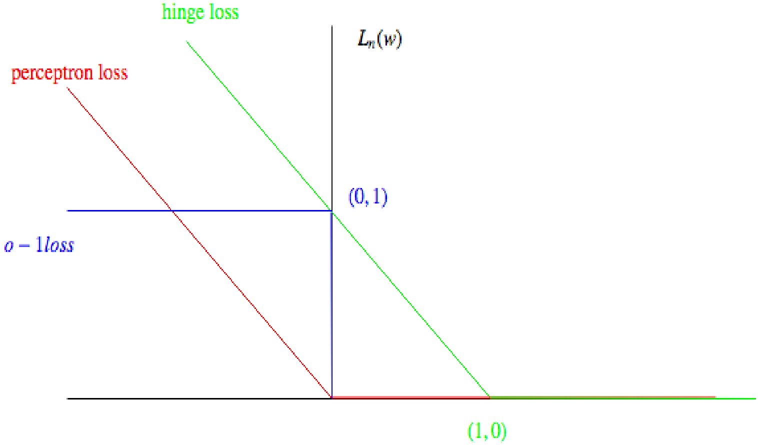
$$Loss = \text{Sum of slacks}$$

$$= \sum_{n=1}^{N} l_n(w,b)$$

$$= \sum_{n=1}^{N} \zeta_n$$

$$= \sum_{n=1}^{N} \max\{0, 1 - y_n(w^T x_n + b)\}$$

Loss Functions in hyperplane based classifier



Loss functions

Recall SVMs

Objective

- Let us consider two class classification problem with class labels $+1$ and -1
- We have the following perceptron objective

$$w^T x_n + b \geq 0 \implies y_n = +1$$

$$w^T x_n + b \leq 0 \implies y_n = -1$$

- We slightly modify our objective

$$w^T x_n + b \geq 1 \implies y_n = +1$$

$$w^T x_n + b \leq -1 \implies y_n = -1$$

Data: $\{(x_1, y_1), \ldots (x_N, y_N)\}$

Modal: $w^T x + b = 0$

Parameters: w a d-dimensional vector and b a number

Optimization Problem:

$$\text{minimize } f(w, b) = \frac{||w||^2}{2}$$

$$\text{subject to } y_n(w^T x_n + b) \geq 1$$

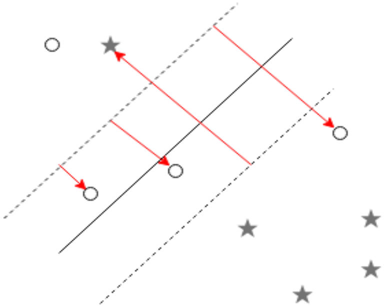
which is a quadratic program with N linearity constraints.

Soft Margin

Allow some training examples

- fall within the margin
- misclassified (i.e fall on the wrong side)

ζ : slack : Distance by which it violates the margin



Case 1 : $\zeta_n < 1$: x_n violates the margin but on the right side.
Case 2: $\zeta_n > 0$: x_n not only violates the margin but totally on the wrong side.

Soft SVM (contd . . .)

In the case data satisfies

$$y_n(w^T x_n + b) \geq 1 - \zeta_n, \qquad \zeta_n > 0$$

Goal: Not only maximize margins but also minimize the sum of slacks.

Objective: The principle objective is

$$\min_{w,b,\zeta} f(w,b,\zeta) = \frac{||w||^2}{2} + c\sum_{n=1}^{N} \zeta_n$$

subject to $y_n(w^T x_n + b) \geq 1 - \zeta_n, \qquad \zeta_n \geq 0$

This is also convex objective function which is a quadratic program (QP) with $2N$ inequality constraints.

Solving soft margin SVM (contd . . .)

