Regularized Least Squares and Support Vector Machines

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About this class

Goal To introduce two main examples of Tikhonov regularization algorithms, deriving and comparing their computational properties.

Basics: Data

- Training set: $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, $x_i \in \mathbb{R}^d, \quad i = 1, \ldots, n$
- Inputs: $X = \{x_1, \ldots, x_n\}$.
- Labels: $Y = \{y_1, \ldots, y_n\}$.

- RKHS $\mathcal{H}$ with a positive semidefinite *kernel function* K:

$$\begin{aligned} \text{linear:} \quad & K(x_i, x_j) = x_i^T x_j \\ \text{polynomial:} \quad & K(x_i, x_j) = (x_i^T x_j + 1)^d \\ \text{gaussian:} \quad & K(x_i, x_j) = \exp\left(-\frac{||x_i - x_j||^2}{\sigma^2}\right) \end{aligned}$$

- Define the kernel matrix $\mathbf{K}$ to satisfy $\mathbf{K}_{ij} = K(x_i, x_j)$.
- The kernel function with one argument fixed is $K_x = K(x, \cdot)$.
- Given an arbitrary input x_*, $\mathbf{K}_{x_*}$ is a vector whose ith entry is $K(x_i, x_*)$.

Tikhonov Regularization

We are interested into studying Tikhonov Regularization

$$\underset{f \in \mathcal{H}}{\operatorname{argmin}} \{ \sum_{i=1}^{n} V(y_i, f(x_i)) + \lambda \| f \|_{\mathcal{H}}^2 \}.$$

The representer theorem guarantees that the solution can be written as

$$f = \sum_{j=1}^{n} c_j K_{x_j}$$

for some $c = (c_1, \ldots, c_n) \in \mathbb{R}^n$.
So $\mathbf{K}c$ is a vector whose ith element is $f(x_i)$:

$$f(x_i) = \sum_{j=1}^{n} c_j K_{x_i}(x_j) = \sum_{j=1}^{n} c_j \mathbf{K}_{ij}$$

and $\|f\|_{\mathcal{H}}^2 = c^T \mathbf{K} c$.

Since $f = \sum_{j=1}^{n} c_j K_{x_j}$, then

$$\begin{aligned}
\|f\|_{\mathcal{H}}^2 &= \langle f, f \rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{n} c_i K_{x_i}, \sum_{j=1}^{n} c_j K_{x_j} \rangle_{\mathcal{H}} \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \langle K_{x_i}, K_{x_j} \rangle_{\mathcal{H}} \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x_i, x_j) = c^t \mathbf{K} c
\end{aligned}$$

Plan

- RLS
  - dual problem
  - regularization path
  - linear case
- SVM
  - dual problem
  - linear case
  - historical derivation

Goal: Find the function $f \in \mathcal{H}$ that minimizes the weighted sum of the square loss and the RKHS norm

$$\underset{f \in \mathcal{H}}{\operatorname{argmin}} \{ \frac{1}{2n} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \frac{\lambda}{2} ||f||_{\mathcal{H}}^2 \}.$$

Using the representer theorem the RLS problem is:

$$\underset{c \in \mathbb{R}^n}{\operatorname{argmin}} \frac{1}{2n} \|\mathbf{Y} - \mathbf{K}c\|_2^2 + \frac{\lambda}{2} c^T \mathbf{K} c$$

The above functional is differentiable, we can find the minimum setting the gradient w.r.t c to 0:

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The above functional is differentiable, we can find the minimum setting the gradient w.r.t c to 0:

$$\begin{aligned} -\mathbf{K}(\mathbf{Y} - \mathbf{K}c) + \lambda n \mathbf{K}c &= 0 \\ (\mathbf{K} + \lambda n I)c &= \mathbf{Y} \\ c &= (\mathbf{K} + \lambda n I)^{-1}\mathbf{Y} \end{aligned}$$

We find c by solving a system of linear equations.

Solving RLS for fixed Parameters

$$(\mathbf{K} + \lambda n I)c = \mathbf{Y}.$$

- The matrix $\mathbf{K} + \lambda n I$ is symmetric positive definite (with $\lambda > 0$), so the appropriate algorithm is Cholesky factorization.
- In Matlab, the operator $\backslash$ seems to be using Cholesky, so you can just write `c = (K +lambda*n*I)\Y;`
- To be safe (or in Octave)
  `R = chol(K +lambda*n*I); c = (R\(R'\Y));`.

The above algorithm has complexity $O(n^3)$.

$$c = (\mathbf{K} + \lambda n I)^{-1} \mathbf{Y}$$

The prediction at a new input x_* is:

$$\begin{aligned} f(x_*) &= \sum_{j=1}^{n} c_j \mathbf{K}_{x_j}(x_*) \\ &= \mathbf{K}_{x_*} c \\ &= \mathbf{K}_{x_*} \mathbf{G}^{-1} \mathbf{Y}, \end{aligned}$$

where $\mathbf{G} = \mathbf{K} + \lambda n I$.
Note that the above operation is $O(n^2)$.

RLS Regularization Path

Typically we have to choose λ and hence to compute the solutions corresponding to different values of λ.

- Is there a more efficent method than solving $c(\lambda) = (\mathbf{K} + \lambda n I)^{-1}\mathbf{Y}$ anew for each λ?

