

CS:E4830 Kernel Methods in Machine Learning

Lecture 6 : Kernel Support Vector Machines

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Some Announcements

- Assignment 2 due today
- No lecture next week,
- Next upcoming session - Lecture 7 (20.04)

Course outline so far

- Introduction to kernel methods
 - Kernel Definition and examples
 - RKHS, Representer Theorem and Kernel Least Squares
- Introductory learning theory
 - Generalization, ERM, Consistency
- Convex optimization Introduction
 - Convexity and Duality
- Algorithms - Supervised
 - *Kernel Support Vector Machines*
 - Logistic regression
 - Kernel methods for large-scale problems
- Algorithms - Unsupervised
 - PCA and k-means
 - Kernel variants
- Kernel methods for Structured output and multi-view data
 - Guest lecture

Supervised learning setup

Binary classification

- Input \mathcal{X} , can be in various forms such as images or text documents
- Output $\mathcal{Y} = \{-1, +1\}$ - binary classification. Other formulations include :
 - One-hot encoded binary vector for multi-class classification - Cifar10
 - Multi-label classification - Wikipedia
- Training set $S = (x_i, y_i)_{i=1}^N$ consists of samples that are sampled independently and identically from an unknown joint distribution P over $\mathcal{X} \times \mathcal{Y}$
- The goal is to build a classifier f to predict the label \hat{y} for a test instance x .

Maximum margin hyperplane

One good solution is to choose the hyperplane $\mathbf{w}^T \mathbf{x} = 0$ that lies furthest away from the training data (maximizing the minimum margin of the training examples):

Maximize γ

w.r.t. variables $\mathbf{w} \in \mathbb{R}^d$

Subject to $\frac{y_i \mathbf{w}^T \mathbf{x}_i}{\|\mathbf{w}\|} \geq \gamma$, for all $i = 1, \dots, m$,

The maximum margin hyperplane has good properties:

- Robustness: small change in the training data will not change the classifications too much
- Theoretically a large margin is tied to a low generalization error
- It can be found efficiently through incremental optimization

Support vector machines (SVM) are based on this principle

Hinge Loss Function and Kernel SVM

- Kernel SVM solves the following optimization problem :

$$\min_{f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^N \ell_{\text{hinge}}(y_i f(x_i)) + \lambda \|f\|_{\mathcal{H}}^2$$

where \mathcal{H} is a reproducing kernel Hilbert space

- Hinge loss is a function $\mathbb{R} \mapsto \mathbb{R}_+$ defined as below :

$$\ell_{\text{hinge}}(u) := \max(1 - u, 0) = \begin{cases} 0 & \text{if } u \geq 1 \\ 1 - u & \text{otherwise} \end{cases}$$

Hinge Loss - a convex upper bound

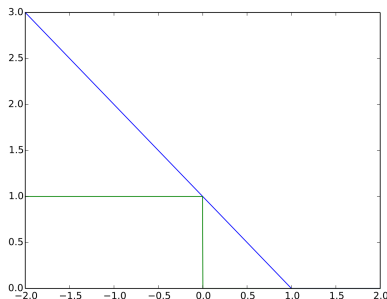


Figure: Hinge and 0-1 loss functions

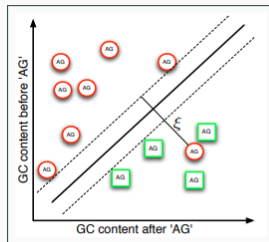
- Hinge Loss (in blue) is given by $\max(1 - yf(x), 0)$
- **Convex Upper bound** on 0-1 loss

Dual representation of the optimal hyperplane

It can be shown theoretically that the **optimal hyperplane** of the soft-margin SVM has a **dual representation** as the linear combination of the training data

$$\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i$$

- The coefficients, also called the **dual variables** are non-negative $\alpha_i \geq 0$
- The positive coefficients $\alpha_i > 0$ appear if and only if \mathbf{x}_i is a support vector, for other training points we have $\alpha_i = 0$



Dual representation of the optimal hyperplane

- Consequently, the functional margin $y\mathbf{w}^T\mathbf{x}$ also can be expressed using the support vectors:

$$y\mathbf{w}^T\mathbf{x} = y \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i^T \mathbf{x}$$

