LEC 6: Support Vector Machine (SVM)

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October 29, 2016

Outline

- Binary SVM
  - Linearly separable, no outliers
  - Linearly separable, with outliers
  - Nonlinearly separable (Kernel SVM)
- Multiclass SVM
  - One-versus-one
  - One-versus-rest
- Practical issues

Main references

- **Olga Veksler's lecture**

  `http://www.csd.uwo.ca/~olga/Courses/CS434a_541a/Lecture11.pdf`

- **Jeff Howbert's lecture**

  `http://courses.washington.edu/css581/lecture_slides/16_support_vector_machines.pdf`

- **Chris Burges' tutorial**

  `http://research.microsoft.com/pubs/67119/svmtutorial.pdf`

What is SVM?

Recall that both LDA and Logistic regression are obtained from probabilistic models:

- Mixture of Gaussians $\mapsto$ LDA
- Bernoulli/multinomial $\mapsto$ Logistic regression

We also know that their decision boundaries (in the input space) are hyperplanes (thus, they are linear classifiers).

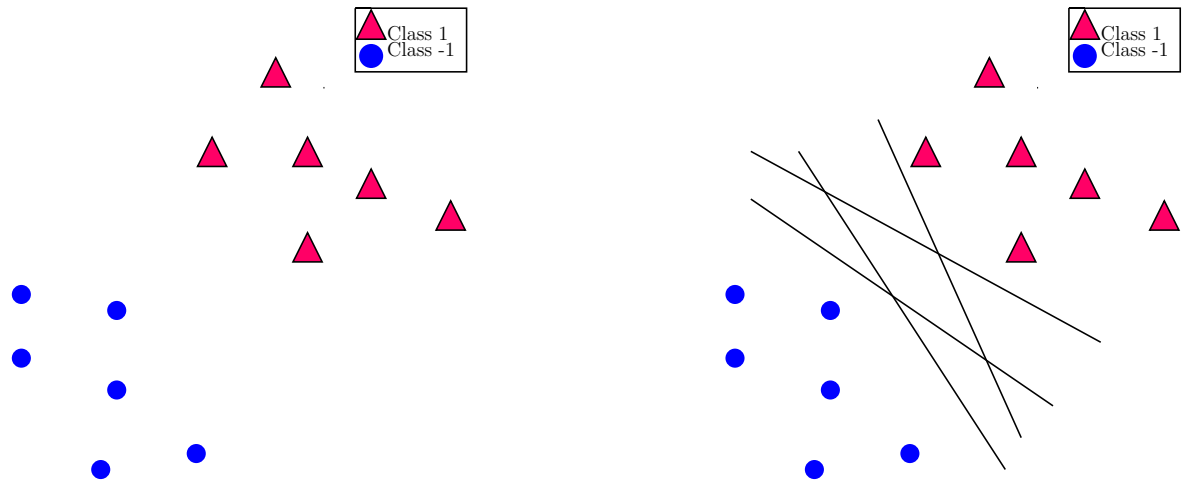
SVM is another linear classifier but seeks to find an '*optimal*' boundary.

It was invented by Vapnik (during the end of last century) and considered one of the major developments in pattern recognition.

Binary SVM: Linearly separable (no outliers)

Support Vector Machine (SVM)

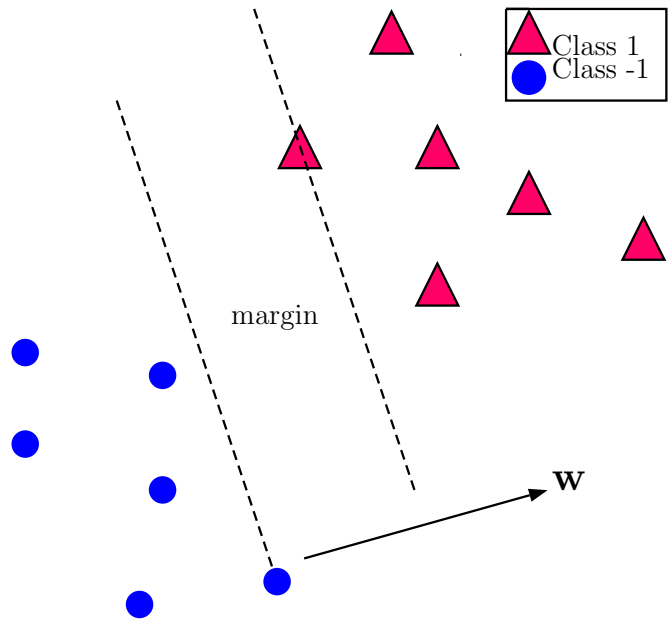
To introduce the idea of SVM, we consider binary classification first.

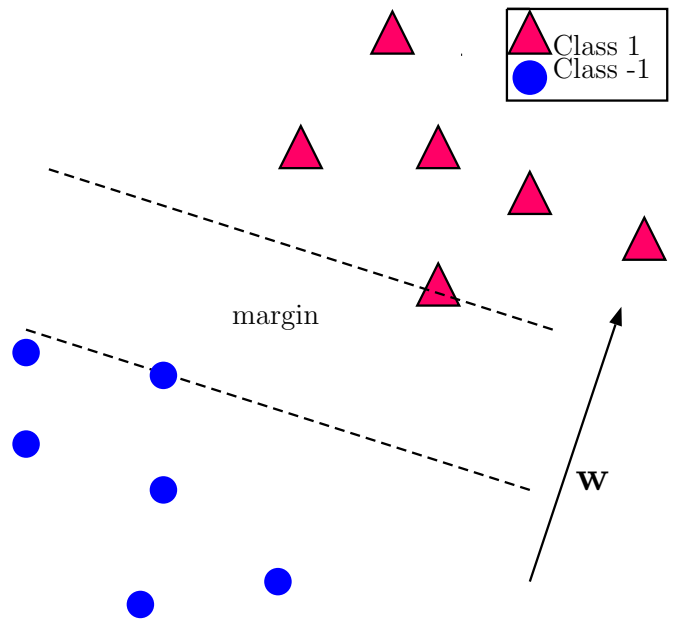


SVM effectively compares (under some criterion) all hyperplanes $\mathbf{w} \cdot \mathbf{x} + b = 0$, where $\mathbf{w}$ is a normal vector while b determines location.

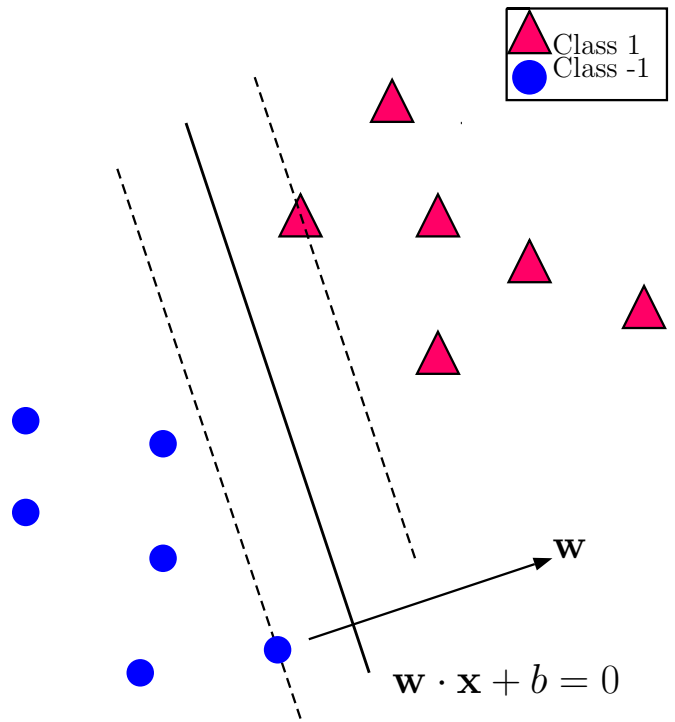
The following specifies how to logically think about the problem:

- Any fixed direction $\mathbf{w}$ determines a unique margin.