RLS Regularization Path

Typically we have to choose λ and hence to compute the solutions corresponding to different values of λ.

- Is there a more efficent method than solving $c(\lambda) = (\mathbf{K} + \lambda n I)^{-1}\mathbf{Y}$ anew for each λ?
- Form the eigendecomposition $\mathbf{K} = \mathbf{Q}\Lambda\mathbf{Q}^T$, where Λ is diagonal with $\Lambda_{ii} \geq 0$ and $\mathbf{Q}\mathbf{Q}^T = I$.
- Then

$$\begin{aligned} \mathbf{G} &= \mathbf{K} + \lambda n I \\ &= \mathbf{Q}\Lambda\mathbf{Q}^T + \lambda n I \\ &= \mathbf{Q}(\Lambda + \lambda n I)\mathbf{Q}^T, \end{aligned}$$

which implies that $\mathbf{G}^{-1} = \mathbf{Q}(\Lambda + \lambda n I)^{-1}\mathbf{Q}^T$.

RLS Regularization Path Cont'd

- $O(n^3)$ time to solve one (dense) linear system, *or* to compute the eigendecomposition (constant is maybe 4x worse). Given $\mathbf{Q}$ and Λ, we can find $c(\lambda)$ in $O(n^2)$ time:

$$c(\lambda) = \mathbf{Q}(\Lambda + \lambda n I)^{-1}\mathbf{Q}^T\mathbf{Y},$$

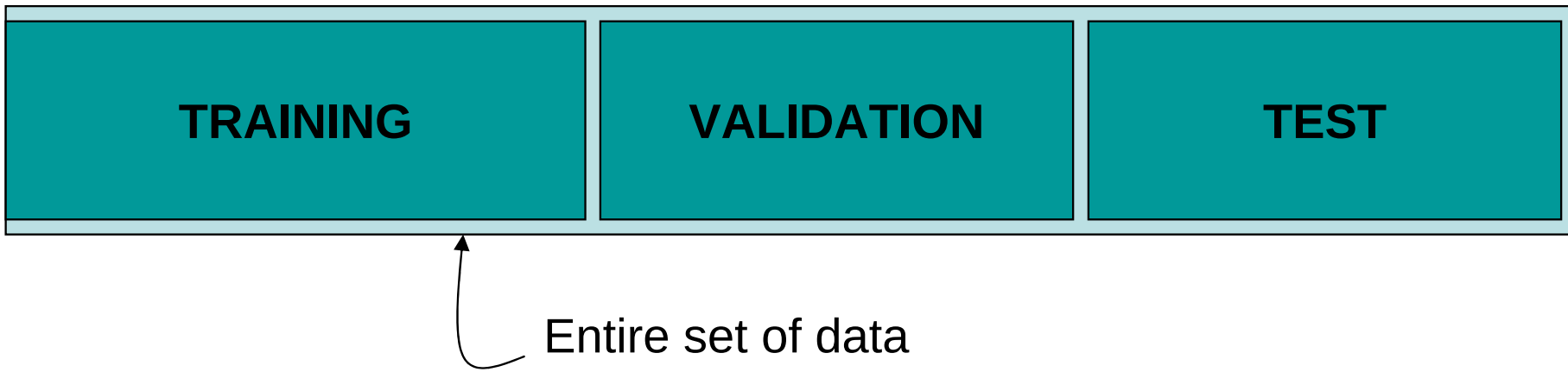
  noting that $(\Lambda + \lambda n I)$ is diagonal.
- Finding $c(\lambda)$ for many λ's is (essentially) free!

PARAMETER CHOICE

- idea: try different λ and see which one performs best
- How to try them? A simple choice is to use a validation set of data
- If we have "enough" training data we may sample out a training and a validation set.
- Otherwise a common practice is K-fold Cross Validation (KCV):
  1. Divide data into K sets of equal size: $S_1, \ldots, S_k$
  2. For each i train on the other $K - 1$ sets and test on the ith set
- If $K = n$ we get the leave-one-out strategy (LOO)

PARAMETER CHOICE

- Notice that some data should *always* be kept aside to be used as test set, to test the generalization performance of the system **after** parameter tuning took place



The Linear Case

- The linear kernel is $K(x_i, x_j) = x_i^T x_j$.
- The linear kernel offers many advantages for computation.
- Key idea: we get a decomposition of the kernel matrix for free: $\mathbf{K} = \mathbf{X}\mathbf{X}^T$
  — where $\mathbf{X} = [x_1^\top, \ldots, x_n^\top]$ is the data matrix $n \times d$
- In the linear case, we will see that we have two different computation options.

Linear kernel, linear function

With a linear kernel, the function we are learning is linear as well:

$$\begin{aligned} f(x_*) &= \mathbf{K}_{x_*} c \\ &= x_*^T \mathbf{X}^T c \\ &= x_*^T w, \end{aligned}$$

where we define w to be $\mathbf{X}^T c$.

