Soft-margin SVM, SMO Algorithm, Decision Trees

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Kernel Linear Regression

When dimensionality of input is D, one step of SGD takes $\mathcal{O}(D^3)$.

Surprisingly, we can do better under some circumstances. We start by noting that we can write the parameters $\boldsymbol{w}$ as a linear combination of the input features $\varphi(\boldsymbol{x}_i)$.

By induction, $\boldsymbol{w} = 0 = \sum_i 0 \cdot \varphi(\boldsymbol{x}_i)$, and assuming $\boldsymbol{w} = \sum_i \beta_i \cdot \varphi(\boldsymbol{x}_i)$, after a SGD update we get

$$\begin{aligned}\boldsymbol{w} &\leftarrow \boldsymbol{w} + \alpha \sum_i \big(t_i - \boldsymbol{w}^T \varphi(\boldsymbol{x}_i)\big)\varphi(\boldsymbol{x}_i) \\ &= \sum_i \Big(\beta_i + \alpha\big(t_i - \boldsymbol{w}^T \varphi(\boldsymbol{x}_i)\big)\Big)\varphi(\boldsymbol{x}_i).\end{aligned}$$

A individual update is $\beta_i \leftarrow \beta_i + \alpha\Big(t_i - \boldsymbol{w}^T \varphi(\boldsymbol{x}_i)\Big)$, and substituting for $\boldsymbol{w}$ we get

$$\beta_i \leftarrow \beta_i + \alpha\Big(t_i - \sum\nolimits_j \beta_j \varphi(\boldsymbol{x}_j)^T \varphi(\boldsymbol{x}_i)\Big).$$

Kernel Linear Regression

We can formulate the alternative linear regression algorithm (it would be called a *dual formulation*):

Input: Dataset ($\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \mathbb{R}^N$), learning rate $\alpha \in \mathbb{R}^+$.

- Set $\beta_i \leftarrow 0$
- Compute all values $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \varphi(\boldsymbol{x}_i)^T \varphi(\boldsymbol{x}_j)$
- Repeat
  - Update the coordinates, either according to a full gradient update:
    - $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} + \alpha(\boldsymbol{t} - K\boldsymbol{\beta})$
  - or alternatively use single-batch SGD, arriving at:
    - for i in random permutation of $\{1, \ldots, N\}$:
      - $\beta_i \leftarrow \beta_i + \alpha\Big(t_i - \sum_j \beta_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)\Big)$

    In vector notation, we can write $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} + \alpha(\boldsymbol{t} - K\boldsymbol{\beta})$.

The predictions are then performed by computing $y(\boldsymbol{x}) = \boldsymbol{w}^T \varphi(\boldsymbol{x}) = \sum_i \beta_i \boldsymbol{\varphi}(\boldsymbol{x}_i)^T \boldsymbol{\varphi}(\boldsymbol{x})$.

Kernels

We define a *kernel* corresponding to a feature map φ as a function

$$K(\boldsymbol{x}, \boldsymbol{z}) \stackrel{\text{def}}{=} \varphi(\boldsymbol{x})^t \varphi(\boldsymbol{z}).$$

There is quite a lot of theory behind kernel construction. The most often used kernels are:

- polynomial kernel or degree d

  $$K(\boldsymbol{x}, \boldsymbol{z}) = (\gamma \boldsymbol{x}^T \boldsymbol{z} + 1)^d,$$

  which corresponds to a feature map generating all combinations of up to d input features;
- Gaussian (or RBF) kernel

  $$K(\boldsymbol{x}, \boldsymbol{z}) = e^{-\gamma ||\boldsymbol{x} - \boldsymbol{z}||^2},$$

  corresponding to a scalar product in an infinite-dimensional space (it is in a sense a combination of polynomial kernels of all degrees).

Support Vector Machines

Assume we have a dataset $\boldsymbol{X} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \{-1, 1\}^N$, feature map φ and model

$$y(\boldsymbol{x}) \stackrel{\text{def}}{=} \boldsymbol{\varphi}(\boldsymbol{x})^T \boldsymbol{w} + b.$$

We already know that the distance of a point $\boldsymbol{x}_i$ to the decision boundary is

$$\frac{|y(\boldsymbol{x}_i)|}{||\boldsymbol{w}||} = \frac{t_i y(\boldsymbol{x}_i)}{||\boldsymbol{w}||}.$$

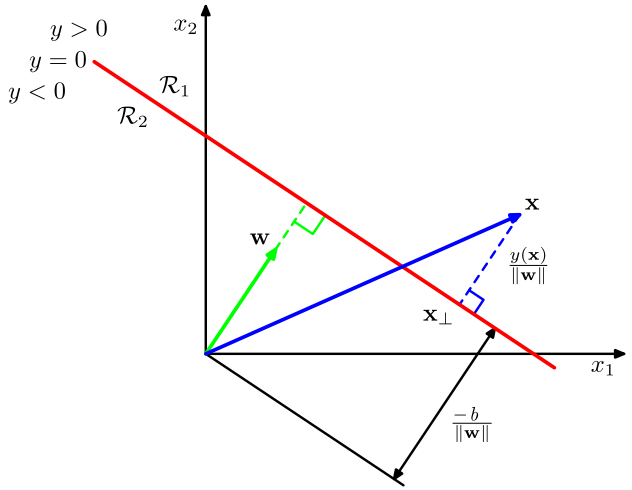


Figure 4.1 of Pattern Recognition and Machine Learning.