- The norm of the weight vector can be expressed as

$$\mathbf{w}^T \mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^m \alpha_j y_j \mathbf{x}_j = \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

- Note that the training data appears in pairwise inner products: $\mathbf{x}_i^T \mathbf{x}_j$

Dual representations

- We can replace the explicit inner products with a kernel function

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$$

which computes an inner product in the space of the arguments, here \mathbb{R}^d

- Plug in:
 - Margin:

$$y\mathbf{w}^T \mathbf{x} = y \sum_{i=1}^m \alpha_i y_i \kappa(\mathbf{x}_i, \mathbf{x})$$

- Squared norm:

$$\|\mathbf{w}\|^2 = \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)$$

From Representer Theorem

- For the following optimization

$$f_{\mathcal{H}} := \arg \min_f \frac{1}{N} \sum_{i=1}^N \ell_{\text{hinge}}(y_i, f(x_i)) + \lambda \theta(\|f\|_{\mathcal{H}}^2)$$

where $\ell_{\text{hinge}}(\cdot, \cdot)$ is the hinge loss function and $\theta : [0, \infty) \mapsto \mathbb{R}$ is non-decreasing function, and \mathcal{H} is an RKHS

- Even though the above problem is potentially an infinite dimensional optimization problem, **Representer Theorem** states its solution can be expressed in the following form

$$f_{\mathcal{H}}(\cdot) = \sum_{j=1}^N \alpha_j k(\cdot, x_j)$$

where $\alpha_j \in \mathbb{R}$, i.e. it is linear combination of kernel evaluations at training points

Implications of Representer Theorem

- Representer Theorem allows us to look for the solutions of the following form:

$$f_{\mathcal{H}}(.) = \sum_{j=1}^N \alpha_j k(., x_j)$$

- Implications

- The desired function just involves kernel computation on **training points only** via $k(., x_i)$ in the above solution
- It reduces the problem of finding $f \in \mathcal{H}$ which could be infinite dimensional to a finite dimensional problem
 - We just need to find the coefficients of the finite linear combination $\alpha_1, \dots, \alpha_N$
- Also, we can reformulate the original objective function in the new form (more in next slides)

Reformulating the Objective using Representer Theorem - I

- Recall the original objective :

$$f_{\mathcal{H}} := \arg \min_f \frac{1}{n} \sum_{i=1}^N \ell(y_i, f(x_i)) + \lambda \theta(\|f\|_{\mathcal{H}})$$

- Using the implication of representer theorem, for the i -th **training point**,

$$f_{\mathcal{H}}(x_i) = \sum_{j=1}^N \alpha_j k(x_i, x_j) = [K\alpha]_i$$

which is the i -th element of the matrix-vector product $K\alpha$

Reformulating the Objective using Representer Theorem - II

- Similarly, rewriting the regularization term :

$$\begin{aligned} \|f\|_{\mathcal{H}}^2 &= \langle f(\cdot), f(\cdot) \rangle \\ &= \left\langle \sum_{i=1}^N \alpha_i k(\cdot, x_i), \sum_{i=1}^N \alpha_i k(\cdot, x_i) \right\rangle \quad (\text{using representer theorem}) \\ &= \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j k(x_i, x_j) \quad (\text{evaluation of dot product}) \\ &= \boldsymbol{\alpha}^T K \boldsymbol{\alpha} \quad (\text{writing in matrix notation}) \end{aligned}$$

Reformulating the Objective using Representer Theorem - III

Using the above substitutions, the original (potentially intractable) objective

$$f_{\mathcal{H}} := \arg \min_f \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i)) + \lambda \theta(\|f\|_{\mathcal{H}})$$

translates to an equivalent (tractable) form below

$$\arg \min_{\alpha \in \mathbb{R}^N} \frac{1}{N} \sum_{i=1}^N \ell(y_i, [K\alpha]_i) + \lambda \theta(\alpha^T K \alpha)$$