For the linear kernel,

$$\begin{aligned} & \min_{c\in\mathbb{R}^n} \frac{1}{2n}||\mathbf{Y}-\mathbf{K}c||_2^2+\frac{\lambda}{2}c^T\mathbf{K}c \\ = & \min_{c\in\mathbb{R}^n} \frac{1}{2n}||\mathbf{Y}-\mathbf{X}\mathbf{X}^Tc||_2^2+\frac{\lambda}{2}c^T\mathbf{X}\mathbf{X}^Tc \\ = & \min_{w\in\mathbb{R}^d} \frac{1}{2n}||\mathbf{Y}-\mathbf{X}w||_2^2+\frac{\lambda}{2}||w||_2^2. \end{aligned}$$

Taking the gradient with respect to w and setting it to zero

$$\mathbf{X}^T\mathbf{X}w-\mathbf{X}^T\mathbf{Y}+\lambda nw=0$$

we get

$$w=(\mathbf{X}^T\mathbf{X}+\lambda nI)^{-1}\mathbf{X}^T\mathbf{Y}.$$

Solution for fixed parameter

$$w = (\mathbf{X}^T\mathbf{X} + \lambda nI)^{-1}\mathbf{X}^T\mathbf{Y}.$$

Choleski decomposition allows us to solve the above problem in $O(d^3)$ for any fixed λ.

- We can work with the *covariance matrix* $\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{d\times d}$.
- The algorithm is identical to solving a general RLS problem replacing the kernel matrix by $\mathbf{X}^T\mathbf{X}$ and the labels vector by $\mathbf{X}^T y$.

We can classify new points in $O(d)$ time, using w, rather than having to compute a weighted sum of n kernel products (which will usually cost $O(nd)$ time).

Regularization Path via SVD

To compute solutions corresponding to multiple values of λ we can again consider an eigendecomposition/svd.

- We need $O(nd)$ memory to store the data in the first place. The SVD also requires $O(nd)$ memory, and $O(nd^2)$ time.

Compared to the nonlinear case, we have replaced an $O(n)$ with an $O(d)$, in both time and memory. If $n >> d$, this can represent a huge savings.

Summary So Far

- When can we solve one RLS problem? (I.e. what are the bottlenecks?)

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- When can we solve one RLS problem? (I.e. what are the bottlenecks?)
- We need to form **K**, which takes $O(n^2 d)$ time and $O(n^2)$ memory. We need to perform a Cholesky factorization or an eigendecomposition of **K**, which takes $O(n^3)$ time.
- In the linear case we have replaced an $O(n)$ with an $O(d)$, in both time and memory. If $n >> d$, this can represent a huge savings.
- **Usually, we run out of memory before we run out of time.**
- **The practical limit on today's workstations is (more-or-less) 10,000 points (using Matlab).**

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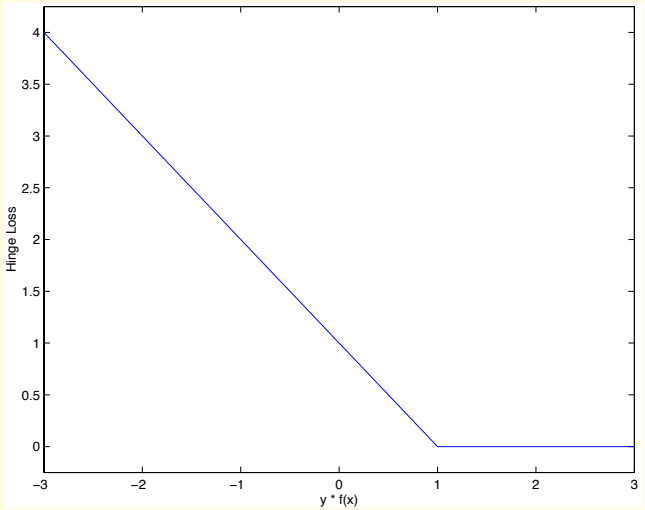
The Hinge Loss

The support vector machine (SVM) for classification arises considering the hinge loss

$$V(f(x), y) \equiv (1 - yf(x))_+,$$

where $(s)_+ \equiv \max(s, 0)$.



SVM Standard Notation

With the hinge loss, our regularization problem becomes

$$\operatorname*{argmin}_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (1 - y_i f(x_i))_+ + \lambda \|f\|_{\mathcal{H}}^2.$$

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In most of the SVM literature, the problem is written as

$$\operatorname*{argmin}_{f \in \mathcal{H}} \; C \sum_{i=1}^{n} (1 - y_i f(x_i))_+ + \frac{1}{2} \|f\|_{\mathcal{H}}^2.$$

The formulations are equivalent setting $C = \frac{1}{2\lambda n}$.
This problem is non-differentiable (because of the "kink" in V).

Slack Variables Formulation

We rewrite the functional using slack variables ξ_i.

$$\begin{aligned} \underset{f \in \mathcal{H}}{\text{argmin}} \quad & C \sum_{i=1}^{n} \xi_i + \frac{1}{2} \|f\|_{\mathcal{H}}^2 \\ \textit{subject to}: \quad & \xi_i \geq 1 - y_i f(x_i) \qquad i = 1, \ldots, n \\ & \xi_i \geq 0 \qquad i = 1, \ldots, n \end{aligned}$$

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Applying the representer theorem we get a constrained quadratic programming problem:

$$\begin{aligned} \underset{c \in \mathbb{R}^n, \xi \in \mathbb{R}^n}{\text{argmin}} \quad & C \sum_{i=1}^{n} \xi_i + \frac{1}{2} c^T \mathbf{K} c \\ \text{subject to} : \quad & \xi_i \geq 1 - y_i \sum_{j=1}^{n} c_j K(x_i, x_j) \qquad i = 1, \ldots, n \\ & \xi_i \geq 0 \qquad\qquad\qquad\qquad\quad i = 1, \ldots, n \end{aligned}$$