- This gives

$$\max_{\alpha \le C, \beta \ge 0} \mathscr{L}_D(\alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (x_m^T x_n)$$

$$\text{such that} \sum_{n=1}^{N} \alpha_n y_n = 0$$

(Note dual variable β does not appear)

$$\Rightarrow \max_{\alpha \le C} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2} \alpha^T G \alpha \qquad s.t \sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\text{where } G_{mn} = y_m y_n x_m^T x_n \text{ a NxN matrix}$$

- **Note:**
  - $\alpha' s$ are again sparse
  - Nonzero $\alpha_n' s$ corresponds to the support vector.

Kernel Methods

The notion of Similarity and Distance

- Consider a d dimensional real space $\mathbb{R}^d$
- Consider two points $x = (x_1, \ldots, x_d)$ and $y = (y_1, \ldots, y_d)$
- When do we say the point x is similar to point y or how do we measure the similarity between x and y
- What is the distance between x and y

Linear models depend on "linear" notion of similarity and distance

$$\text{similarity}(x_n, x_m) = x_n^T x_m$$

$$\text{Distance}(x_n, x_m) = (x_n - x_m)^T (x_n - x_m)$$

Going from one space to another

Use feature mapping function ϕ to map data to new space (usually high dimensional) where the original learning problem becomes easy i.e

$$\phi : \mathbb{X} \rightarrow \mathbb{F}$$

$\mathbb{X}$: space that the original data lies

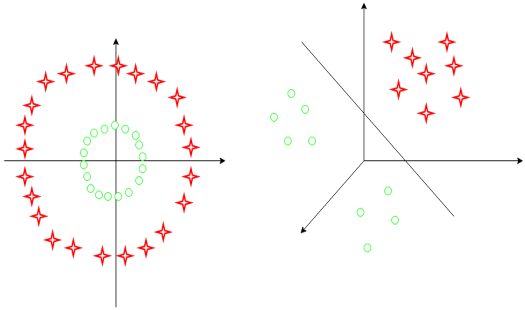
$\mathbb{F}$: some high dimensional space

Feature Mappings

Consider the following mapping

$$\phi : \mathbb{R}^2 \to \mathbb{R}^3$$

$$(x_1, x_2) \to (x_1^2, \sqrt{2}x_1x_2, x_2^2) = (z_1, z_2, z_3)$$



Cover's Theorem on the Seperability of Patterns

By Thomas Cover, 1965

A complex pattern-classification problem, cast in a high-dimensional space nonlinearly, is more likely to be linearly seperable than in a low-dimensional space, provided that the space is not densely populated

- This motivates use of nonlinear kernels in various machine learning methods.
- Kernel methods dominated ML for many years.

Thomas Cover was an information theoretist

What could be the problem with the mappings?

- Constructing these mappings can be expensive, specially when the new space is high dimension.
- Storing and using the mappings in later computation can be way expensive.
- Kernels side-step these issues by defining on "implicit" feature map.

Kernel : Example

Consider $x = (x_1, x_2) \in \mathbb{R}^2$, $z = (z_1, z_2) \in \mathbb{R}^2$

Define a function

$$
\begin{aligned}
K : \mathbb{R}^2 \times \mathbb{R}^2 &\to \mathbb{R} \\
K(x, z) &= (x^T z)^2 \\
&= (x_1 z_1 + x_2 z_2)^2 \\
&= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 \\
&= (x_1^2, \sqrt{2} x_1 x_2, x_2^2)(z_1^2, \sqrt{2} z_1 z_2, z_2^2) \\
&= \phi(x)^T \phi(z)
\end{aligned}
$$

We have

$$
\begin{aligned}
K : \mathbb{R}^2 \times \mathbb{R}^2 &\to \mathbb{R} \\
K(x, z) &= (x^T z)^2 \\
&= \phi(x)^T \phi(z)
\end{aligned}
$$

K implicitly defines a mappings ϕ to a higher dimensional space $\phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$ and computes inner product based similarity $\phi(x)^T\phi(x)$ in that space

- We did not need to predefine/compute the mapping ϕ to compute $K(x, z)$
- The function K is known as the kernel function
- Evaluating K is almost as fast as computing inner product.
- Any kernel function K implicitly defines an associated feature mapping ϕ