We therefore want to maximize

$$\arg\max_{w,b} \frac{1}{||\boldsymbol{w}||} \min_i \left[t_i (\boldsymbol{\varphi}(\boldsymbol{x})^T \boldsymbol{w} + b) \right].$$

However, this problem is difficult to optimize directly.

Because the model is invariant to multiplying $\boldsymbol{w}$ and b by a constant, we can say that for the points closest to the decision boundary, it will hold that

$$t_i y(\boldsymbol{x}_i) = 1.$$

Then for all the points we will have $t_i y(\boldsymbol{x}_i) \geq 1$ and we can simplify

$$\arg\max_{w,b} \frac{1}{||\boldsymbol{w}||} \min_i \left[t_i (\boldsymbol{\varphi}(\boldsymbol{x})^T \boldsymbol{w} + b) \right]$$

to

$$\arg\min_{w,b} \frac{1}{2} ||\boldsymbol{w}||^2 \text{ given that } t_i y(\boldsymbol{x}_i) \geq 1.$$

In order to solve the constrained problem of

$$\arg\min_{w,b} \frac{1}{2}||\boldsymbol{w}||^2 \text{ given that } t_i y(\boldsymbol{x}_i) \geq 1,$$

we write the Lagrangian with multipliers $\boldsymbol{a} = (a_1, \ldots, a_N)$ as

$$L = \frac{1}{2}||\boldsymbol{w}||^2 - \sum_i a_i \left[t_i y(\boldsymbol{x}_i) - 1\right].$$

Setting the derivatives with respect to $\boldsymbol{w}$ and b to zero, we get

$$\boldsymbol{w} = \sum_i a_i t_i \varphi(\boldsymbol{x}_i)$$
$$0 = \sum_i a_i t_i$$

Substituting these to the Lagrangian, we get

$$L = \sum_i a_i - \frac{1}{2} \sum_i \sum_j a_i a_j t_i t_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

with respect to the constraints $\forall_i : a_i \geq 0$, $\sum_i a_i t_i = 0$ and kernel $K(\boldsymbol{x}, \boldsymbol{z}) = \varphi(\boldsymbol{x})^T \varphi(\boldsymbol{z})$.

The solution of this Lagrangian will fulfil the KKT conditions, meaning that

$$\begin{aligned} a_i &\geq 0 \\ t_i y(\boldsymbol{x}_i) - 1 &\geq 0 \\ a_i \big(t_i y(\boldsymbol{x}_i) - 1\big) &= 0. \end{aligned}$$

Therefore, either a point is on a boundary, or $a_i = 0$. Given that the predictions for point $\boldsymbol{x}$ are given by $y(\boldsymbol{x}) = \sum a_i t_i K(\boldsymbol{x}, \boldsymbol{x}_i) + b$, we need to keep only the points on the boundary, the so-called **support vectors**.

Support Vector Machines

The dual formulation allows us to use non-linear kernels.

Figure 7.2 Example of synthetic data from two classes in two dimensions showing contours of constant $y(\mathbf{x})$ obtained from a support vector machine having a Gaussian kernel function. Also shown are the decision boundary, the margin boundaries, and the support vectors.