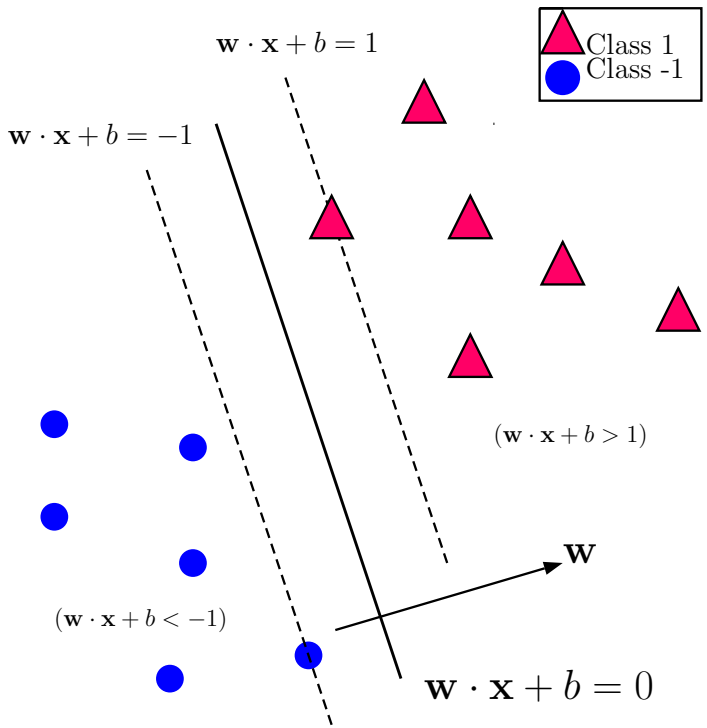




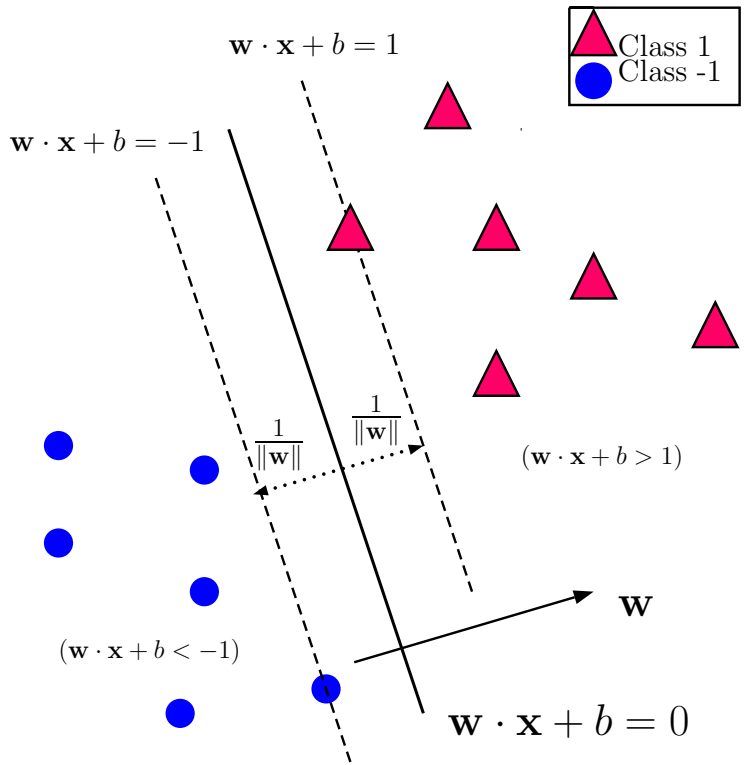
- We select b such that the center hyperplane is given by $\mathbf{w} \cdot \mathbf{x} + b = 0$. This is the **optimal** boundary *orthogonal to the given direction* $\mathbf{w}$, as it is equally far from the two classes.



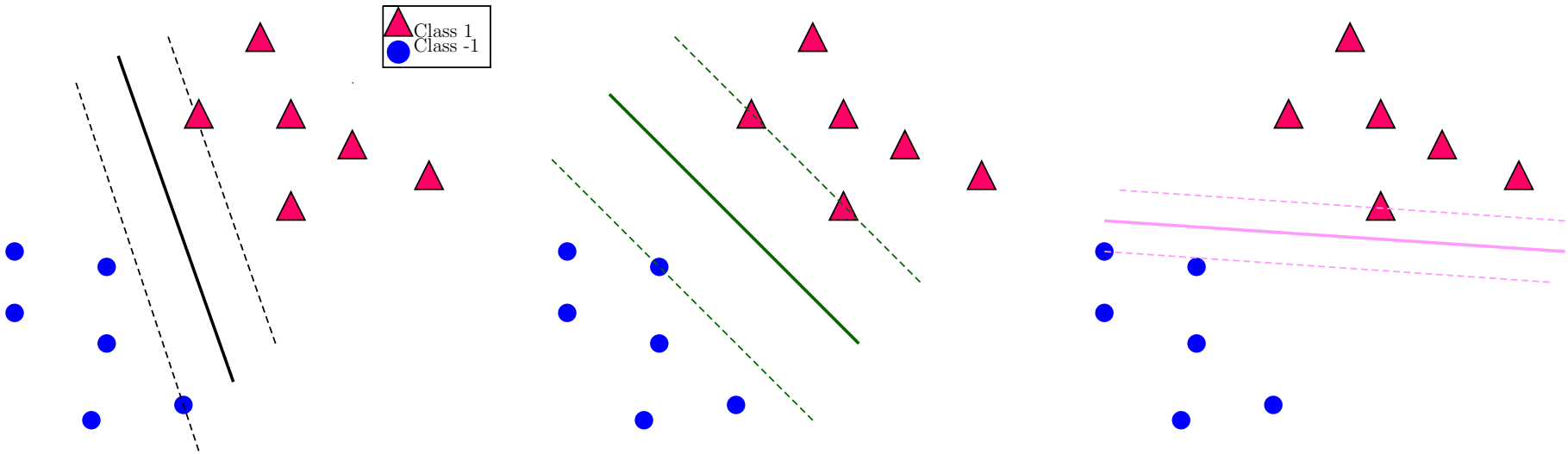
- Any scalar multiple of $\mathbf{w}$ and b denotes the same hyperplane. To uniquely fix the two parameters, we require the margin boundaries to have equations $\mathbf{w} \cdot \mathbf{x} + b = \pm 1$.



- Under such requirements, we can show that the margin between the two classes is exactly $\frac{2}{\|\mathbf{w}\|_2}$.



