

Lecture 5

Support Vector Machines Support Vector Machines

Outline

- ► Lagrange Duality
- ► KKT optimality conditions
- ► Large margin classifiers
- Hard-margin SVM (Primal / Dual)
- ► Soft-margin SVM (Primal)
- Kernel SVM
- SVM and Hinge Loss
- ► SVM beyond Classification
- Applications

Lagrange Duality (1)

▶ We consider optimization problem in **canonical** form:

minimize
$$f_0(x)$$

subject to $f_i(x) \leq 0$, $i = 1, ..., m$
 $h_i(x) = 0$, $i = 1, ..., p$

▶ The **Lagrange function** \mathcal{L} : $\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ is defined as a weighted sum of the objective and constraint functions:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f_0(\mathbf{x}) + \sum_{i=1}^m \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^p \mu_i h_i(\mathbf{x}),$$

where x is called **primal** and (λ, μ) the **dual** variables.

Lagrange Duality (2)

▶ The (Lagrange) dual function $g: \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ is defined as:

$$g(\lambda, \mu) = \inf_{x \in domain(f_0)} \mathcal{L}(x, \lambda, \mu).$$

The (convex!) optimization problem

maximize
$$g(\lambda, \mu)$$
 subject to $\lambda \succeq 0$

is called the (Lagrange) dual problem.

▶ The inequality $d^* \leq p^*$ always holds, where p^* , d^* are the optimal values of the primal and dual problem, respectively.

Lagrange Duality (3)

▶ The (Lagrange) **dual function** $g: \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ is defined as:

$$g(\lambda, \mu) = \inf_{x \in \text{domain}(f_0)} \mathcal{L}(x, \lambda, \mu).$$

► The (convex!) optimization problem

maximize
$$g(\lambda, \mu)$$
 subject to $\lambda \succ 0$

is called the (Lagrange) dual problem.

▶ The inequality $d^* \leq p^*$ always holds, where p^* , d^* are the optimal values of the primal and dual problem, respectively. We refer to the difference $p^* - d^*$ as duality gap. In the case $p^* = d^*$ we talk about **strong duality**.

Karush–Kuhn–Tucker (KKT) Conditions

Theorem: Optimality Conditions

For any optimization problem with differentiable objective and constraint functions for which strong duality obtains, any pair of primal and dual optimal (x^*, λ^*, μ^*) must satisfy KKT-conditions:

$$abla_{x}\mathcal{L}(\mathbf{x}^{*}, \boldsymbol{\lambda}^{*}, \boldsymbol{\mu}^{*}) = 0,$$
 (stationarity)
 $f_{i}(\mathbf{x}^{*}) \leqslant 0,$ (primal feasibility)
 $h_{i}(\mathbf{x}^{*}) = 0,$ (primal feasibility)
 $\lambda_{i}^{*} \geqslant 0,$ (dual feasibility)
 $\lambda_{i}^{*} \cdot f_{i}(\mathbf{x}^{*}) = 0$ (complementary slackness)

For any convex problem, the KKT-conditions are sufficient for (x^*, λ^*, μ^*) to be optimal with zero duality gap.

Slater's Theorem

We say that a convex optimization problem

minimize
$$f_0(\mathbf{x})$$

subject to $f_i(\mathbf{x}) \leq 0$, $i = 1, ..., m$
 $h_i(\mathbf{x}) = 0$, $i = 1, ..., p$

satisfies the Slater's condition if there exists a strictly feasible point x, i.e., $f_i(x) < 0$ and $h_j(x) = 0$ for all i, j.

Slater's Theorem

For any convex problem for which Slater's condition holds, the KKT-conditions provide necessary and sufficient condition for (x^*, λ^*, μ^*) to be primal and dual optimal with zero duality gap.