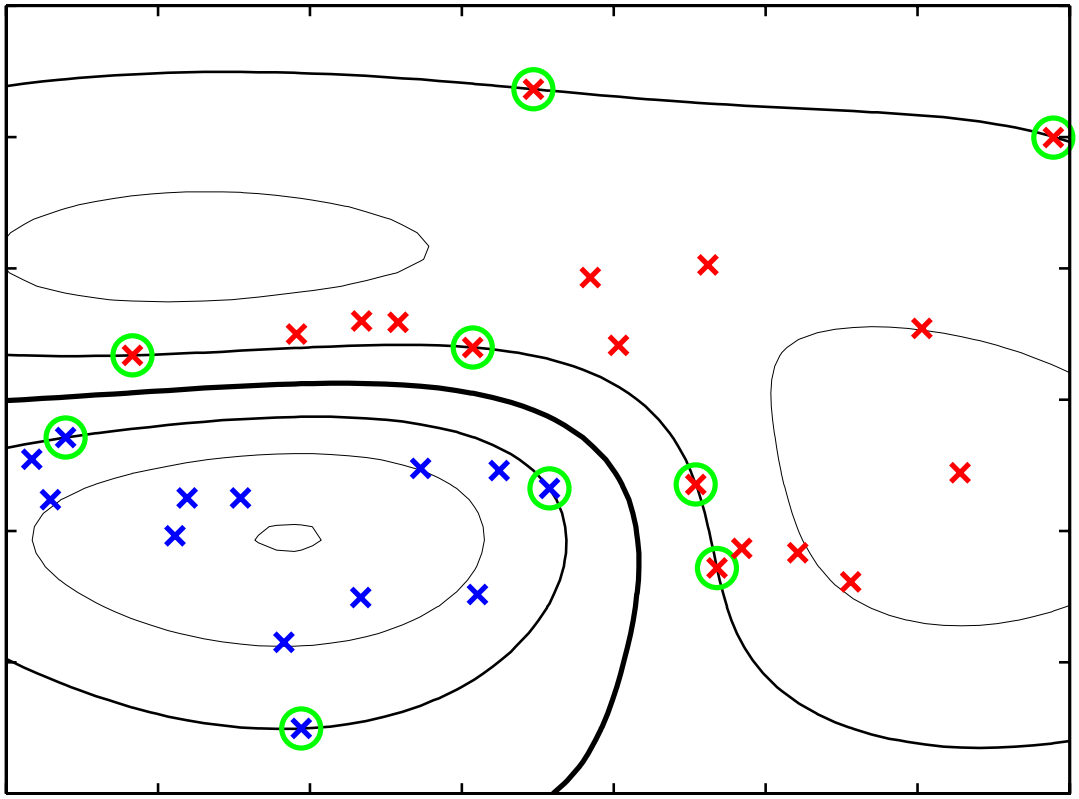


Figure 7.2 of Pattern Recognition and Machine Learning.

Support Vector Machines for Non-linearly Separable Data

Until now, we assumed the data to be linearly separable – the **hard-margin SVM** variant. We now relax this condition to arrive at **soft-margin SVM**. The idea is to allow points to be in the margin or even on the *wrong side* of the decision boundary. We introduce *slack variables* $\xi_i \geq 0$, one for each training instance, defined as

$$\xi_i = \begin{cases} 0 & \text{for points fulfilling } t_i y(\boldsymbol{x}_i) \geq 1, \\ |t_i - y(\boldsymbol{x}_i)| & \text{otherwise.} \end{cases}$$

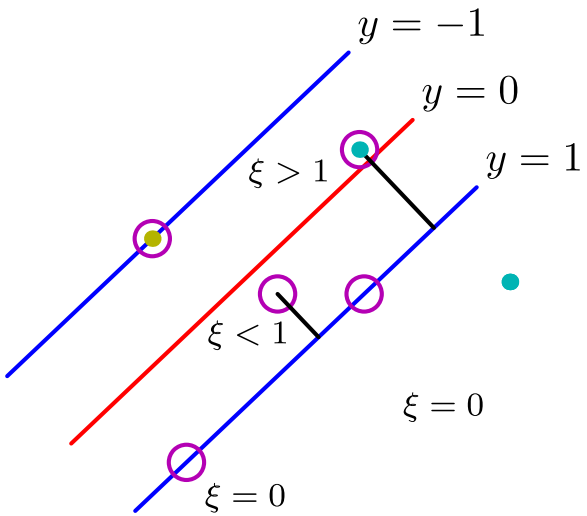


Figure 7.3 of Pattern Recognition and Machine Learning.

Therefore, $\xi_i = 0$ signifies a point outside of margin, $0 < \xi_i < 1$ denotes a point inside the margin, $\xi_i = 1$ is a point on the decision boundary and $\xi_i > 1$ indicates the point is on the opposite side of the separating hyperplane.

Therefore, we want to optimize

$$\arg\min_{w,b} C \sum_i \xi_i + \frac{1}{2}||\boldsymbol{w}||^2 \text{ given that } t_i y(\boldsymbol{x}_i) \geq 1 - \xi_i \text{ and } \xi_i \geq 0.$$

Support Vector Machines for Non-linearly Separable Data

We again create a Lagrangian, this time with multipliers $\boldsymbol{a} = (a_1, \ldots, a_N)$ and also $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_N)$:

$$L = \frac{1}{2}||\boldsymbol{w}||^2 + C\sum_i \xi_i - \sum_i a_i \left[t_i y(\boldsymbol{x}_i) - 1 + \xi_i\right] - \sum_i \mu_i \xi_i .$$

Solving for the critical points and substituting for $\boldsymbol{w}$, b and $\boldsymbol{\xi}$ (obtaining an additional constraint $\mu_i = C - a_i$ compared to the previous case), we obtain the Lagrangian in the form

$$L = \sum_i a_i - \frac{1}{2}\sum_i \sum_j a_i a_j t_i t_j K(\boldsymbol{x}_i, \boldsymbol{x}_j),$$

which is identical to the previous case, but the constraints are a bit different:

$$\forall_i : C \geq a_i \geq 0 \text{ and } \sum_i a_i t_i = 0.$$

Support Vector Machines for Non-linearly Separable Data

Using KKT conditions, we can see that the support vectors (examples with $a_i > 0$) are the ones with $t_i y(\boldsymbol{x}_i) = 1 - \xi_i$, i.e., the examples on the margin boundary, inside the margin and on the opposite side of the decision boundary.