How to Solve?

$$\begin{aligned} \underset{c\in\mathbb{R}^n,\xi\in\mathbb{R}^n}{\text{argmin}} \quad & C\sum_{i=1}^n \xi_i + \frac{1}{2}c^T\mathbf{K}c \\ \text{subject to :} \quad & \xi_i \geq 1 - y_i\left(\sum_{j=1}^n c_j K(x_i, x_j)\right) \quad i = 1, \ldots, n \\ & \xi_i \geq 0 \quad i = 1, \ldots, n \end{aligned}$$

- This is a constrained optimization problem. The general approach:
  - Form the *primal* problem – we did this.
  - *Lagrangian* from primal – just like Lagrange multipliers.
  - *Dual* – one dual variable associated to each primal constraint in the Lagrangian.

The Primal and Dual Problems

$$\begin{aligned} \underset{c\in\mathbb{R}^n,\xi\in\mathbb{R}^n}{\text{argmin}} \quad & C\sum_{i=1}^n \xi_i + \tfrac{1}{2}c^T\mathbf{K}c \\ \text{subject to :} \quad & \xi_i \geq 1 - y_i\left(\sum_{j=1}^n c_j K(x_i,x_j)\right) \quad i = 1,\ldots,n \\ & \xi_i \geq 0 \quad i = 1,\ldots,n \end{aligned}$$

$$\begin{aligned} \max_{\alpha\in\mathbb{R}^{\mathbf{n}}} \quad & \sum_{i=1}^n \alpha_i - \tfrac{1}{2}\alpha^T(\text{diag}\mathbf{Y})\mathbf{K}(\text{diag}\mathbf{Y})\alpha \\ & 0 \leq \alpha_i \leq C \quad i = 1,\ldots,n \end{aligned}$$

The dual problem is easier to solve: simple box constraints.

Support Vectors

- Basic idea: solve the dual problem to find the optimal α's, and use them to find c

$$c_i = \alpha_i y_i$$

- The dual problem is easier to solve than the primal problem. It has simple box constraints and a single equality constraint, and the problem can be decomposed into a sequence of smaller problems.

Optimality Conditions

All optimal solutions (c, ξ) to the primal problem must satisfy the following conditions for some (α, ζ):

$$\frac{\partial L}{\partial c_i} = \sum_{j=1}^{n} c_j K(x_i, x_j) - \sum_{j=1}^{n} y_i \alpha_j K(x_i, x_j) = 0 \qquad i = 1, \ldots, n$$

$$\frac{\partial L}{\partial \xi_i} = C - \alpha_i - \zeta_i = 0 \qquad i = 1, \ldots, n$$

$$y_i(\sum_{j=1}^{n} y_j \alpha_j K(x_i, x_j)) - 1 + \xi_i \geq 0 \qquad i = 1, \ldots, n$$

$$\alpha_i[y_i(\sum_{j=1}^{n} y_j \alpha_j K(x_i, x_j)) - 1 + \xi_i] = 0 \qquad i = 1, \ldots, n$$

$$\zeta_i \xi_i = 0 \qquad i = 1, \ldots, n$$

$$\xi_i, \alpha_i, \zeta_i \geq 0 \qquad i = 1, \ldots, n$$

Optimality Conditions

- They are also known as the Karush-Kuhn-Tucker (KKT) conditions.
- These optimality conditions are both necessary and sufficient for optimality: (c, ξ, α, ζ) satisfy all of the conditions if and only if they are optimal for both the primal and the dual.

Solution

$$f(x) = \sum_{i=1}^{n} y_i \alpha_i K(x, x_i)$$

From the KKT conditions we can derive the following:

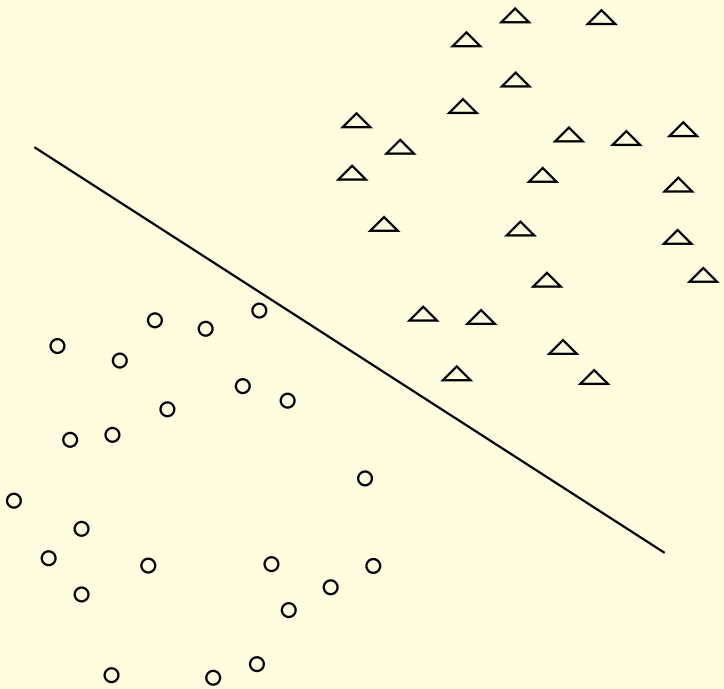
$$\begin{aligned} \alpha_i = 0 &\implies y_i f(x_i) \geq 1 \\ 0 < \alpha_i < C &\implies y_i f(x_i) = 1 \\ \alpha_i = C &\implies y_i f(x_i) \leq 1 \end{aligned}$$

$$\begin{aligned} \alpha_i = 0 &\impliedby y_i f(x_i) > 1 \\ \alpha_i = C &\impliedby y_i f(x_i) < 1 \end{aligned}$$