Linear Classifiers with Margin

- Let $\phi(\mathbf{x})$ be some feature map mapping the data in \mathbb{R}^d to some feature space \mathbb{R}^D .
- We consider functions of the type $f_{\theta}: \mathbb{R}^d \to \mathbb{R}$ with $f_{\theta}(\mathbf{x}) = \text{sign}(\mathbf{w}^{\top} \phi(\mathbf{x}) + b)$, where $\theta = (\mathbf{w}, b)$ denotes the parameters.
- We consider functions that classify with some margin:

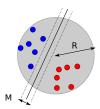
$$\mathcal{F} = \left\{ \mathit{f}_{\theta} \colon \theta \in \mathbb{R}^{d+1} \right.$$
 ,

$$\forall_{i=1}^n: |\mathbf{w}^\top \phi(\mathbf{x}_i) + b| \ge 1, \frac{2}{\|\mathbf{w}\|} = M$$

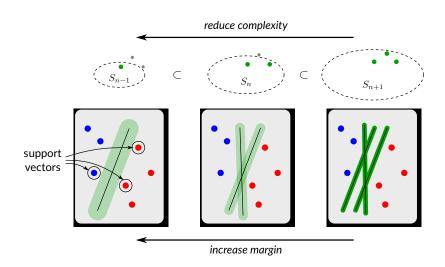
The VC-dimension can be bounded as

$$h_{\mathcal{F}} \leq \min\left\{d+1, \left\lceil \frac{4R^2}{M^2} \right\rceil + 1\right\}$$

(cf. Burges 1998).



Support Vector Machine (SVM)

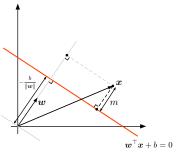


Hard-Margin SVM (Derivation)

▶ Given data $\{(x_1, y_1), ..., (x_n, y_n)\}$ with $y_i \in \{-1, 1\}$, we want to maximize the separation margin of the linear classifier $y(x) = w^\top x + b$:

$$\underset{\boldsymbol{w},b}{\mathsf{maximize}} \ \frac{1}{\|\boldsymbol{w}\|} \underset{i=1,\dots,n}{\mathsf{min}} y_i (\boldsymbol{w}^\top \boldsymbol{x_i} + b)$$

▶ Observation: rescaling $\mathbf{w} \mapsto k\mathbf{w}$ and $\mathbf{b} \mapsto k\mathbf{b}$, $k \neq 0$ results in the same objective value. We can use this fact to set $\min_{i=1,...,n} y_i(\mathbf{w}^\top \mathbf{x}_i + b) = 1$.



$$m = \frac{\boldsymbol{w}^{\top} \boldsymbol{x}}{\|\boldsymbol{w}\|} - (-\frac{b}{\|\boldsymbol{w}\|}) = \frac{\boldsymbol{w}^{\top} \boldsymbol{x} + b}{\|\boldsymbol{w}\|}$$

Hard-Margin SVM (Derivation)

► This gives the following optimization problem

$$\underset{\boldsymbol{w},b}{\text{maximize}} \ \frac{1}{\|\boldsymbol{w}\|} \quad \text{subject to} \quad \underset{i=1,\dots,n}{\text{min}} y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) = 1$$

or equivalently

minimize
$$\frac{1}{2} \| \mathbf{w} \|^2$$
 subject to $y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geqslant 1, i = 1, ..., n$

Replacing x by (non-linear) features $\phi(x)$ gives the (primal) hard-margin formulation of the Support Vector Machine:

minimize
$$\frac{1}{2} \| \boldsymbol{w} \|^2$$
 subject to $y_i(\boldsymbol{w}^{\top} \phi(\boldsymbol{x}_i) + b) \geqslant 1, i = 1, ..., n$

Hard-Margin SVM (Primal Problem)

1. The classifier with largest margin between the positive and negative data points $\{(x_i, y_i)\}_{i=1,\dots,n}$ can be obtained by solving a convex optimization problem:

minimize
$$\frac{1}{2} \| \boldsymbol{w} \|^2$$

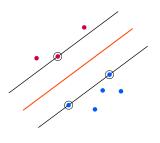
subject to $y_i(\boldsymbol{w}^{\top} \boldsymbol{\phi}(\boldsymbol{x}_i) + b) \geqslant 1$, $i = 1, ..., n$

2. The decision function $f: \mathbb{R}^d \to \{1, -1\}$ is given by

$$f(\mathbf{x}) = \operatorname{sign}(\mathbf{w}^{\top} \phi(\mathbf{x}) + b)$$

and it can be used to classify new data.

3. Data points (\mathbf{x}_i, y_i) where a corresponding constraint is active, i. e., $y_i(\mathbf{w}^{\top}\phi(\mathbf{x}_i) + b) = 1$ are called **support vectors**.