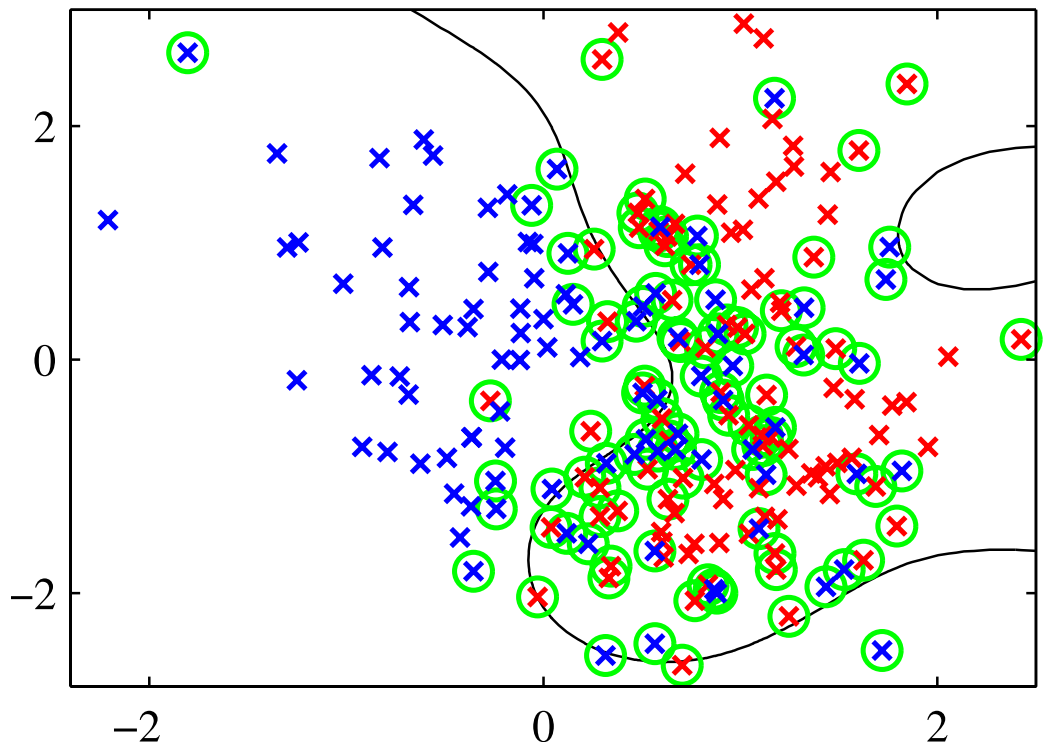


Figure 7.4 of Pattern Recognition and Machine Learning.

SGD-like Formulation of Soft-Margin SVM

Note that the slack variables can be written as

$$\xi_i = \max\left(0, 1 - t_i y(\boldsymbol{x}_i)\right),$$

so we can reformulate the soft-margin SVM objective using **hinge loss**

$$\mathcal{L}_{\text{hinge}}(t, y) \stackrel{\text{def}}{=} \max(0, 1 - ty)$$

to

$$\arg\min_{w,b} C \sum_i \mathcal{L}_{\text{hinge}}\left(t_i, y(\boldsymbol{x}_i)\right) + \frac{1}{2}||\boldsymbol{w}||^2.$$

Such formulation is analogous to a regularized loss, where C is an *inverse* regularization strength, so $C = \infty$ implies no regularization and $C = 0$ ignores the data entirely.

Comparison of Linear and Logistic Regression and SVM

For $f(\boldsymbol{x}; \boldsymbol{w}, b) \stackrel{\text{def}}{=} \boldsymbol{\varphi}(\boldsymbol{x})^T \boldsymbol{w} + b$, we have seen the following losses:

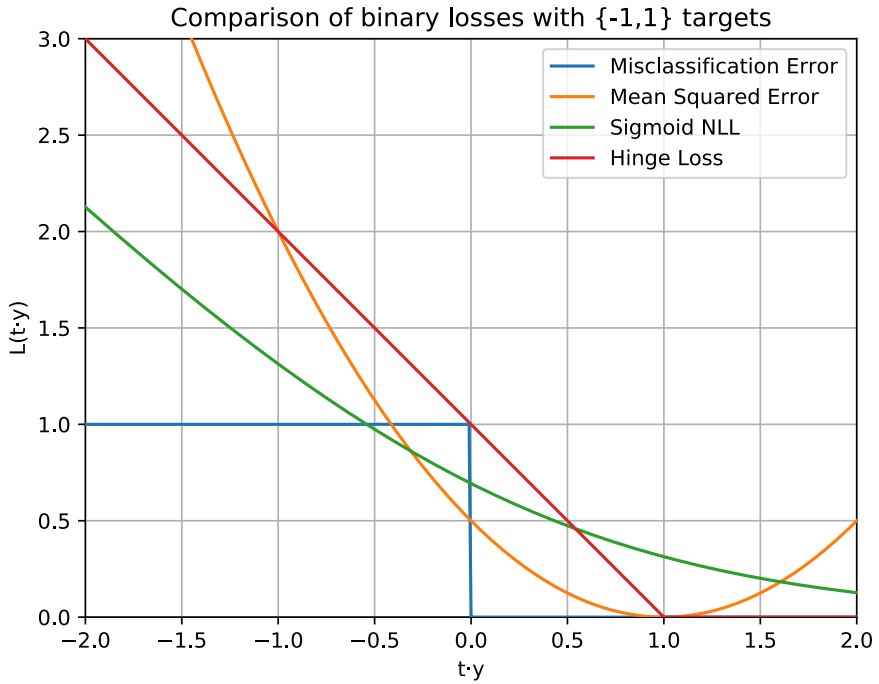
Model	Objective	Per-Instance Loss
Linear Regression	$\arg\min_{\boldsymbol{w},b} \sum_i \mathcal{L}_{\text{MSE}}\big(t_i, f(\boldsymbol{x}_i)\big) + \frac{1}{2}\lambda\|\boldsymbol{w}\|^2$	$\mathcal{L}_{\text{MSE}}(t, y) = \frac{1}{2}(t-y)^2$
Logistic regression	$\arg\min_{\boldsymbol{w},b} \sum_i \mathcal{L}_{\text{σ-NLL}}\big(t_i, f(\boldsymbol{x}_i)\big) + \frac{1}{2}\lambda\|\boldsymbol{w}\|^2$	$\mathcal{L}_{\text{σ-NLL}}(t, y) = -\log \begin{pmatrix} \sigma(y)^t + \\ \big(1-\sigma(y)\big)^{1-t} \end{pmatrix}$
Softmax regression	$\arg\min_{\boldsymbol{W},\boldsymbol{b}} \sum_i \mathcal{L}_{\text{s-NLL}}\big(t_i, f(\boldsymbol{x}_i)\big) + \frac{1}{2}\lambda\|\boldsymbol{w}\|^2$	$\mathcal{L}_{\text{s-NLL}}(t, \boldsymbol{y}) = -\log \text{softmax}(\boldsymbol{y})_t$
SVM	$\arg\min_{\boldsymbol{w},b} C\sum_i \mathcal{L}_{\text{hinge}}\big(t_i, f(\boldsymbol{x}_i)\big) + \frac{1}{2}\|\boldsymbol{w}\|^2$	$\mathcal{L}_{\text{hinge}}(t, y) = \max(0, 1-ty)$

Note that $\mathcal{L}_{\text{MSE}}(t, y) \propto -\log\big(\mathcal{N}(t; \mu = y, \sigma^2 = 1)\big)$ and that $\mathcal{L}_{\text{σ-NLL}}(t, y) = \mathcal{L}_{\text{s-NLL}}(t, [y, 0])$.

Binary Classification Loss Functions Comparison

To compare various functions for binary classification, we need to formulate them all in the same settings, with $t \in \{-1, 1\}$.

- MSE: $(ty - 1)^2$, because it is $(y - 1)^2$ for $t = 1$ and $(-y - t)^2$ for $t = -1$
- LR: $\sigma(ty)$, because it is $\sigma(y)$ for $t = 1$ and $1 - \sigma(y) = \sigma(-y)$ for $t = -1$
- SVM: $\max(0, 1 - ty)$



Sequential Minimal Optimization Algorithm

To solve the dual formulation of a SVM, usually Sequential Minimal Optimization (SMO; John Platt, 1998) algorithm is used.

Before we introduce it, we start by introducing **coordinate descent** optimization algorithm.

Consider solving unconstrained optimization problem

$$\arg\min_{\boldsymbol{w}} L(w_1, w_2, \ldots, w_D).$$

Instead of the usual SGD approach, we could optimize the weights one by one, using the following algorithm