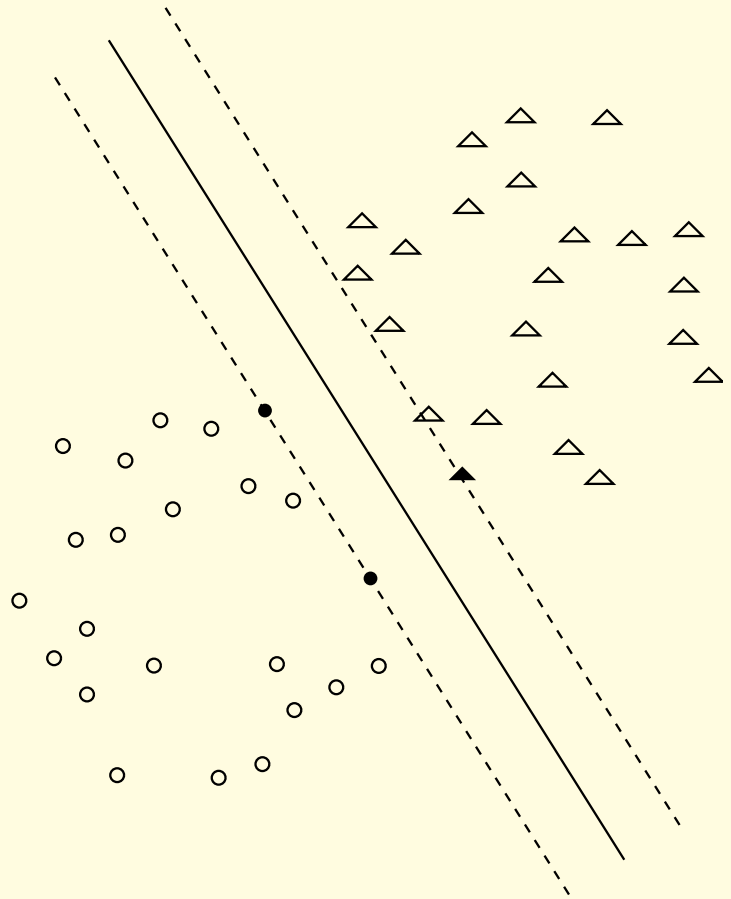
The Geometric Approach

- The "traditional" approach to describe SVM is to start with the concepts of *separating hyperplanes* and *margin*.
- The theory is usually developed in a linear space, beginning with the idea of a perceptron, a linear hyperplane that separates the positive and the negative examples.
- Defining the margin as the distance from the hyperplane to the nearest example, the basic observation is that intuitively, we expect a hyperplane with larger margin to generalize better than one with smaller margin.

Large and Small Margin Hyperplanes

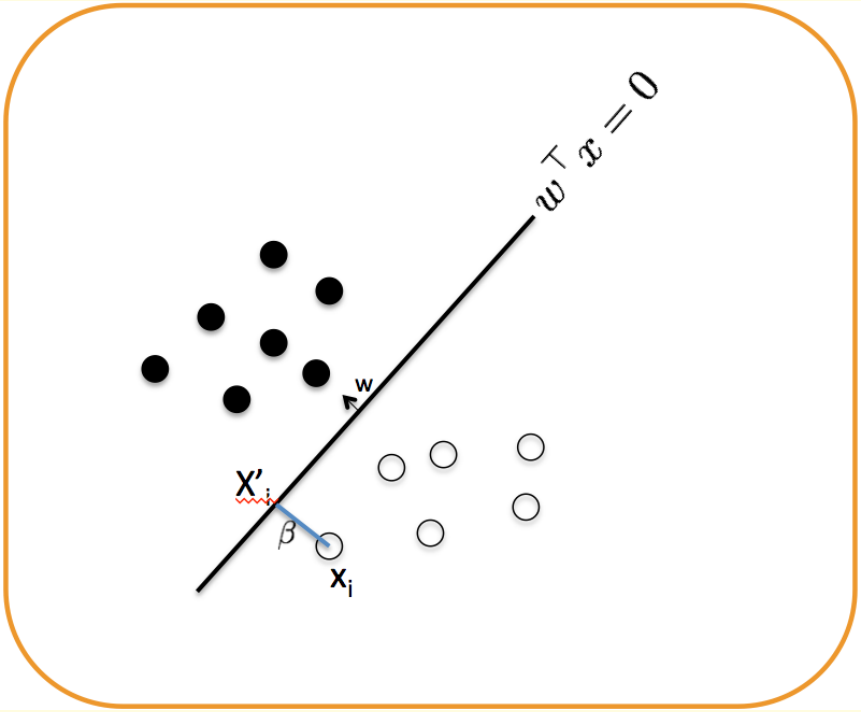


(a)