The larger the margin, the better the classifier



The binary SVM problem

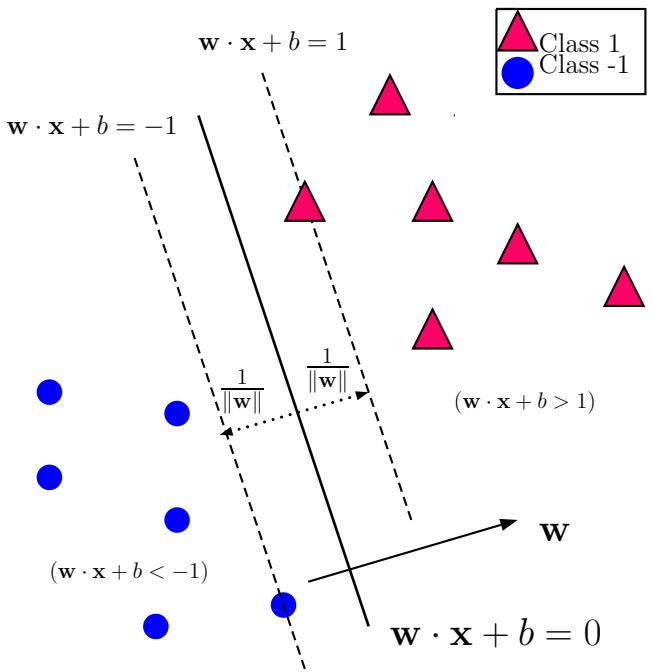
Problem. Given training data $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ with labels $y_i = \pm 1$, SVM finds the optimal separating hyperplane by maximizing the class margin.

Specifically, it tries to solve

$$\max_{\mathbf{w},b} \frac{2}{\|\mathbf{w}\|_2} \quad \text{subject to}$$

$$\mathbf{w} \cdot \mathbf{x}_i + b \geq 1, \quad \text{if } y_i = +1;$$

$$\mathbf{w} \cdot \mathbf{x}_i + b \leq -1, \quad \text{if } y_i = -1$$



Remark. The classification rule for new data $\mathbf{x}$ is $y = \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$.

A more convenient formulation

The previous problem is equivalent to

$$\min_{\mathbf{w},b} \ \frac{1}{2}\|\mathbf{w}\|_2^2 \qquad \text{subject to} \quad y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 \text{ for all } 1 \leq i \leq n.$$

This is an optimization problem with linear, inequality constraints.

Remarks:

- The constraints determine a convex region enclosed by hyperplanes.
- The objective function is quadratic (also convex).
- This problem thus has a unique global solution.

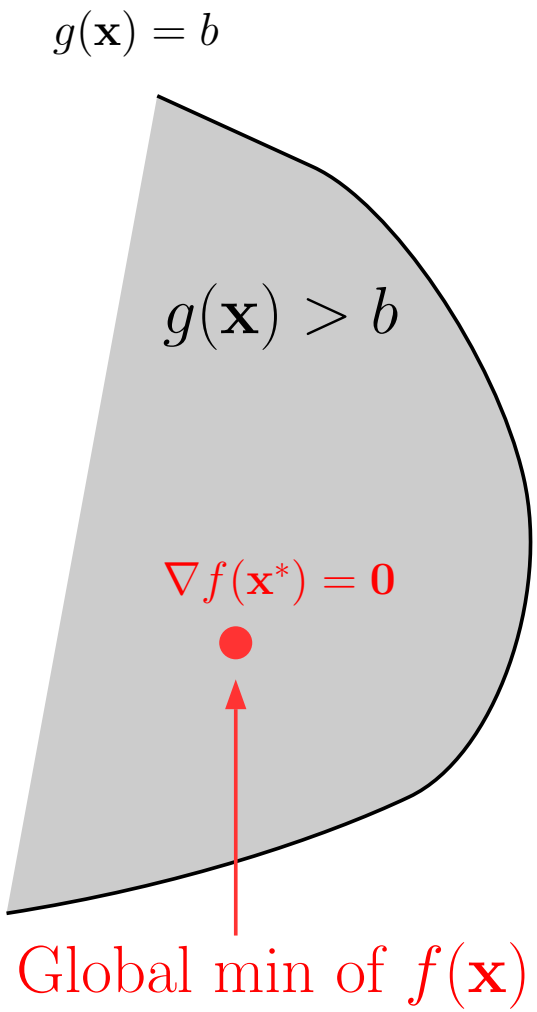
Review of multivariable calculus

Consider the following **constrained optimization** problem

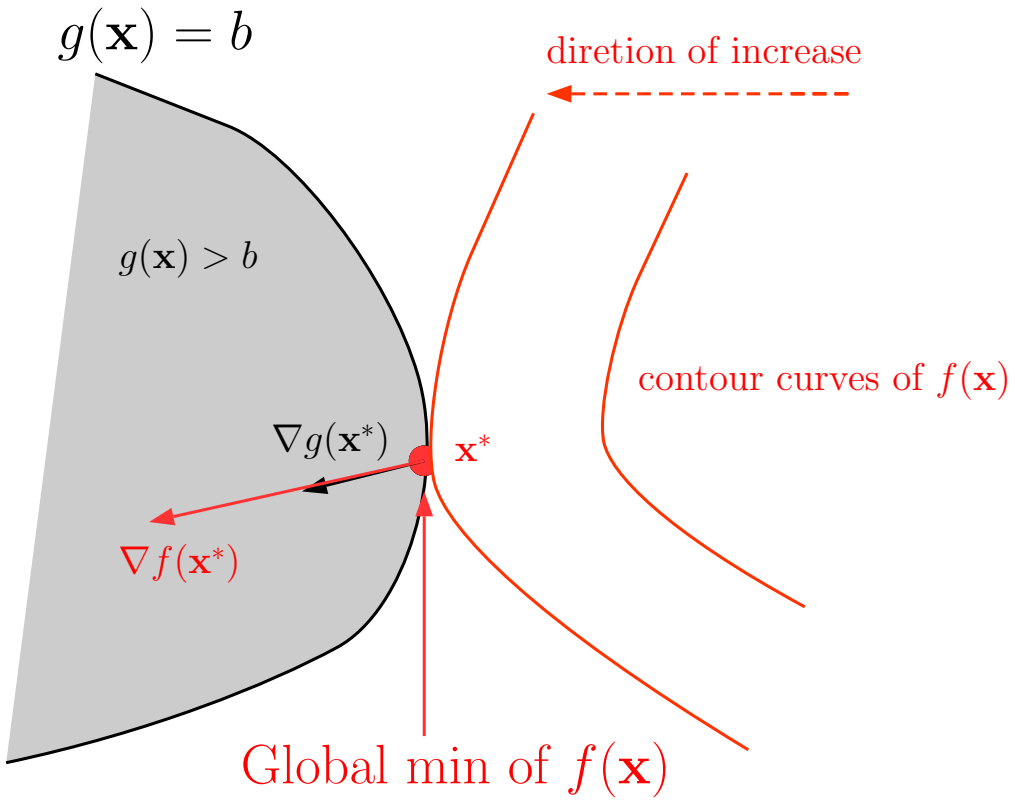
$$\min f(\mathbf{x}) \qquad \text{subject to} \quad g(\mathbf{x}) \geq b$$

There are two cases regarding where the global minimum of $f(\mathbf{x})$ is attained:

(1) At an *interior* point $\mathbf{x}^*$ (i.e., $g(\mathbf{x}^*) > b$). In this case $\mathbf{x}^*$ is just a critical point of $f(\mathbf{x})$.


$g(\mathbf{x}) = b$
$g(\mathbf{x}) > b$
$\nabla f(\mathbf{x}^*) = \mathbf{0}$
Global min of $f(\mathbf{x})$

(2) At a *boundary* point $\mathbf{x}^*$ (i.e., $g(\mathbf{x}^*) = b$). In this case, there exists a constant $\lambda > 0$ such that $\nabla f(\mathbf{x}^*) = \lambda \cdot \nabla g(\mathbf{x}^*)$.