Kernel : Definition

Feature mapping:

$$\phi : \mathcal{X} \to \mathcal{F}$$

Kernel function:

$$K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

$$(x, z) \to \phi(x)^T \phi(z)$$

Note: Not every K with $K(x, z) = \phi(x)^T \phi(z)$, for some ϕ is not a kernel. K needs to satisfy Mercer's condition

Mercer Condition

- K is symmetric and positive semidefinite

  $$\Downarrow$$

  K must define a dot product for some higher space $\mathcal{F}$

- The function K is p.s.d if

  $$\int\int f(x)K(x,z)f(z)\mathrm{d}x\mathrm{d}z \geq 0$$

  for every function f that is square integral i.e

  $$\int f(x)\mathrm{d}x < \infty$$

Algebraic operations on Kernels

$$K(x,z) = K_1(x,z) + K_2(x,z)$$
$$K(x,z) = \alpha K_1(x,z)$$
$$K(x,z) = K_1(x,z)K_2(x,z)$$

Examples of Kernels

- Linear kernel : $K(x,z) = x^T z$
- Quadratic kernel : $K(x,z) = (x^T z)^2$ or $(1 + x^T z)^2$
- Polynomial kernel : $K(x,z) = (x^T z)^d$ or $(1 + x^T z)^d$
- Radial basis function(RBF) : $K(x,z) = \exp(-r||x-z||^2)$

Kernel Matrix

Given the data $\{x_1, x_2, \ldots, x_N\}$, where $x_n \in \mathcal{X}$, $n = 1, 2, \ldots N$, kernel K is a function

$$K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$
$$K(x_i, x_j) \mapsto \phi(x_i)^T \phi(x_j)$$

that defines a $N \times N$ matrix K as

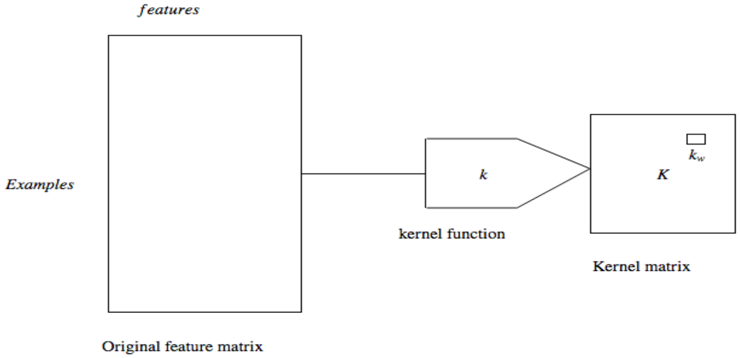
$$K_{ij} = K(x_i, x_j)$$

which gives similarity between i^{th} and j^{th} example in the feature space $\mathcal{F}$.

Important Properties of Kernel Matrix

- The matrix K is
  - Symmetric i.e. $K = K^T$
  - Positive definite i.e $z^T K z > 0, \qquad \forall z \in \mathbb{R}^N$
    $\Rightarrow$ all eigenvalues are positive.

Kernel Matrix (contd. . .)



Kernel matrix

On using kernels

- Kernels can turn linear models to nonlinear models. In any model during training and test if input appear as $x_i^T x_j$ then these models can be kernalised by replacing $x_i^T x_j$ with $\phi(x_i^T)\phi(x_j) = K(x_i, x_j)$
- The following learning algorithm can be kernalized
  - Distance based methods, Perceptron, SVM, linear regression.
  - Many unsupervised learning algorithms like k-means clustering, PCA.

Kernalized SVM training

- The soft margin SVM dual problem is

$$\max_{\alpha \leq C} \mathscr{L}_D(\alpha) = \alpha^T 1 - \frac{1}{2}\alpha^T G \alpha \qquad s.t \sum_{n=1}^{N} \alpha_n y_n = 0$$

  -

$$G_{mm} = y_m y_n x_m^T x_n = y_m y_n K_{mn}$$

  - we can replace the inner product with a kernel function as

$$K_{mn} = K(x_m, x_n) = \phi(x_m)^T \phi(x_n)$$

- Now SVM learn a linear separator in the kernel induced feature space $\mathbb{F}$, which is a nonlinear separators in the original space.