SVM Problem Refomulation

- Using Representer theorem, the problem can be reformulated as

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^N} \left\{ \frac{1}{N} \sum_{i=1}^N \ell_{\text{hinge}}(y_i [K\boldsymbol{\alpha}]_i) + \lambda \boldsymbol{\alpha}^T K \boldsymbol{\alpha} \right\}$$

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- The above optimization problem is convex (why?)
- However, it is non-smooth/non-differentiable optimization problem

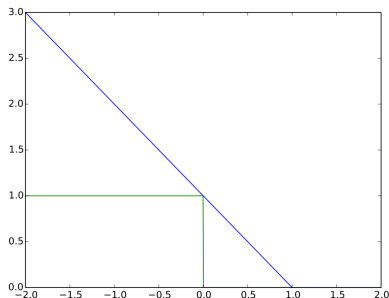


Figure: $\ell_{\text{hinge}}(\cdot)$ is the function in blue, $z = yf(x)$ in the above graph

Another Equivalent Reformulation

- The optimization problem on the previous slide is equivalent (even though not immediately obvious) to the following with an extra optimization variable ξ , one for each example in the training set. If we re-write it in terms of slack variables $\xi_i \in \mathbb{R}$ for $i = 1, \dots, N$

$$\min_{\alpha \in \mathbb{R}^N, \xi \in \mathbb{R}^N} \left\{ \frac{1}{N} \sum_{i=1}^N \xi_i + \lambda \alpha^T K \alpha \right\} \text{ such that } \xi_i \geq \ell_{\text{hinge}}(y_i [K\alpha]_i)$$

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- In the above formulation, the objective is smooth but not the constraints
- Recall the definition of hinge loss

$$\ell_{\text{hinge}}(u) = \max(1 - u, 0) \iff \begin{cases} 0 & \text{if } u \geq 1 \\ 1 - u & \text{otherwise} \end{cases}$$

- Using above, the N constraints ($\xi_i \geq \ell_{\text{hinge}}(y_i[K\alpha]_i)$) can be replaced by $2N$ constraints to make the problem smooth as follows :

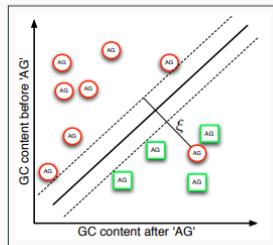
$$\xi_i \geq \ell_{\text{hinge}}(y_i[K\alpha]_i) \iff \begin{cases} \xi_i \geq 0 \\ \xi_i \geq 1 - y_i[K\alpha]_i \end{cases}$$

Non-separable data

- To allow non-separable data, we allow the functional margin of some data points to be smaller than 1 by a slack variable $\xi_i \geq 0$
- The relaxed margin constraint will be expressed as

$$y_i \mathbf{w}^T \mathbf{x}_i \geq 1 - \xi_i, \xi_i \geq 0$$

- $\xi_i = 0$ corresponds to having large enough margin > 1
- $\xi_i > 1$ corresponds to negative margin, misclassified point
- The set of support vectors includes all \mathbf{x}_i that have non-zero slack ξ_i (functional margin ≤ 1)



SVM Primal Formulation

$$\min_{\alpha \in \mathbb{R}^N, \xi \in \mathbb{R}^N} \left\{ \frac{1}{n} \sum_{i=1}^N \xi_i + \lambda \alpha^T K \alpha \right\}$$

such that

$$\begin{cases} 1 - y_i [K\alpha]_i - \xi_i \leq 0 & \text{for } i = 1, \dots, N \\ -\xi_i \leq 0 & \text{for } i = 1, \dots, N \end{cases}$$

Putting in the standard convex optimization problem framework where the inequality constraints should in the less than (\leq) form

- The Lagrangian of the problem is :

$$L(\boldsymbol{\alpha}, \boldsymbol{\xi}, \boldsymbol{\mu}, \boldsymbol{\nu}) = \frac{1}{N} \sum_{i=1}^N \xi_i + \lambda \boldsymbol{\alpha}^T K \boldsymbol{\alpha} + \sum_{i=1}^N \mu_i [1 - y_i [K \boldsymbol{\alpha}]_i - \xi_i] - \sum_{i=1}^N \nu_i \xi_i$$

- $\boldsymbol{\mu}, \boldsymbol{\nu} \in \mathbb{R}^N$, $\boldsymbol{\mu} \geq 0$ and $\boldsymbol{\nu} \geq 0$
- Note that constraints have moved to the Lagrangian.