Deriving the Dual of the Hard-Margin SVM

► Consider the hard-margin formulation of SVM

minimize
$$\frac{1}{2} \| \boldsymbol{w} \|^2$$
 subject to $y_i(\boldsymbol{w}^{\top} \phi(\boldsymbol{x}_i) + b) \geqslant 1$, $i = 1, ..., n$

Write the Lagrangian

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \|\boldsymbol{w}\|^2 + \sum_{i=1}^{n} \alpha_i (1 - y_i(\boldsymbol{w}^{\top} \phi(\boldsymbol{x}) + b))$$

▶ Compute the dual function $g(\alpha) = \inf_{w,b} \mathcal{L}(w, b, \alpha)$:

$$g(\boldsymbol{\alpha}) = \begin{cases} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle, & \text{if } \sum_{i=1}^{n} \alpha_i y_i = 0 \\ -\infty & \text{else} \end{cases}$$

where we used the fact that \mathcal{L} is strictly convex and

$$\nabla_{\mathbf{w}} \mathcal{L} = \mathbf{0} \implies \mathbf{w} = \sum_{i=1}^{n} \alpha_{i} y_{i} \phi(\mathbf{x}_{i})$$
 and $\frac{\partial \mathcal{L}}{\partial b} = 0 \implies \sum_{i=1}^{n} \alpha_{i} y_{i} = 0$

Hard-Margin SVM (Dual Problem)

▶ The dual problem has the following form:

Due to the relationship $\mathbf{w} = \sum \alpha_i y_i \phi(\mathbf{x}_i)$ the decision function is given as

$$f(x) = \sum_{i=1}^{n} \alpha_{i} y_{i} \langle \phi(x_{i}), \phi(x) \rangle + b$$

How do we find the bias b? Note that for each support vector $x_i \in S$, it holds $y_i \cdot f(x_i) = 1$, where S denotes the set of support vectors. Here, it is enough to use one arbitrary support vector to compute b. However, the following provides numerically more stable solution:

$$b = \frac{1}{|S|} \sum_{i \in S} (y_i - \sum_{j \in S} \alpha_j y_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle)$$

Hard-Margin SVM (Dual Problem)

On the previous slide we saw how to compute bias in the dual formulation:

$$b = \frac{1}{|S|} \sum_{i \in S} (y_i - \sum_{j \in S} \alpha_j y_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle)$$

The remaining question here is how to find S.

▶ Based on the complementary slackness in the KKT-conditions

$$\alpha_i \cdot (1 - y_i(\mathbf{w}^{\top} \phi(\mathbf{x}_i) + b)) = 0$$

we conclude

 x_i is a support vector $\Leftrightarrow \alpha_i > 0$.

Soft-Margin SVM (Primal Problem)

F. (松弛变量): 用于度量样本 g. 违反间隔的程度 确保数据点可以在某种程度上被错误分类。

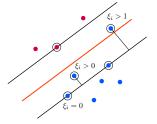
C(正则化参数): 权衡间隔大小和误分类代价。C越大,模型对误分类的容忍度越低(趋向 Hard Marqin);C越小,模型允许更多误分类(更趋向 Soft Marqin)。

1. If the data $\{(x_i, y_i)\}_{i=1,\dots,n}$ is not separable (e.g. due to noise), we introduce slack variables $(\xi_i)_i$ that allows for data points to violate the margin constraints at the cost of additional penalty. We refer to this formulation as **soft-margin** SVM:

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$$

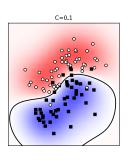
subject to
$$y_i(\mathbf{w}^\top \phi(\mathbf{x}_i) + b) \geqslant 1 - \xi_i, \quad i = 1, ..., n$$
$$\xi_i \geqslant 0, \qquad \qquad i = 1, ..., n$$

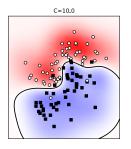
- 2. Here, $C \in (0,\infty)$ is a regularization constant controlling the trade-off between the margin size and the constraint violation. For $C \to \infty$ we recover the hard-margin formulation.
- 3. Data points (x_i, y_i) for which either $\xi_i > 0$ or $y_i(\mathbf{w}^{\top}\phi(x_i) + b) = 1$ holds are called **support vectors**.

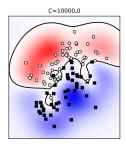


Effect of the parameter C

The larger the parameter C the more the decision boundary is forced to correctly classify every data point. For $C \to \infty$ we recover the hard-margin formulation. For $C \to 0$ the robustness of "correctly" classified points increases.