The above two cases are unified by the **method of Lagrange multipliers**:

- Form the Lagrange function

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda(g(\mathbf{x}) - b)$$

- Find all critical points by solving

$$\begin{aligned} \nabla_{\mathbf{x}} L = \mathbf{0}: \quad \nabla f(\mathbf{x}) &= \lambda \nabla g(\mathbf{x}) \\ \lambda(g(\mathbf{x}) - b) &= 0 \\ \lambda &\geq 0 \\ g(\mathbf{x}) &\geq b \end{aligned}$$

Remark. The solutions give all candidate points for the global minimizer (one needs to compare them and pick the best one).

Remarks:

- The above equations are called Karush-Kuhn-Tucker (KKT) conditions.
- When there are multiple inequality constraints

$$\min f(\mathbf{x}) \qquad \text{subject to} \quad g_1(\mathbf{x}) \geq b_1, \ldots, g_k(\mathbf{x}) \geq b_k$$

  the method works very similarly:

– Form the Lagrange function

$$L(\mathbf{x}, \lambda_1, \ldots, \lambda_k) = f(\mathbf{x}) - \lambda_1(g_1(\mathbf{x}) - b_1) - \cdots - \lambda_k(g_k(\mathbf{x}) - b_k)$$

– Find all critical points by solving

$$\nabla_{\mathbf{x}} L = \mathbf{0}: \quad \frac{\partial L}{\partial x_1} = 0, \ldots, \frac{\partial L}{\partial x_n} = 0$$
$$\lambda_1(g_1(\mathbf{x}) - b_1) = 0, \ldots, \lambda_k(g_k(\mathbf{x}) - b_k) = 0$$
$$\lambda_1 \geq 0, \ldots, \lambda_k \geq 0$$
$$g_1(\mathbf{x}) \geq b_1, \ldots, g_k(\mathbf{x}) \geq b_k$$

and compare them to pick the best one.

Lagrange method applied to binary SVM

- The Lagrange function is

$$L(\mathbf{w}, b, \lambda_1, \ldots, \lambda_n) = \frac{1}{2}\|\mathbf{w}\|_2^2 - \sum_{i=1}^{n} \lambda_i (y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1)$$

- The KKT conditions are

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum \lambda_i y_i \mathbf{x}_i = 0, \quad \frac{\partial L}{\partial b} = \sum \lambda_i y_i = 0$$

$$\lambda_i (y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1) = 0, \ \forall i$$

$$\lambda_i \geq 0, \ \forall i$$

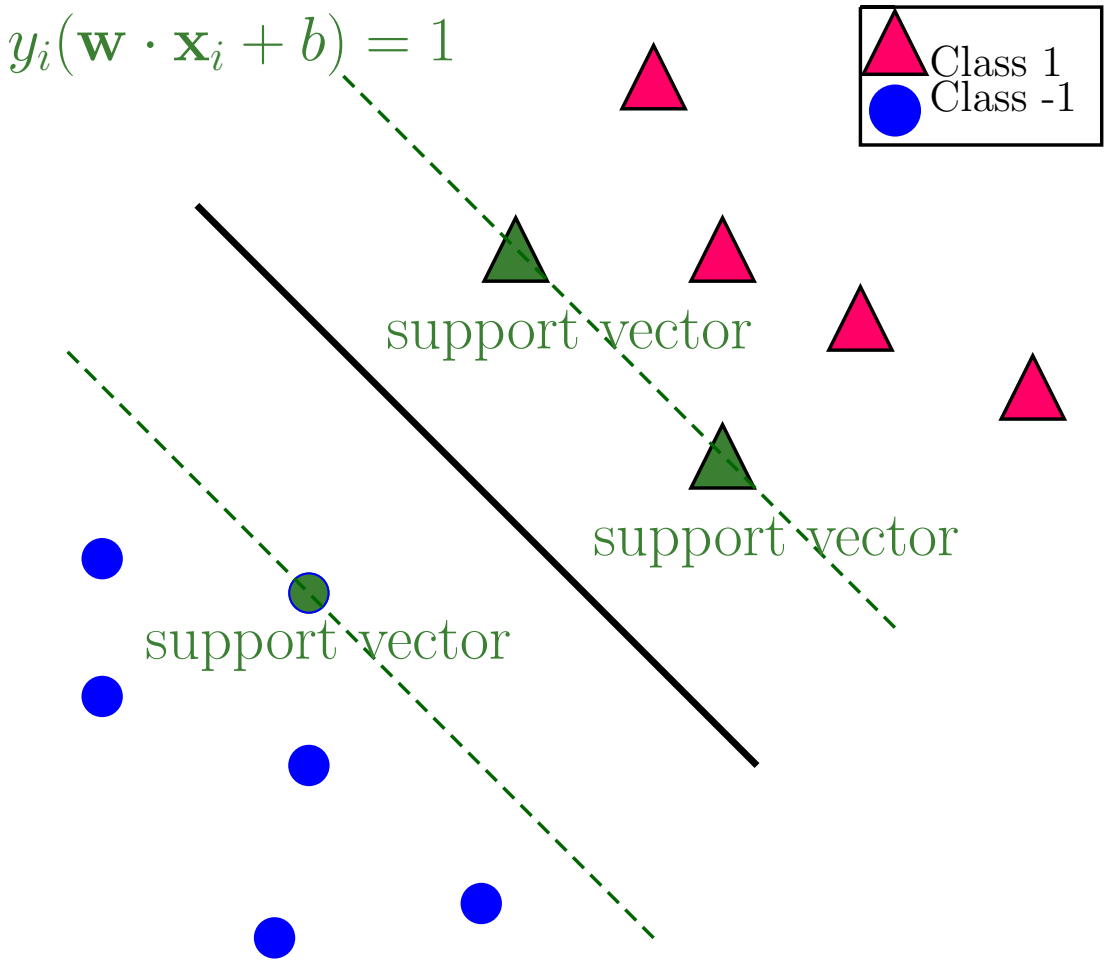
$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1, \ \forall i$$