Computing derivatives w.r.t ξ

- The lagrangian of the problem is :

$$L(\alpha, \xi, \mu, \nu) = \frac{1}{N} \sum_{i=1}^N \xi_i + \lambda \alpha^T K \alpha + \sum_{i=1}^N \mu_i [1 - y_i [K \alpha]_i - \xi_i] - \sum_{i=1}^N \nu_i \xi_i$$

Lagrangian wrt ξ

- $L(\alpha, \xi, \mu, \nu)$ is a linear function in ξ . What is its minimum value

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Lagrangian wrt ξ

- $L(\alpha, \xi, \mu, \nu)$ is a linear function in ξ . What is its minimum value
- Its minimum value is $-\infty$, except when it is constant,

$$\nabla_{\xi} L(\alpha, \xi, \mu, \nu) = \frac{1}{N} - \mu - \nu = 0$$

equivalently,

$$\frac{1}{N} = \mu + \nu$$

Computing derivatives w.r.t α

- The lagrangian of the problem is :

$$L(\alpha, \xi, \mu, \nu) = \frac{1}{N} \sum_{i=1}^N \xi_i + \lambda \alpha^T K \alpha + \sum_{i=1}^N \mu_i [1 - y_i [K \alpha]_i - \xi_i] - \sum_{i=1}^N \nu_i \xi_i$$

Lagrangian wrt α

- $L(\alpha, \xi, \mu, \nu)$ is a convex quadratic function in α . To find the optimal value, set the gradient to $\mathbf{0}$ (the zero vector) :

$$\nabla_{\alpha} L = \mathbf{0}$$

- The optimal solution α^* is given by

$$\alpha_i^* = \frac{y_i \mu_i}{2\lambda}$$

Lagrange Dual Function and Dual Problem

Lagrange Dual Function

- The Lagrange dual function by substituting the optimal values (with those obtained in previous two slides) is given by :

$$\begin{aligned} q(\boldsymbol{\mu}, \boldsymbol{\nu}) &= \min_{\boldsymbol{\alpha} \in \mathbb{R}^N, \boldsymbol{\xi} \in \mathbb{R}^N} L(\boldsymbol{\alpha}, \boldsymbol{\xi}, \boldsymbol{\mu}, \boldsymbol{\nu}) \\ &= \begin{cases} \sum_{i=1}^N \mu_i - \frac{1}{4\lambda} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \mu_i \mu_j K(x_i, x_j) & \text{if } \boldsymbol{\mu} + \boldsymbol{\nu} = \frac{1}{N} \\ -\infty & \text{otherwise} \end{cases} \end{aligned}$$

Lagrange Dual Problem

- The Lagrange dual problem is

$$\max q(\boldsymbol{\nu}, \boldsymbol{\mu}) \text{ such that } \boldsymbol{\mu} \geq 0, \boldsymbol{\nu} \geq 0$$

Closer Look At The Dual Problem

- The Lagrange dual problem is

$$\max q(\boldsymbol{\nu}, \boldsymbol{\mu}) \text{ such that } \boldsymbol{\mu} \geq 0, \boldsymbol{\nu} \geq 0$$

- If $0 \leq \mu_i \leq 1/N$ for all i , then the dual function takes finite values. Also, the value of ν_i is fixed at $\nu_i = 1/N - \mu_i$ in this case.
- The dual problem is therefore given by

$$\max_{\mathbf{0} \leq \boldsymbol{\mu} \leq \mathbf{1}/N} \sum_{i=1}^N \mu_i - \frac{1}{4\lambda} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \mu_i \mu_j K(x_i, x_j)$$