Kernel Functions

Definition (Kernel function)

A kernel is a function $\kappa \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ that for all $x, y \in \mathcal{X}$ satisfies

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

where $\phi \colon \mathcal{X} \to \mathcal{F}$ is a mapping from some \mathcal{X} to a Hilbert space $(\mathcal{F}, \langle \cdot, \cdot \rangle)$.

Definition (Finitely positive semi-definite functions)

A function $\kappa\colon \mathcal{X}\times\mathcal{X}\to\mathbb{R}$ satisfies the finitely positive semi-definite property if it is symmetric and for which the matrices formed by restriction to any finite subset of the space \mathcal{X} are positive semi-definite.

Theorem (Kernel matrices)

The kernel functions satisfy the finitely positive semi-definite property. That is, the corresponding kernel matrices are positive semi-definite.

Examples of Kernels

Observation: In the SVM dual form, we never need to access the feature map $\phi(\cdot)$ explicitly. Instead, we can always express computations in terms of the kernel function.

Examples of commonly used kernels satisfying the Mercer property are:

$$\begin{array}{ll} \text{Linear} & k(\mathbf{x},\mathbf{x}') = \langle \mathbf{x},\mathbf{x}' \rangle \\ \text{Polynomial} & k(\mathbf{x},\mathbf{x}') = (\langle \mathbf{x},\mathbf{x}' \rangle + \beta)^{\gamma} & \beta \in \mathbb{R}_{\geq 0}, \gamma \in \mathbb{N} \\ \text{Gaussian} & k(\mathbf{x},\mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2) & \gamma \in \mathbb{R}_{> 0} \end{array}$$

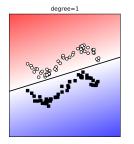
Note: The feature map associated to the Gaussian kernel is infinite-dimensional. However, in the dual form, we never need to access it for training and prediction, and we only need the kernel function.

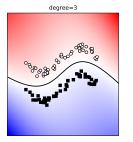
SVM with Polynomial Kernel

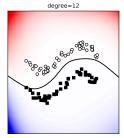
The SVM decision function

$$g(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i y_i \underbrace{(\langle \mathbf{x}_i, \mathbf{x} \rangle + a)^{\gamma}}_{k(\mathbf{x}_i, \mathbf{x})} + b$$

is polynomial of degree γ .







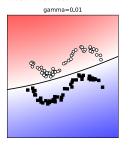
Observation: The polynomial decision function has very high value in the extrapolation regime.

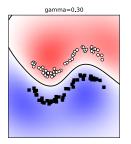
SVM with Gaussian Kernel

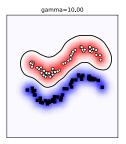
The SVM decision function

$$g(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i y_i \underbrace{\exp(-\gamma \|\mathbf{x}_i - \mathbf{x}\|^2)}_{k(\mathbf{x}_i, \mathbf{x})} + b$$

is a superposition of 'bump' functions. Intermediate values of γ usually give the best results.







More Advanced Kernels

More advanced kernels can be used to incorporate prior knowledge into the classifier, and to let the algorithm operate on non-vector data.

Examples:

- Bag-of-words kernels (text classification, image recognition)
- Tree kernels (text classification)
- Weighted degree kernel (bioinformatics)
- Graph kernels

Some of these kernels will be studied in Machine Learning 2.

Computational Requirements of SVMs

Computation required by the primal

- ▶ Optimization of a vector (\mathbf{w}, b) in \mathbb{R}^{d+1} subject to n constraints.
- \triangleright Primal is infeasible when d is very large (e.g. infinite-dimensional).

Computation required by the dual

- Computation of a kernel matrix K of size $n \times n$ with $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$
- \triangleright Dual is infeasible when n is large (e.g. 1 million data points).

What if both n and d are large?

- Random features (approximates infinite-dimensional feature maps through randomization).
- Neural networks (learns an efficient feature map of size $\ll D$).