(b)

For simplicity we consider the linear separable case



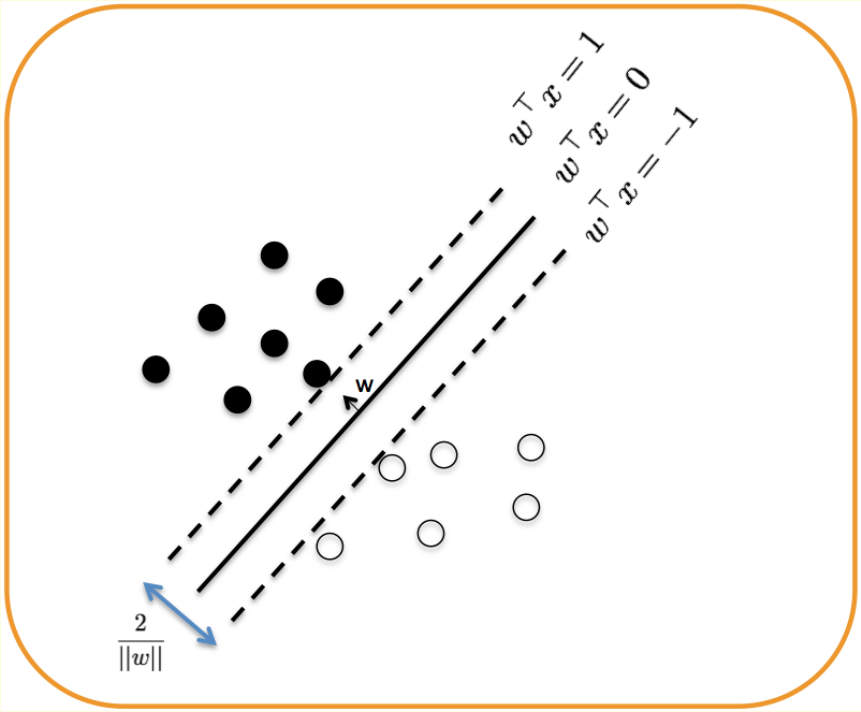
- Consider the decision surface $D = \{x : w^\top x = 0\}$
- Given a point x_i its projection on the decision surface is $x_i' = x_i - \beta \frac{w}{||w||}$.

$$w^\top x_i - \beta \frac{w}{||w||} = 0 \text{ iff } \beta = y_i \frac{w^\top}{||w||} x$$

β is often called a *geometrical margin* which is scale invariant.

Maximizing the margin

separable case

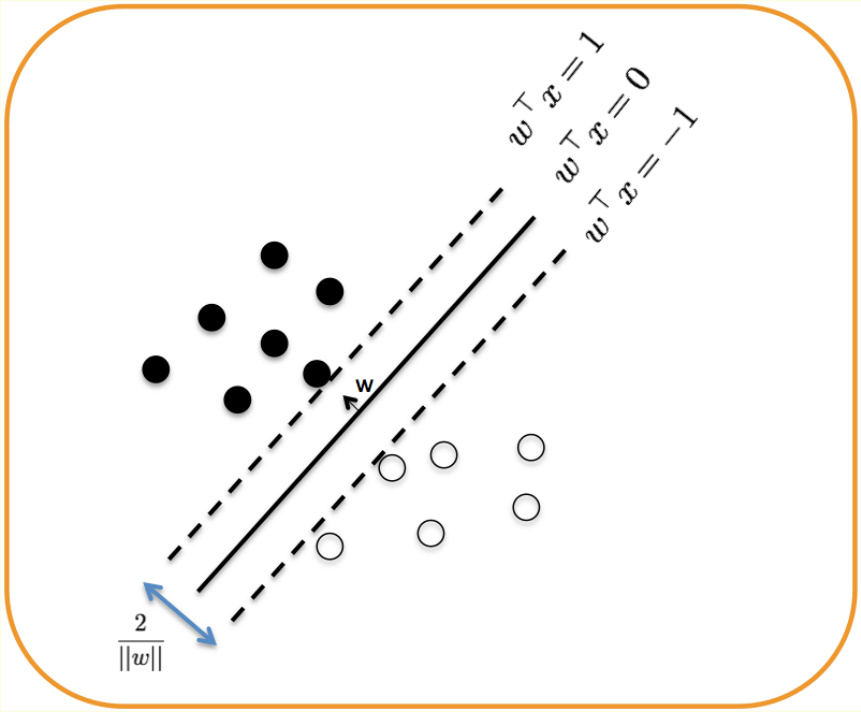


- $\beta_w = \min_{i=1\ldots n} \beta_i$
-

$$\begin{aligned} \max_{w \in \mathbb{R}^d} \quad & \beta_w \\ \text{subject to} \quad & \beta_w \geq 0 \\ & ||w|| = 1 \end{aligned}$$