Dual Soft-Margin SVM

A dual optimization problem for the soft-margin SVM with kernels is given by

$$\text{Maximize } OBJ(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{w.r.t} \quad \text{variables } \alpha \in \mathbb{R}^m$$

$$\text{Subject to} \quad 0 \leq \alpha_i \leq C/m$$

for all $i = 1, \dots, m$

- It is a QP with variables α_i , again with a unique optimum
- At optimum, will have implicitly computed the optimal hyperplane $\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i$
- The data only appears through the kernel function $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- Full derivation requires techniques of optimization theory, which we will skip here

Rewriting in terms of Primal Variables

Dual problem (from previous slide)

$$\max_{0 \leq \mu_i \leq 1/N} \sum_{i=1}^N \mu_i - \frac{1}{4\lambda} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \mu_i \mu_j K(x_i, x_j)$$

Since the primal variable α and the dual variable μ are related by $\alpha_i = \frac{\mu_i y_i}{2\lambda}$, it can be written in the form of primal variables as follows

writing in terms of primal variable α

$$\max_{\alpha \in \mathbb{R}^N} 2 \sum_{i=1}^N \alpha_i y_i - \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j K(x_i, x_j)$$

such that

$$0 \leq y_i \alpha_i \leq \frac{1}{2\lambda N} \text{ for } i = 1, \dots, N$$

The above can be solved using a standard Quadratic program solver.

Back to Representer Theorem

- Once we have the α from the previous slide, the decision function in RKHS is constructed using representer theorem:

$$f(.) = \sum_{j=1}^N \alpha_j k(., x_j)$$

- However, if N is large, this might still be computationally expensive for prediction
- In order to tackle this, the complementarity conditions (next) motivate the idea of *support vectors*, which we see next.

Complementarity conditions at the optimum

(Check corresponding slide from previous Lecture on Complementary Slackness)

- These are given by the product of the dual variables and the corresponding constraint as follows :

$$\mu_i[y_i f(x_i) + \xi_i - 1] = 0$$

$$\nu_i \xi_i = 0$$

- Recalling that $\mu_i = \frac{2\lambda\alpha_i}{y_i}$ and $\nu_i = \frac{1}{N} - \frac{2\lambda\alpha_i}{y_i}$
- In terms of the primal variable α , the above can be re-written as

$$\alpha_i[y_i f(x_i) + \xi_i - 1] = 0$$

$$\left(\alpha_i - \frac{y_i}{2\lambda N}\right) \xi_i = 0$$

Complementarity Conditions

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- If $\alpha_i = 0$, then the second constraint is active : $\xi_i = 0$. This implies $y_i f(x_i) \geq 1$ (Why?). (*These are correctly classified points with some margin*)

Complementarity Conditions

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- If $\alpha_i = 0$, then the second constraint is active : $\xi_i = 0$. This implies $y_i f(x_i) \geq 1$ (Why?). (*These are correctly classified points with some margin*)
- If $0 < y_i \alpha_i < \frac{1}{2\lambda N}$, then both the constraints are active, i.e., $\xi_i = 0$ and $y_i f(x_i) + \xi_i - 1 = 0$. This leads to $y_i f(x_i) = 1$. (*These are correctly classified points right at the margin*)

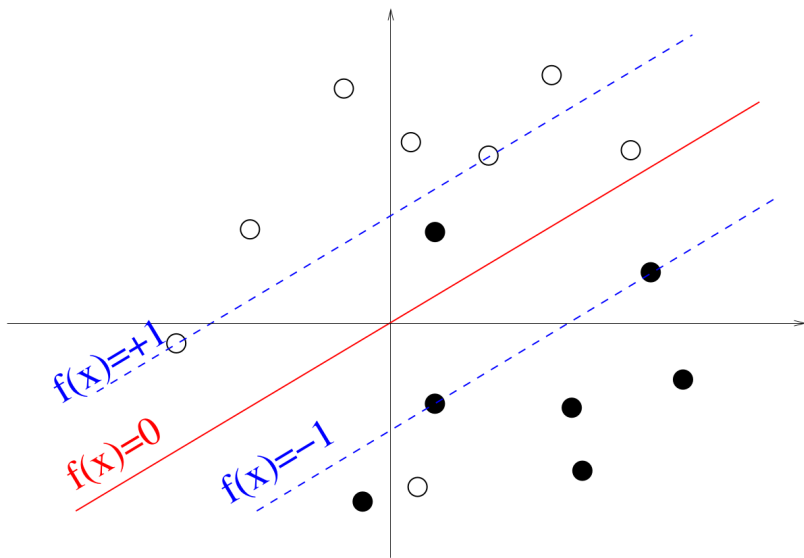
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- If $0 < y_i \alpha_i < \frac{1}{2\lambda N}$, then both the constraints are active, i.e., $\xi_i = 0$ and $y_i f(x_i) + \xi_i - 1 = 0$. This leads to $y_i f(x_i) = 1$. (*These are correctly classified points right at the margin*)
- If $\alpha_i = \frac{y_i}{2\lambda N}$, then the second constraint is not active ($\xi_i \geq 0$) but the first one is active : $y_i f(x_i) + \xi_i = 1$. This implies that $y_i f(x_i) \leq 1$. (*These points may be correctly or incorrectly classified points*)