Discussions

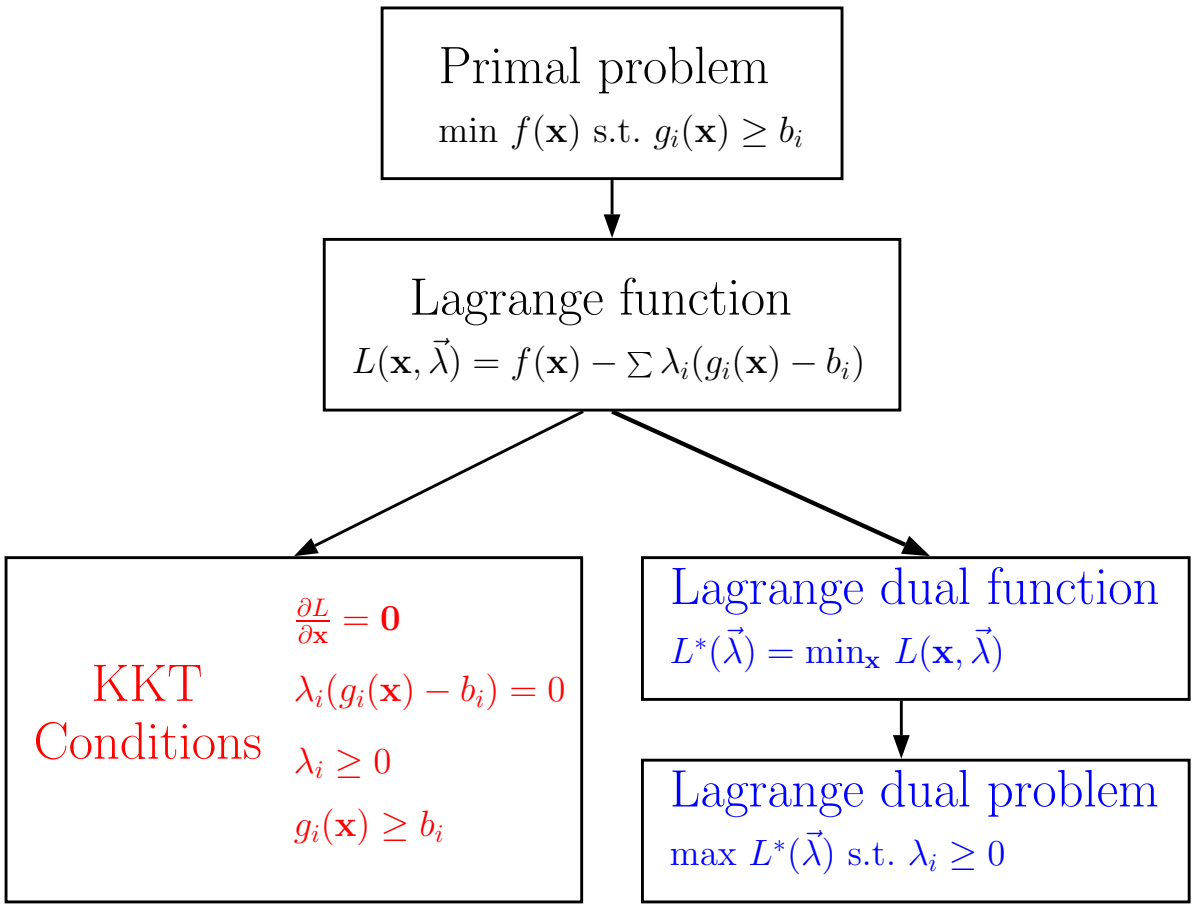
- The first condition implies that the optimal $\mathbf{w}$ is a linear combination of the training vectors:
$$\mathbf{w} = \sum \lambda_i y_i \mathbf{x}_i$$

- The second line implies that whenever $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) > 1$ (i.e., $\mathbf{x}_i$ is an interior point), we have $\lambda_i = 0$. Therefore, the optimal $\mathbf{w}$ is only a linear combination of the support vectors (i.e., those satisfying $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$).

- The optimal b can be found from any support vector $\mathbf{x}_i$ (with $\lambda_i > 0$):
$$b = \frac{1}{y_i} - \mathbf{w} \cdot \mathbf{x}_i = y_i - \mathbf{w} \cdot \mathbf{x}_i$$


$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$
Class 1
Class -1
support vector
support vector
support vector

The Lagrange dual problem



For binary SVM, the **primal** problem is

$$\min_{\mathbf{w},b} \ \frac{1}{2}\|\mathbf{w}\|_2^2 \qquad \text{subject to} \quad y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 \text{ for all } i.$$

The associated Lagrange function is

$$L(\mathbf{w}, b, \lambda_1, \ldots, \lambda_n) = \frac{1}{2}\|\mathbf{w}\|_2^2 - \sum_{i=1}^{n} \lambda_i (y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1)$$

By definition, the **Lagrange dual function** is

$$L^*(\lambda_1, \ldots, \lambda_n) = \min_{\mathbf{w},b} L(\mathbf{w}, b, \lambda_1, \ldots, \lambda_n), \quad \lambda_1 \geq 0, \ldots, \lambda_n \geq 0$$

To find the minimum of L over $\mathbf{w}, b$ (while fixing all λ_i), we set the gradient vector to zero to obtain

$$\mathbf{w} = \sum \lambda_i y_i \mathbf{x}_i, \quad \sum \lambda_i y_i = 0$$

Plugging the formula for $\mathbf{w}$ into L gives that

$$\begin{aligned} L^*(\lambda_1, \ldots, \lambda_n) &= \frac{1}{2} \left\| \sum_i \lambda_i y_i \mathbf{x}_i \right\|_2^2 - \sum_i \lambda_i \left(y_i \left(\left(\sum_j \lambda_j y_j \mathbf{x}_j \right) \cdot \mathbf{x}_i + b \right) - 1 \right) \\ &= \sum_i \lambda_i - \frac{1}{2} \sum_i \sum_j \lambda_i \lambda_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j \end{aligned}$$

with the constraints

$$\lambda_i \geq 0, \quad \sum \lambda_i y_i = 0$$

We have obtained the Lagrange dual problem for binary SVM (without outliers)

$$\max_{\lambda_1,\ldots,\lambda_n} \sum \lambda_i - \frac{1}{2}\sum_{i,j} \lambda_i \lambda_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

$$\text{subject to} \quad \lambda_i \geq 0 \text{ and } \sum \lambda_i y_i = 0$$

Remarks:

- The primal and dual problems are equivalent.
- The dual problem only depends on the number of samples (one λ per $\mathbf{x}_i$), not on their dimension.
- The dual problem can also be solved by quadratic programming.
- Samples appear only through their dot products $\mathbf{x}_i \cdot \mathbf{x}_j$, an observation to be exploited for designing nonlinear SVM classifiers.

Quadratic programming in Matlab

'**quadprog**' - Quadratic programming function (requires Optimization toolbox).

x = quadprog(H,f,A,b) attempts to solve the quadratic programming problem:

$$\min_{\mathbf{x}} \ \frac{1}{2} \cdot \mathbf{x}^T \cdot \mathbf{H} \cdot \mathbf{x} + \mathbf{f}^T \cdot \mathbf{x} \qquad \text{subject to :} \quad \mathbf{A} \cdot \mathbf{x} \leq \mathbf{b}$$

x = quadprog(H,f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints **Aeq** $\cdot$ **x = beq**.

Binary SVM via quadratic programming

In order to use the Matlab *quadprog* function, we first need to transfrom the previous formulation to the standard form

$$\min_{\lambda_1,\ldots,\lambda_n} \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x}_i\cdot\mathbf{x}_j - \sum\lambda_i$$