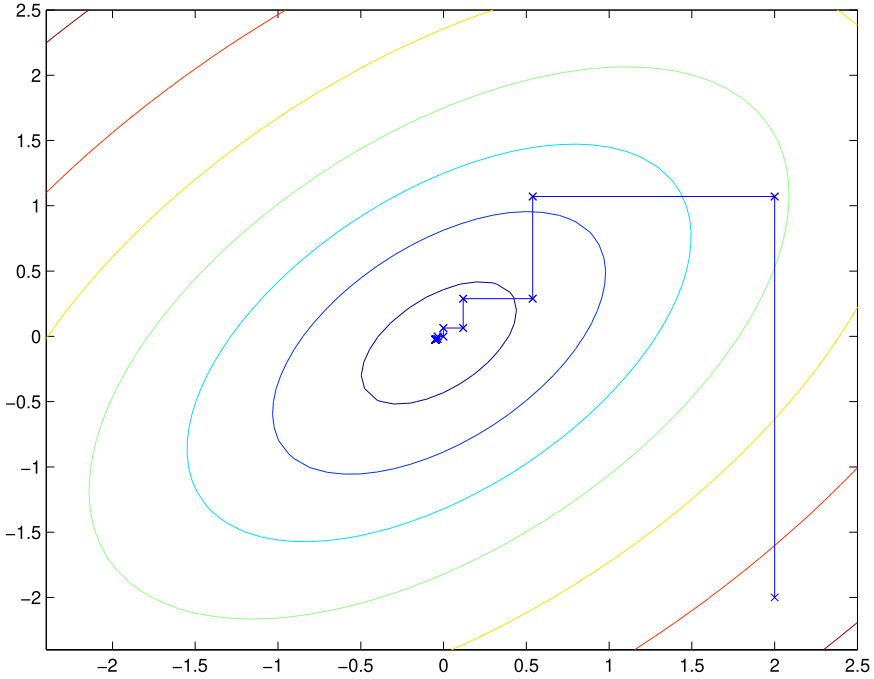
- loop until convergence
  - for i in $\{1, 2, \ldots, D\}$:
    - $w_i \leftarrow \arg\min_{w_i} L(w_1, w_2, \ldots, w_D)$

Sequential Minimal Optimization Algorithm

- loop until convergence
- for i in $\{1, 2, \ldots, D\}$:
  - $w_i \leftarrow \arg\min_{w_i} L(w_1, w_2, \ldots, w_D)$

If the inner $\arg\min$ can be performed efficiently, the coordinate descent can be fairly efficient.

Note that we might want to choose w_i in different order, for example by trying to choose w_i providing the largest decrease of L.



CS229 Lecture 3 Notes, http://cs229.stanford.edu/notes/cs229-notes3.pdf

Sequential Minimal Optimization Algorithm

In soft-margin SVM, we try to minimize

$$L = \sum_i a_i - \frac{1}{2} \sum_i \sum_j a_i a_j t_i t_j K(\boldsymbol{x}_i, \boldsymbol{x}_j),$$

such that

$$\forall_i : C \geq a_i \geq 0 \text{ and } \sum_i a_i t_i = 0.$$

The KKT conditions for the solution can be reformulated (while staying equivalent) as

$$\begin{aligned}
a_i > 0 &\Rightarrow t_i y(\boldsymbol{x}_i) \leq 1, \quad \text{because } a_i > 0 \Rightarrow t_i y(\boldsymbol{x}_i) = 1 - \xi_i \text{ and we have } \xi_i \geq 0, \\
a_i < C &\Rightarrow t_i y(\boldsymbol{x}_i) \geq 1, \quad \text{because } a_i < C \Rightarrow \mu_i > 0 \Rightarrow \xi_i = 0 \text{ and } t_i y(\boldsymbol{x}_i) \geq 1 - \xi_i, \\
0 < a_i < C &\Rightarrow t_i y(\boldsymbol{x}_i) = 1, \quad \text{a combination of both.}
\end{aligned}$$

Sequential Minimal Optimization Algorithm

At its core, the SMO algorithm is just a coordinate descent.

It tries to find such α_i fulfilling the KKT conditions – for soft-margin SVM, KKT conditions are sufficient conditions for optimality (the loss is convex and inequality constraints affine).

However, note that because of the $\sum a_i t_i = 0$ constraint we cannot optimize just one a_i, because a single a_i is determined from the others.

Therefore, in each step we pick two a_i, a_j coefficients and try to minimize the loss while fulfilling the constraints.

- loop until convergence (until $\forall i : a_i < C \Rightarrow t_i y(\boldsymbol{x}_i) \geq 1$ and $a_i > 0 \Rightarrow t_i y(\boldsymbol{x}_i) \leq 1$)
  - for i in $\{1, 2, \ldots, D\}$, for $j \neq i$ in ${1, 2, ..., D}:
    - $a_i, a_j \leftarrow \arg\min_{a_i, a_j} L(a_1, a_2, \ldots, a_D)$ such that $C \geq a_i \geq 0$, $\sum_i a_i t_i = 0$

Sequential Minimal Optimization Algorithm

The SMO is an efficient algorithm, because we can compute the update to a_i, a_j efficiently, because there exists an closed form solution.

Assume that we are updating a_i and a_j. Then from the $\sum_k a_k t_k = 0$ condition we can write $a_i t_i = -\sum_{k \neq i} a_k t_k$. Given that $t_i^2 = 1$ and denoting $\zeta = -\sum_{k \neq i, k \neq j} a_k t_k$, we get

$$a_i = t_i(\zeta - a_j t_j).$$

Minimizing $L(\boldsymbol{a})$ with respect to a_i and a_j then amounts to minimizing a quadratic function of a_j, which has an analytical solution.