MAXIMIZING THE MARGIN

SEPARABLE CASE



- $\beta_w = \min_{i=1\ldots n} \beta_i$
-

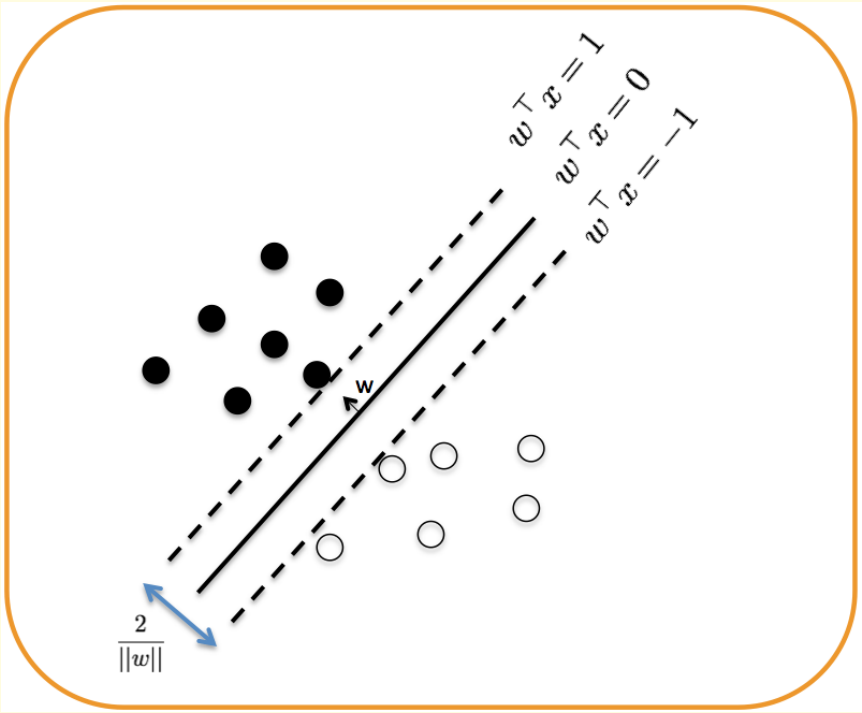
$$\max_{w \in R^d} \quad \beta_w$$

$$\text{subject to} \quad y_i \frac{w^\top}{||w||} x_i \geq \beta_w$$

$$||w|| = 1, \beta_w \geq 0$$

Maximizing the margin

Separable case



- we consider $\alpha = \beta_w ||w||$,
- because of the scale invariance we may set $\alpha = 1$, thus we obtain

$$\begin{aligned} \max_{w \in R^d} \quad & \frac{1}{||w||} \\ \text{subject to} \quad & y_i w^\top x_i \geq 1 \end{aligned}$$

- or equivalently

$$\begin{aligned} \min_{w \in R^d} \quad & \frac{1}{2}||w||^2 \\ \text{subject to} \quad & y_i w^\top x_i \geq 1 \end{aligned}$$

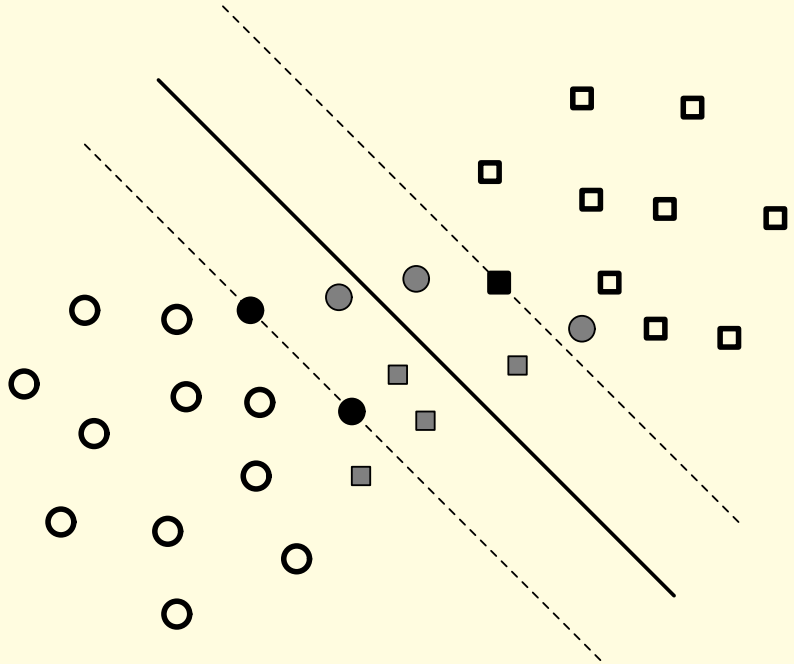
Non-separable means there are points on the wrong side of the margin, i.e.

$$\exists i \text{ s.t. } y_i w^\top x_i < 1 \ .$$

We add slack variables to account for the wrongness:

$$\begin{aligned} \underset{\xi_i, w}{\text{argmin}} \quad & \sum_{i=1}^n \xi_i + \frac{1}{2}\|w\|^2 \\ \text{s.t.} \quad & y_i w^\top x_i \geq 1 - \xi_i \ , \ \forall i \end{aligned}$$

Geometric Interpretation of Reduced Optimality Conditions



$$\begin{aligned}
\alpha_i = 0 &\implies y_i f(x_i) \geq 1 \\
0 < \alpha_i < C &\implies y_i f(x_i) = 1 \\
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\end{aligned}$$