Kernalized SVM training (contd...)

- For a new test sample x

$$y = \text{sign}(w^T x) = \text{sign}\left(\sum_{n=1}^{N} \alpha_n y_n x_n^T x\right)$$
$$= \text{sign}\left(\sum_{n=1}^{N} \alpha_n y_n K(x_n, x)\right)$$

- The SVM weight vectors is

$$w = \sum_{n=1}^{N} \alpha_n y_n \phi(x_n) = \sum_{n=1}^{N} \alpha_n y_n K(x_n, .)$$

- Note w can be explicitly computed and stored only if the feature map ϕ of K can be explicitly written i.e K can be written as

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

which is not always possible.

kernel Ridge regression

Ridge repgression problem

$$w = arg \min_{w} \sum_{n=1}^{N} (y_n - w^T x_n)^2 + \lambda w^T w$$

The solution is

$$w = \left(\sum_{n=1}^{N} x_n x_n^T + \lambda I_d \right) \left(\sum_{n=1}^{N} y_n x_n \right) = (X^T X + \lambda I_d)^{-1} X^T Y \qquad X =$$

Kernel Ridge regression (contd. . .)

Matrix Identity: We use the following identity from the matrix algebra

$$(B^T R^{-1} B + P^{-1})^{-1} B^T R^{-1} = P B^T (B P B^T + R)^{-1}$$

Substitute the following

$$R = I_N$$

$$B = X$$

$$P = I_D$$

Kernel Ridge regression (contd...)

We get

$$\begin{aligned} w &= X^T(XX^T + \lambda I_n)^{-1}y \\ &= X^T\alpha \\ &= \sum_{n=1}^{N} \alpha_n x_n \end{aligned}$$

where

$$\alpha = (XX^T + \lambda I_n)^{-1}y = (K + \lambda I_N)^{-1}y$$

$$K_{nm} = x_n^T x_m \Rightarrow K = XX^T$$

Here α is a vector of dual variables with dimension N

Kernel Ridge regression (contd...)

Now we kernalize the model.

$$w = \sum_{n=1}^{N} \alpha_n \phi(x_n)$$
$$= \sum_{n=1}^{N} \alpha_n K(x_n, .)$$

where

$$\alpha = (K + \lambda I_N)^{-1} y$$

We have

$$K_{nm} = \phi(x_n)^T \phi(x_m)$$
$$= K(x_n, x_m)$$

Kernel Ridge regression (contd . . .)

For a test input x, predict the output y as

$$y = w^T \phi(x) = \sum_{n=1}^{N} \alpha_n \phi(x_n)^T \phi(x)$$
$$= \sum_{n=1}^{N} \alpha_n K(x_n, x)$$

Learning from kernels: Some remarks

- RBF kernel works well in practice.
- Hyperparameters of the kernel may need to be tuned via cross validation
- There are approaches that use multiple kernel which called "Multiple kernel learning".

On kernels and Feature learning

Let $x_1, x_2, \ldots, x_N$ be given data in $\mathbb{R}^D$. Then Gram matrix is defined as

$$K = \begin{bmatrix} K(x_1, x_1) & K(x_1, x_2) & \ldots & K(x_1, x_N) \\ K(x_2, x_1) & K(x_2, x_2) & \ldots & K(x_2, x_N) \\ & & & \\ & & & \\ K(x_N, x_1) & K(x_N, x_2) & \ldots & K(x_N, x_N) \end{bmatrix}$$

For any x_n define the following N-dim vectors:

$$\begin{aligned} \psi(x_n) &= K(x_n, .) \\ &= (K(x_n, x_1), K(x_n, x_2), \ldots, K(x_n, x_N)) \end{aligned}$$

- $\psi(x_n)$ can be considered as the new feature representation of x_n
- Each feature represents similarity of x_n with other inputs.