Note that the real SMO algorithm has several heuristics for choosing a_i, a_j such that the L can be minimized the most.

Sequential Minimal Optimization Algorithm Sketch

Input: Dataset ($\boldsymbol{X} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \{-1, 1\}^N$), kernel $\boldsymbol{K}$, regularization parameter C, tolerance tol, $max\_passes\_without\_a\_changing$ value

- Initialize $a_i \leftarrow 0$, $b \leftarrow 0$, $passes \leftarrow 0$
- **while** $passes < max\_passes\_without\_a\_changing$:
  - $changed\_as \leftarrow 0$
  - **for** i in $1, 2, \ldots, N$:
    - $E_i \leftarrow y(\boldsymbol{x}_i) - t_i$
    - **if** ($a_i < C$ **and** $t_i E_i < -tol$) **or** ($a_i > 0$ **and** $t_i E_i > tol$):
      - Choose $j \neq i$ randomly
      - Update a_i, a_j and b
      - $changed\_as \leftarrow changed\_as + 1$
  - **if** $changed\_as = 0$: $passes \leftarrow passes + 1$
  - **else**: $passes \leftarrow 0$

Sequential Minimal Optimization Algorithm Sketch

Input: Dataset ($\boldsymbol{X} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \{-1, 1\}^N$), kernel $\boldsymbol{K}$, regularization parameter C, tolerance tol, $max\_passes\_without\_a\_changing$ value

- Update a_i, a_j, b:
  - Express a_i using a_j
  - Find a_j optimizing the loss L quadratic with respect to a_j
  - Clip a_j so that $0 \leq a_i, a_j \leq C$
  - Compute corresponding a_i
  - Compute b matching to updated a_i, a_j

Primal versus Dual Formulation

Assume we have a dataset with N training examples, each with D features. Also assume the used feature map φ generates F features.

Property	**Primal Formulation**	**Dual Formulation**
Parameters	F	N
Model size	F	$s \cdot D$ for s support vectors
Usual training time	$c \cdot N \cdot F$ for c iterations	between $\Omega(ND)$ and $\mathcal{O}(N^2 D)$
Inference time	$\Theta(F)$	$\Theta(s \cdot D)$ for s support vectors

Decision Trees

The idea of decision trees is to partition the input space into usually cuboid regions and solving each region with a simpler model.

We focus on **Classification and Regression Trees** (CART; Breiman et al., 1984), but there are additional variants like ID3, C4.5, ...

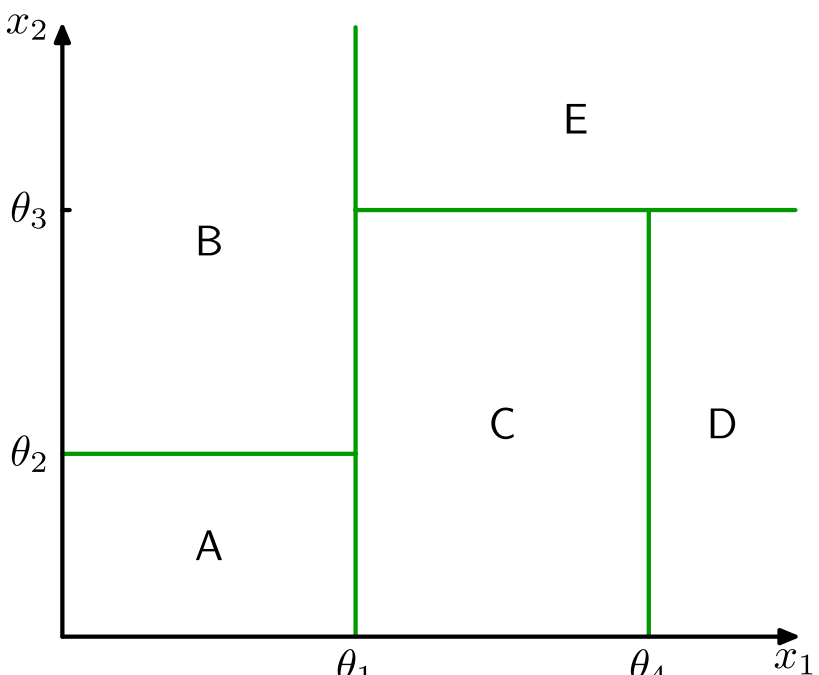


Figure 14.6 of Pattern Recognition and Machine Learning.