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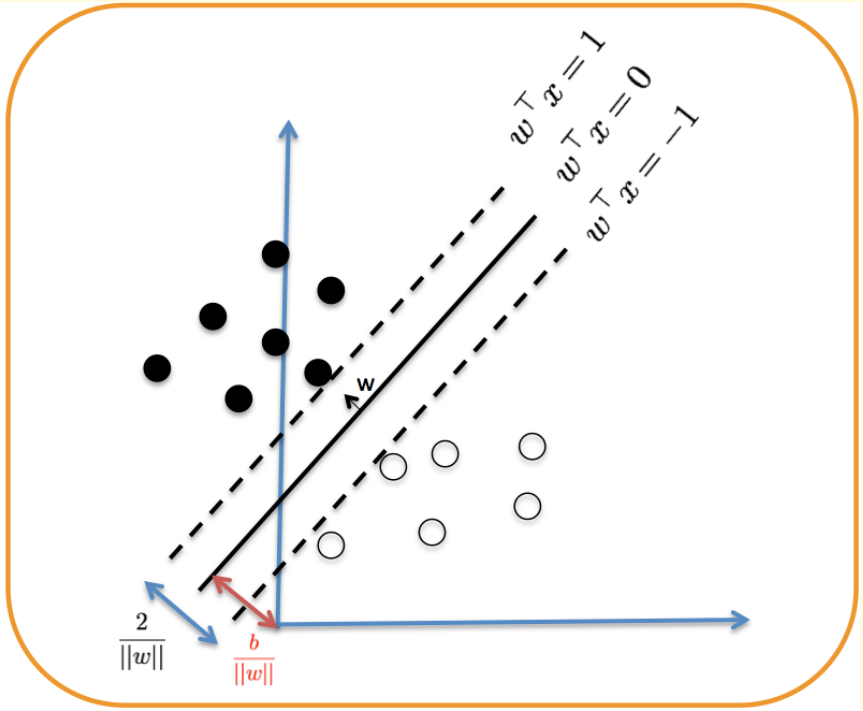
Adding a bias term



- The original SVM formulation includes a bias term, so that $f(x) = w^\top x + b$
- This amounts at adding a further constraint $\sum_{i=1}^{n} y_i \alpha_i x_i = 0$

SVM - Summary

- The SVM is a Tikhonov regularization problem, with the hinge loss.
- Solving the SVM means solving a constrained quadratic program, roughly $O(n^3)$
  - It's better to work with the dual program.
- Solutions can be *sparse* – few non-zero coefficients, this can have impact for memory and computational requirements.
- The non-zero coefficients correspond to points not classified correctly enough – a.k.a. "support vectors."

Multi-output

- In many practical problems, it is convenient to model the object of interest as a function with multiple outputs.
- In machine learning, this problem typically goes under the name of multi-output learning.
- A possible approach is to do re-write penalized empirical risk minimization

$$\min_{f^1,\ldots,f^T} ERR[f^1,\ldots,f^T] + \lambda PEN(f^1,\ldots,f^T)$$

Typically

- The error term is the sum of the empirical risks.
- The penalty term enforces similarity among the tasks.

MULTI-CLASS CODING

A classical problem is *multi-category classification* where each input can be assigned to one of T classes.

- We can consider T labels $Y = \{1, 2, \ldots T\}$: this choice forces an unnatural ordering among classes

MULTI-CLASS CODING

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- We can consider T labels $Y = \{1, 2, \dots T\}$: this choice forces an unnatural ordering among classes
- We can define a coding, that is a one-to-one map $C : Y \to \mathcal{Y}$ where $\mathcal{Y} = (\ell_1, \dots, \ell_T)$ are a set of coding vectors

MULTI-CLASS

In multi-category classification each input can be assigned to one of T classes. We can think of encoding each class with a vector, for example: class one can be $(1, 0 \ldots, 0)$, class 2 $(0, 1 \ldots, 0)$ etc.

Multi-class and Multi-label

Multi-class

In multi-category classification each input can be assigned to one of T classes. We can think of encoding each class with a vector, for example: class one can be $(1, 0 \ldots, 0)$, class 2 $(0, 1 \ldots, 0)$ etc.

Multilabel

Images contain at most T objects each input image is associate to a vector

$$(1, 0, 1 \ldots, 0)$$

where $1/0$ indicate presence/absence of the an object.

MULTI-CLASS RLS - ONE VS ALL

Consider the coding where class 1 is $(1, -1, \ldots, -1)$, class 2 is $(-1, 1, \ldots, -1)$ ...

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One can easily check that the problem

$$\min_{f_1,\ldots,f_T} \{\frac{1}{n} \sum_{j=1}^{T} \sum_{i=1}^{n} (y_i^j - f^j(x_i))^2 + \lambda \sum_{j=1}^{T} \|f^j\|_K^2$$

is exactly the one versus all scheme with regularized least squares.

MULTI-CLASS RLS - SOLUTION

$$(\mathbf{K} + \lambda n I) W = \mathbf{Y}$$

with W a $d \times T$ matrix and $\mathbf{Y}$ a $n \times T$ matrix whose i-th column contains 1s if input belongs to class i, -1 otherwise.

The classification rule can be written as

$$c : X \to \{1, ..., T\}$$

$$c(x) = \arg \max_{t=1,...,T} \sum_{j=1}^{n} W_i^t K(x, x_i)$$