Decision Hyperplanes



Pictorial Depiction for α values

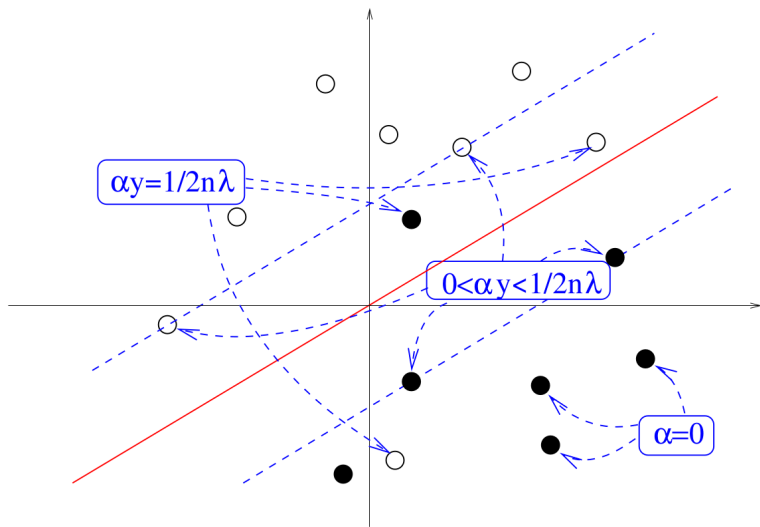


Figure: n in the figure above corresponds to N in our notation

- From Representer theorem, the function evaluation at any $x \in \mathcal{X}$ (the input space) is given by

$$f(x) = \sum_{i=1}^N \alpha_i k(x_i, x) = \sum_{i \in SV} \alpha_i k(x_i, x)$$

where SV is the set of support vectors i.e. those training points for which $\alpha_i \neq 0$

- Hence the name Support Vector Machines
- The above sparsity of $\alpha \in \mathbb{R}^N$ can be used for
 - Faster prediction since one needs to go over only the support vectors

Another variant - C-SVM

Sometimes, instead of the regularization parameter λ , the SVM problem is written in the following form :

$$\min_{f \in \mathcal{H}} \left\{ C \sum_{i=1}^N (\ell_{\text{hinge}}(y_i [K\alpha]_i))^2 + \frac{1}{2} \|f\|_{\mathcal{H}}^2 \right\}$$

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- This is equivalent to the original formulation on the first slide ($\min_{f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^N \ell_{\text{hinge}}(y_i f(x_i)) + \lambda \|f\|_{\mathcal{H}}^2$) with $C = \frac{1}{2N\lambda}$

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- Using the Lagrangian formulation, the dual can be written as

$$\max_{\alpha \in \mathbb{R}^N} 2 \sum_{i=1}^N \alpha_i y_i - \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j K(x_i, x_j)$$

such that

$$0 \leq y_i \alpha_i \leq C \text{ for } i = 1, \dots, N \text{ (also called box constraints)}$$

- Most of the material for this lecture is based on a similar course by Julien Mairal's at ENS Paris
- Further details (with somewhat different notation) on SVMs - JST & Christianini book, Chapter 7