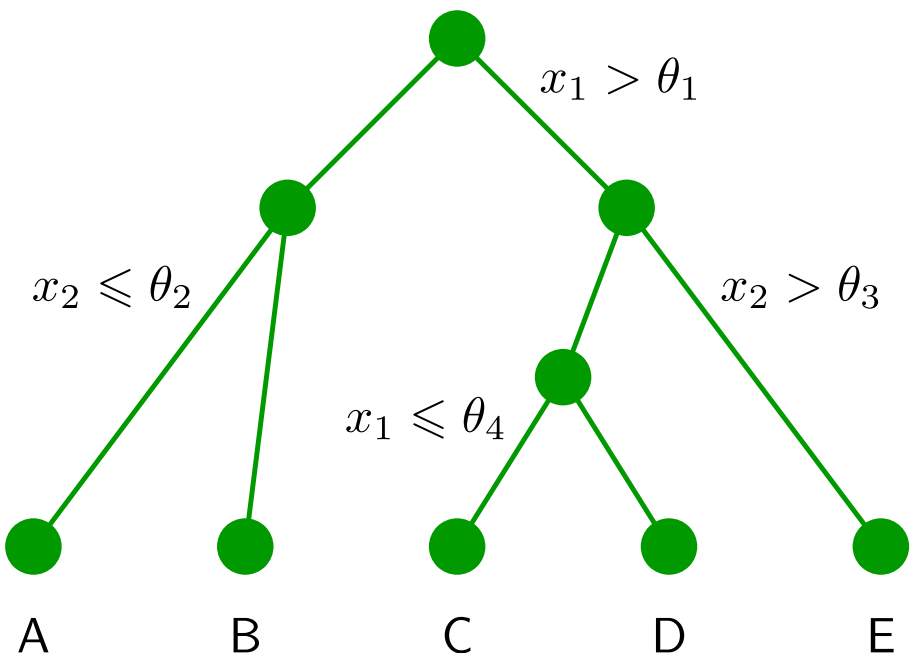


Figure 14.5 of Pattern Recognition and Machine Learning.

Regression Decision Trees

Assume we have an input dataset $\boldsymbol{X} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \mathbb{R}^N$. At the beginning, the decision tree is just a single node and all input examples belong to this node. We denote $I_{\mathcal{T}}$ the set of training example indices belonging to a leaf node $\mathcal{T}$.

For each leaf, our model will predict the average of the training examples belonging to that leaf, $\hat{t}_{\mathcal{T}} = \frac{1}{|I_{\mathcal{T}}|} \sum_{i \in I_{\mathcal{T}}} t_i$.

We will use a *criterion* $c_{\mathcal{T}}$ telling us how *uniform* or *homogeneous* are the training examples belonging to a leaf node $\mathcal{T}$ – for regression, we will employ the sum of squares error between the examples belonging to the node and the predicted value in that node; this is proportional to variance of the training examples belonging to the leaf node $\mathcal{T}$, multiplied by the number of the examples. Note that even if it not *mean* squared error, it is sometimes denoted as MSE.

$$c_{\text{SE}}(\mathcal{T}) \stackrel{\text{def}}{=} \sum_{i \in I_{\mathcal{T}}} (t_i - \hat{t}_{\mathcal{T}})^2, \text{ where } \hat{t}_{\mathcal{T}} = \frac{1}{|I_{\mathcal{T}}|} \sum_{i \in I_{\mathcal{T}}} t_i.$$

Tree Construction

To split a node, the goal is to find a feature and its value such that when splitting a node $\mathcal{T}$ into $\mathcal{T}_L$ and $\mathcal{T}_R$, the resulting regions decrease the overall criterion value the most, i.e., the difference $c_{\mathcal{T}_L} + c_{\mathcal{T}_R} - c_{\mathcal{T}}$ is the lowest.

Usually we have several constraints, we mention on the most common ones:

- **maximum tree depth**: we do not split nodes with this depth;
- **minimum examples to split**: we only split nodes with this many training examples;
- **maximum number of leaf nodes**

The tree is usually built in one of two ways:

- if the number of leaf nodes is unlimited, we usually build the tree in a depth-first manner, recursively splitting every leaf until some above constraint is invalidated;
- if the maximum number of leaf nodes is give, we usually split such leaf $\mathcal{T}$ where the criterion difference $c_{\mathcal{T}_L} + c_{\mathcal{T}_R} - c_{\mathcal{T}}$ is the lowest.

Classification Decision Trees

For multi-class classification, we predict such class most frequent in the training examples belonging to a leaf $\mathcal{T}$.

To define the criterions, let us denote the average probability for class k in a region $\mathcal{T}$ at $p_{\mathcal{T}}(k)$.

For classification trees, one of the following two criterions is usually used:

- **Gini index**:

$$c_{\text{Gini}}(\mathcal{T}) \stackrel{\text{def}}{=} |I_{\mathcal{T}}| \sum_k p_{\mathcal{T}}(k)\big(1 - p_{\mathcal{T}}(k)\big)$$

- **Entropy Criterion**

$$c_{\text{entropy}}(\mathcal{T}) \stackrel{\text{def}}{=} |I_{\mathcal{T}}| H(p_{\mathcal{T}}) = -|I_{\mathcal{T}}| \sum_k p_{\mathcal{T}}(k) \log p_{\mathcal{T}}(k)$$