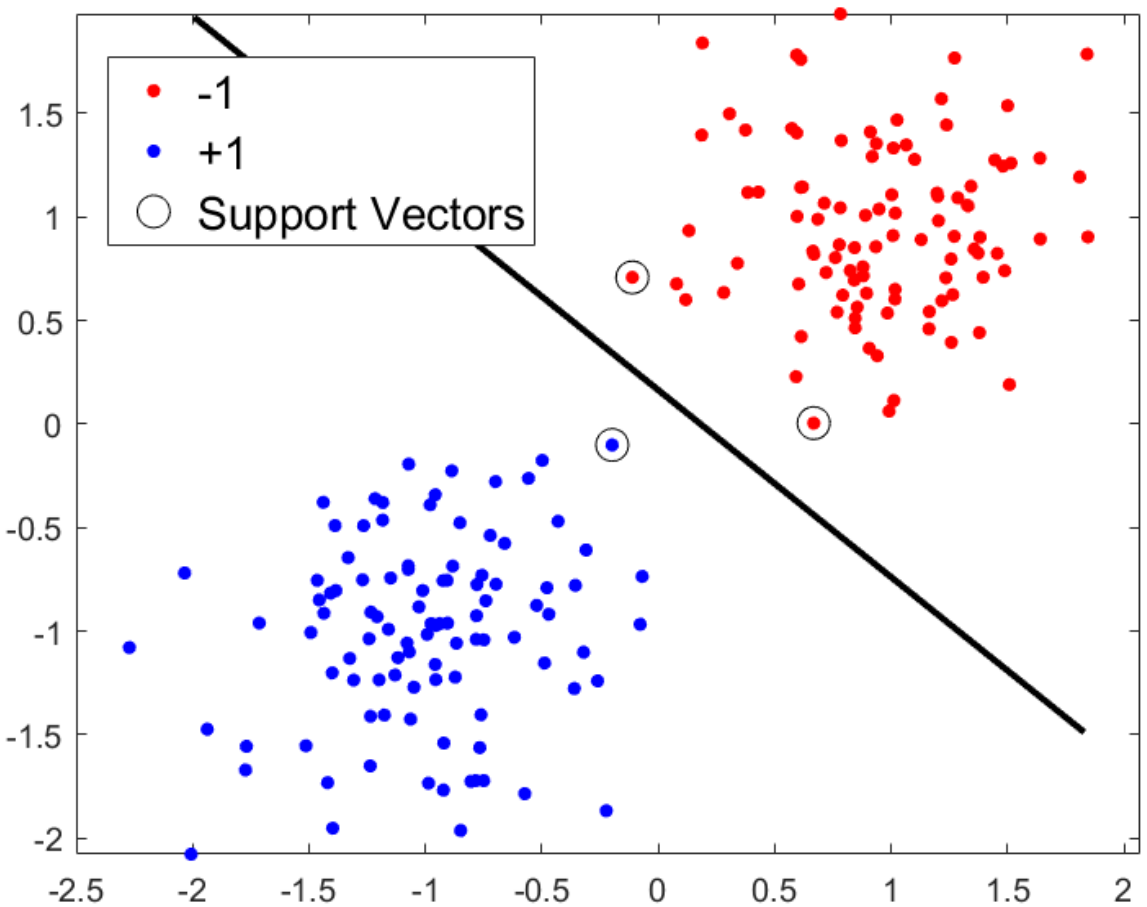
$$\text{subject to} \quad -\lambda_i \le 0 \text{ and } \sum\lambda_i y_i = 0$$

and then matrice/vectorize it:

$$\min_{\vec{\lambda}} \frac{1}{2}\vec{\lambda}^T\mathbf{H}\vec{\lambda} + \mathbf{f}^T\vec{\lambda}$$

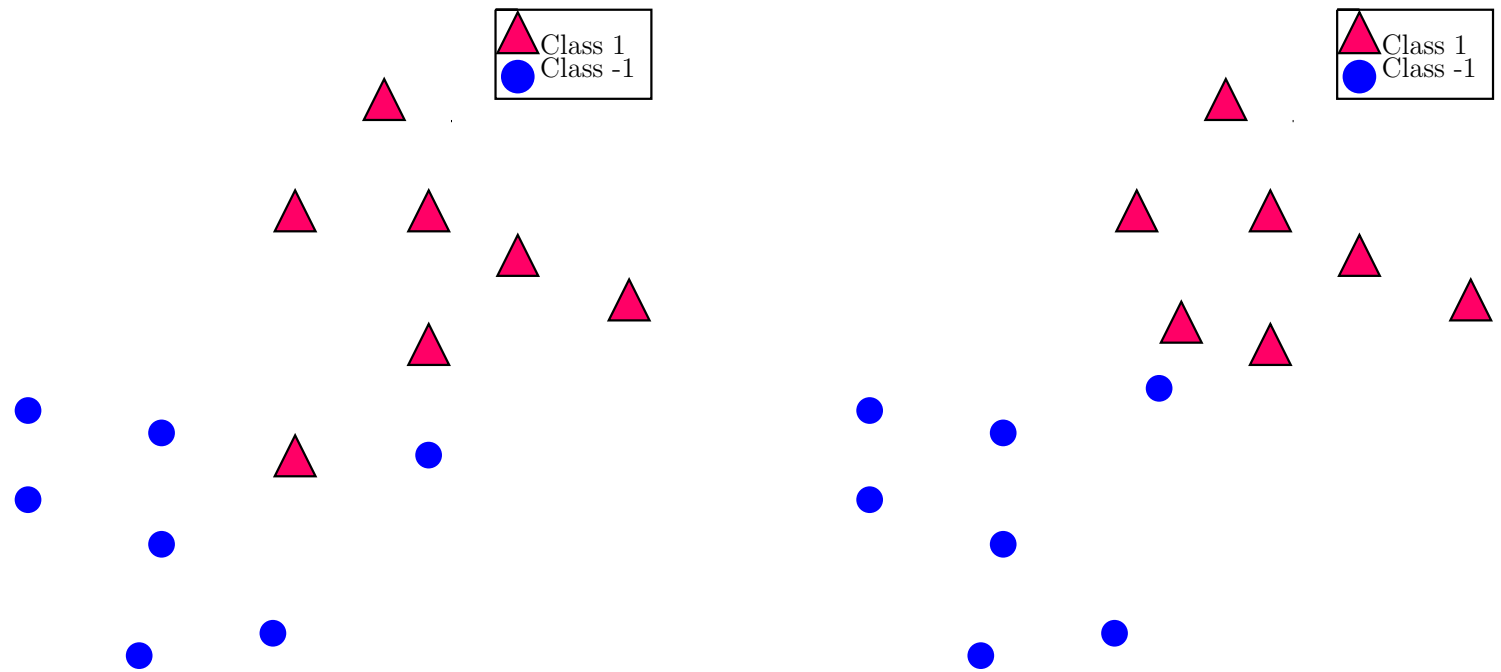
$$\text{subject to} \quad \mathbf{A}\vec{\lambda} \le \mathbf{b} \text{ and } \mathbf{A}_{\text{eq}}\vec{\lambda} = \mathbf{b}_{\text{eq}}$$