SVM and **Hinge** Loss

Recall that our decision boundary is defined by $g(\mathbf{x}) = \mathbf{w}^{\top} \phi(\mathbf{x}_i) + b$, and therefore, we can write the constraint as:

$$\xi_i \geq 1 - y_i \cdot g(\mathbf{x})$$

Together with $\xi_i \geqslant 0$ this implies

$$\xi_i = \max(0, 1 - y_i \cdot g(\mathbf{x}))$$

By injecting it directly in the objective we get an unconstrained optimization problem

$$\min_{\mathbf{w}, b, \boldsymbol{\xi}} \quad \underbrace{\frac{1}{2} \|\mathbf{w}\|^2}_{\mathcal{E}_{\text{reg}}} + \underbrace{C \sum_{i=1}^{N} \underbrace{\max \left(0, 1 - y_i \cdot g(\mathbf{x})\right)}_{\mathcal{E}_{\text{emp}}}}_{\mathcal{E}_{\text{emp}}}$$

i.e. we optimize the sum of a fitting term and a regularization term (as we do e.g. for logistic regression but with a different loss function).

SVM Beyond Classification

Support vector data description (SVDD):

Consider an *unlabeled* dataset $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$. We would like to find the smallest enclosing sphere of the data, i.e.

$$\min_{R,c} R^2$$

subject to the constraints

$$\forall_{i=1}^n: \|\phi(\mathbf{x}_i) - \mathbf{c}\|^2 \le R^2.$$

We consider a point to be anomalous if the point exceeds a certain distance from the center \mathbf{c} , i.e.

$$f(\mathbf{x}) = \text{sign}(\|\phi(\mathbf{x}) - \mathbf{c}\| - \tau)$$

Note: Like for the SVM, the SVDD algorithm also has a dual form, it can expressed in terms of kernels, and we can add slack variables to it.



SVM Beyond Classification

Support vector regression (SVR):

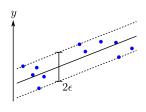
Consider a *labeled* regression dataset $\mathcal{D} = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)\}$ with $y_i \in \mathbb{R}$. We would like to build the regression model

$$\min_{\mathbf{w},b} \|\mathbf{w}\|^2$$

subject to the constraints

$$\forall_{i=1}^n: |w^\top \phi(\mathbf{x}_i) + b - y_i| \le \epsilon$$

Note: Like for the SVM, support vector regression has a dual form, it can be kernelized, and we can add slack variables to it. With the slack variables, the constraints above can also be seen as applying an ϵ -sensitive loss.



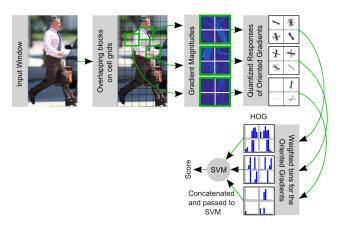
SVM for Text Categorization

Precision/recall-breakeven point on the ten most frequent Reuters categories and microaveraged performance over all Reuters categories.

					SVM (poly)					SVM (rbf)			
					degree $d =$					width $\gamma =$			
	Bayes	Rocchio	C4.5	k-NN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	98.5	98.4	98.3	98.5	98.5	98.4	98.3
acq	91.5	92.1	85.3						95.3				
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	76.2	74.0	75.4	76.3	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	92.4	91.3	89.9	93.1	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	88.9	87.8	88.9	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	77.1	76.9	78.0	77.8	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	76.2	74.4	75.0	76.2	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	86.5	86.0	85.4	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	85.9	83.8	85.2	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	85.7	83.9	85.1	85.7	85.7	84.5
microavg.	72.0	79.9	79.4	82.3	84.2				85.9				
					combined: 86.0				combined: 86.4				

Source: Joachims et al. 1998, Text categorization with Support Vector Machines: Learning with many relevant features

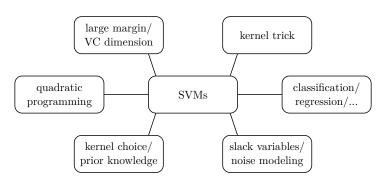
SVM/HoG for Pedestrian Detection



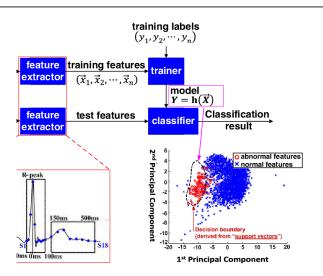
Source: Dutta 2015, Pedestrian Detection using HOG and SVM in Automotives

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Visual Summary



SVM for **ECG**-based arrhythmia Detection



Wang et al. (2014), Hardware Specialization in Low-power Sensing Applications to Address Energy and Resilience