Support Vector Machine



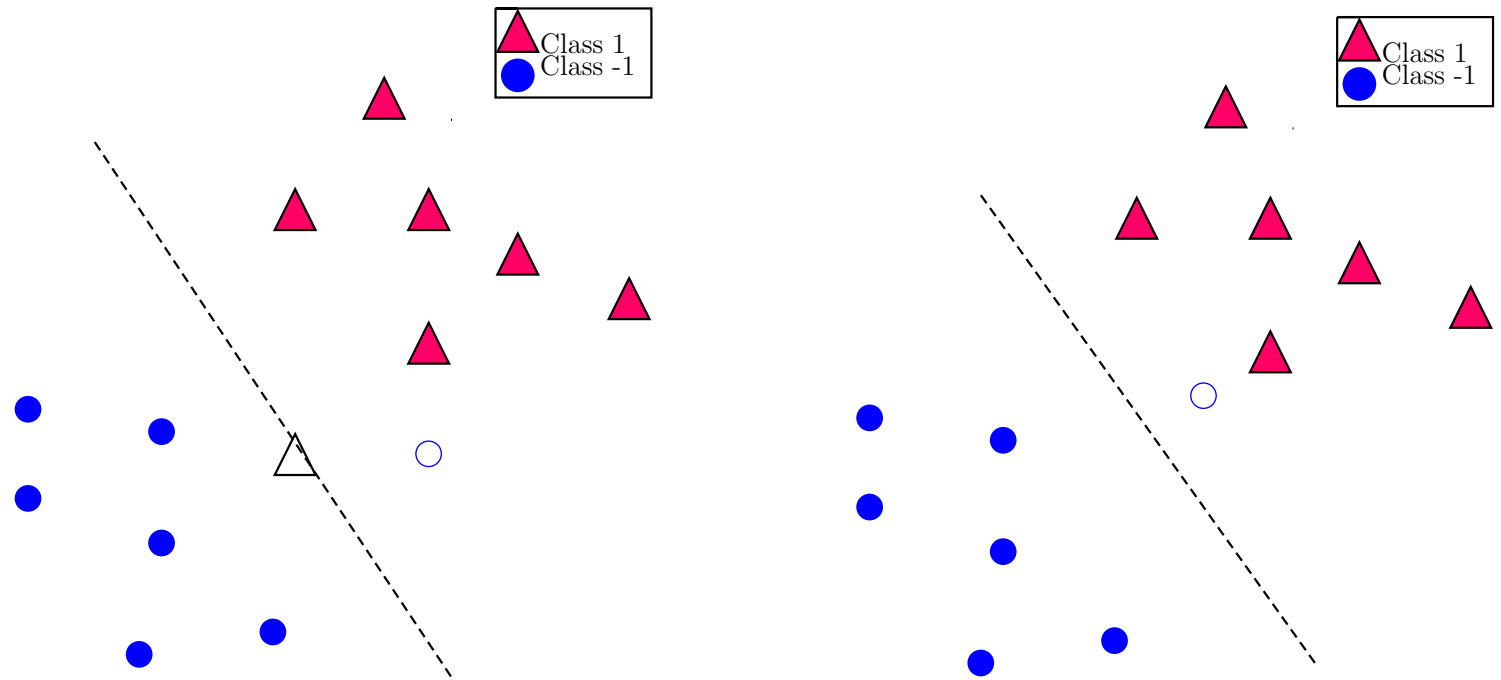
Binary SVM: Linearly separable with outliers

What is the optimal separating line?



(Left: not linearly separable; right: linearly separable but quite weakly)

What is the optimal separating line?



(Both data sets are much better linearly separated if several points are ignored).

Introducing slack variables

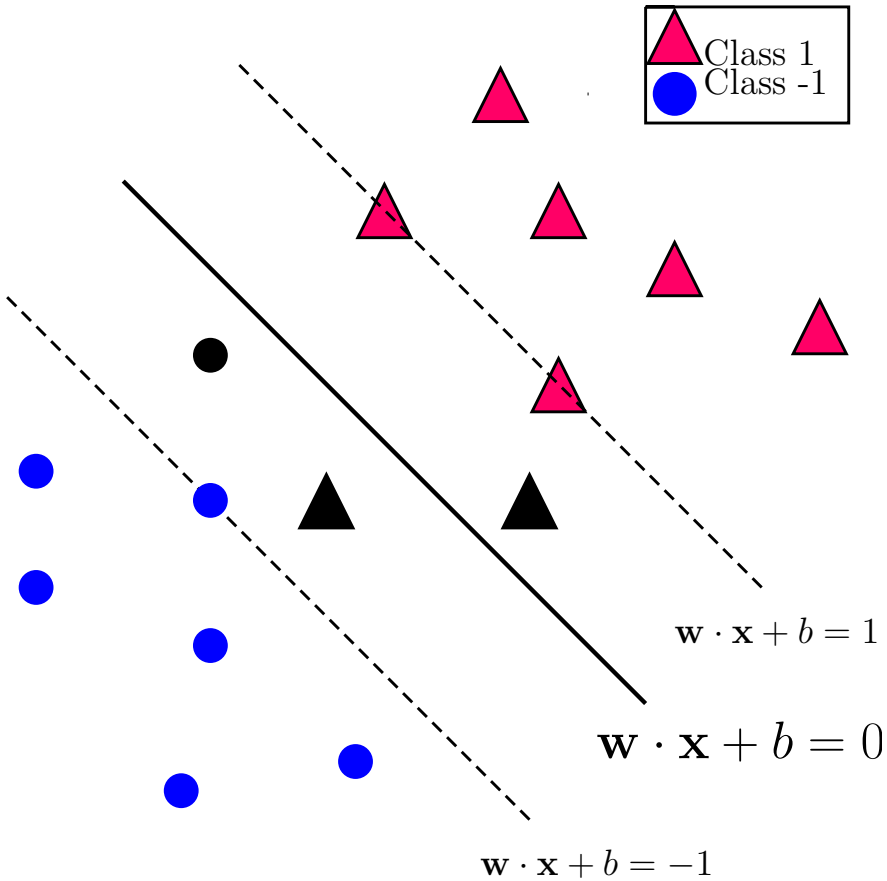
To find a linear boundary with a large margin, we must allow violations of the constraint $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$.

That is, we allow a few points to fall within the margin. They will satisfy

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) < 1$$

There are two cases:

- $y_i = +1$: $\mathbf{w} \cdot \mathbf{x}_i + b < 1$;
- $y_i = -1$: $\mathbf{w} \cdot \mathbf{x}_i + b > -1$.



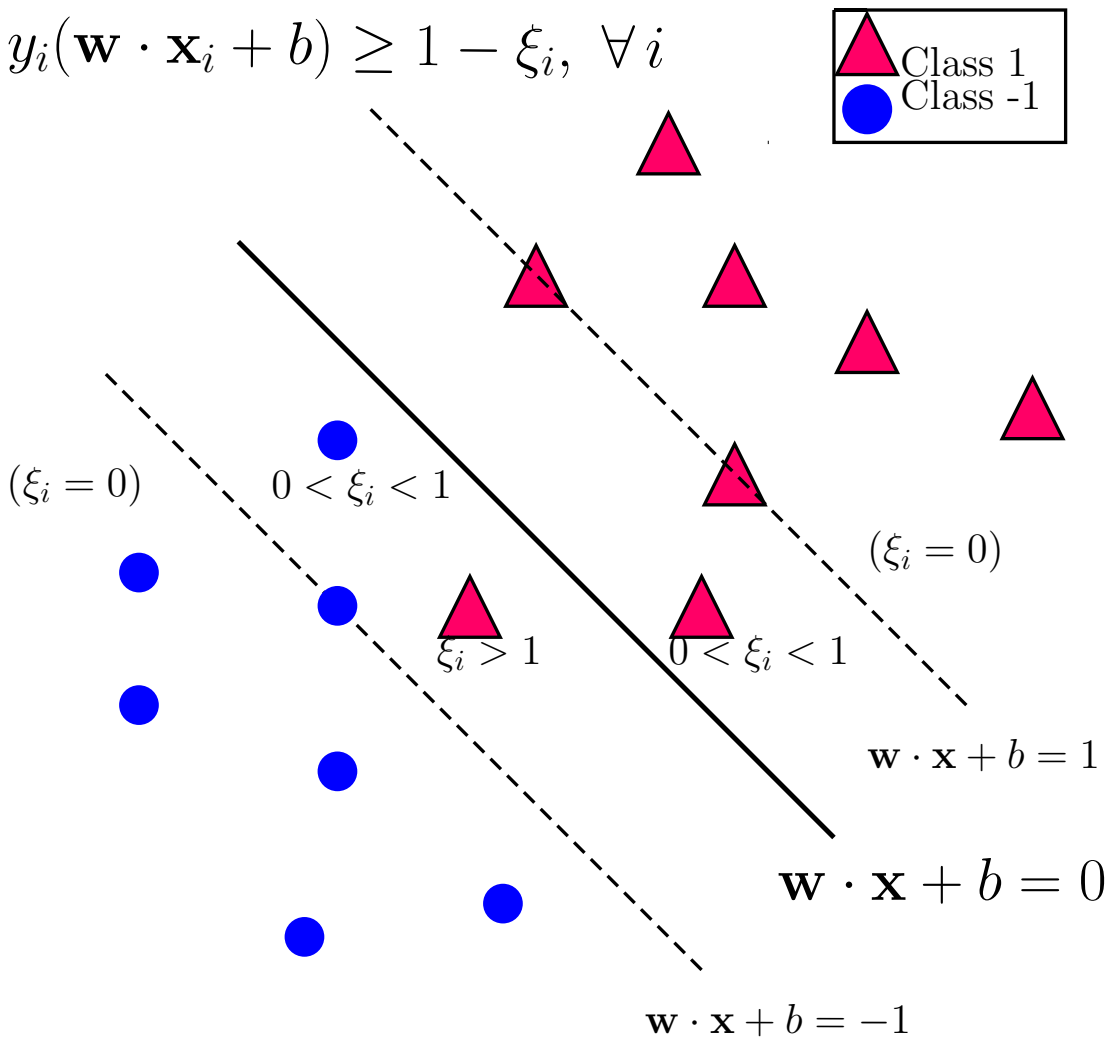
Formally, we introduce slack variables $\xi_1, \ldots, \xi_n \geq 0$ (one for each sample) to allow for *exceptions*:

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i, \quad \forall\ i$$

where $\xi_i = 0$ for the points in ideal locations, and $\xi_i > 0$ for the violations (chosen precisely so that the equality will hold true):

- $0 < \xi_i < 1$: Still on correct side of hyperplane but within the margin
- $\xi_i > 1$: Already on wrong side of hyperplane

We say that such an SVM has a **soft margin** to distinguish from the previous *hard margin*.


$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i, \ \forall i$
Class 1
Class -1
$(\xi_i = 0)$
$0 < \xi_i < 1$
$(\xi_i = 0)$
$\xi_i > 1$
$0 < \xi_i < 1$
$\mathbf{w} \cdot \mathbf{x} + b = 1$
$\mathbf{w} \cdot \mathbf{x} + b = 0$
$\mathbf{w} \cdot \mathbf{x} + b = -1$

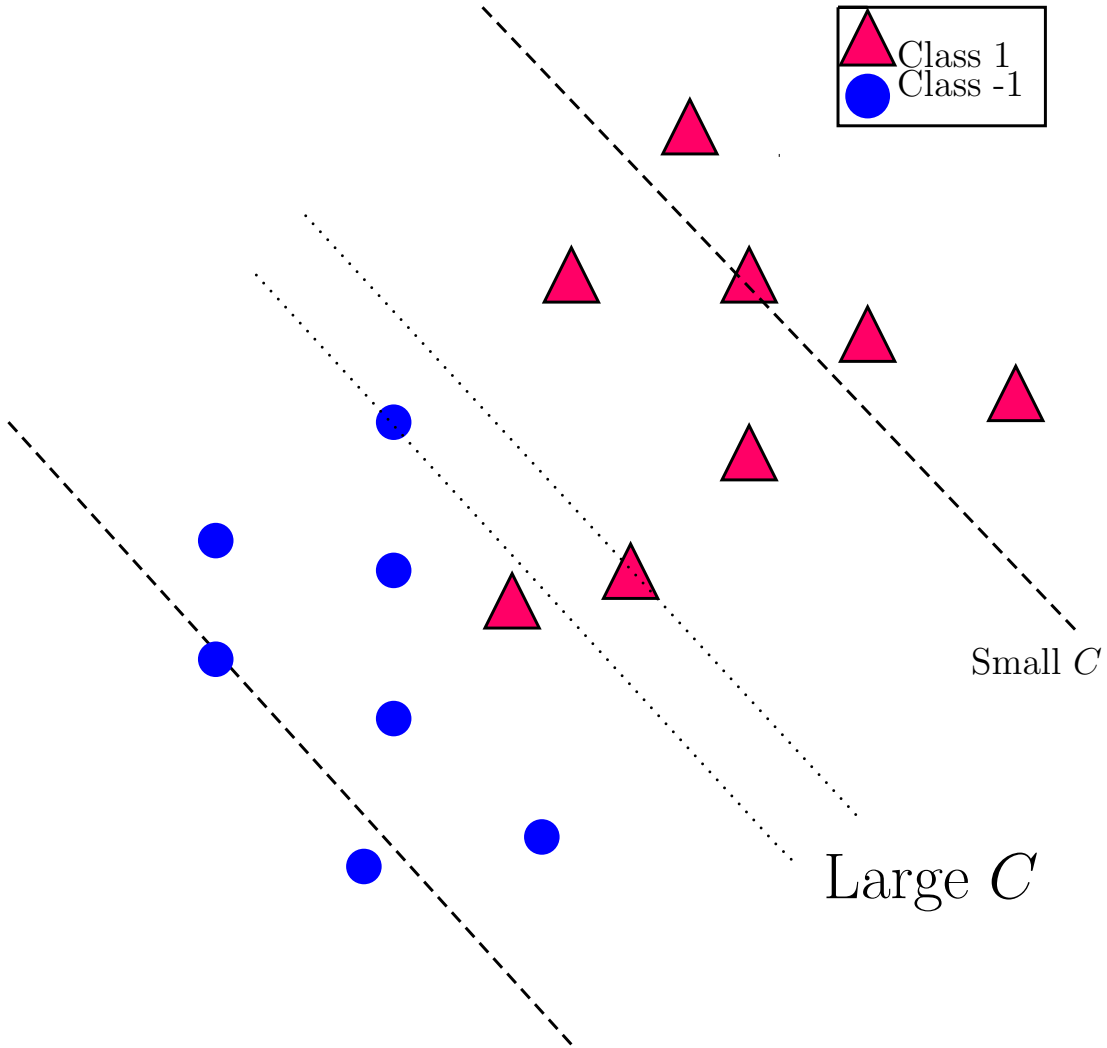
Because we want most of the points to be in ideal locations, we incorporate the slack variables into the objective function as follows

$$\min_{\mathbf{w},b,\vec{\xi}} \frac{1}{2}\|\mathbf{w}\|_2^2 + C \cdot \underbrace{\sum_i 1_{\xi_i>0}}_{\#\text{ exceptions}}$$

where $C > 0$ is a regularization constant:

- Larger C leads to fewer exceptions (smaller margin, possible overfitting).
- Smaller C tolerates more exceptions (larger margin, possible underfitting).

Clearly, there must be a tradeoff between margin and #exceptions when selecting the optimal C (often based on cross validation).


Class 1
Class -1
Small C
Large C

ℓ_1 relaxation of the penalty term

The discrete nature of the penalty term on previous slide, $\sum_i 1_{\xi_i > 0} = \|\vec{\xi}\|_0$, makes the problem intractable.

A common strategy is to replace the ℓ_0 penalty with a ℓ_1 penalty: $\sum_i \xi_i = \|\vec{\xi}\|_1$, resulting in the following full problem

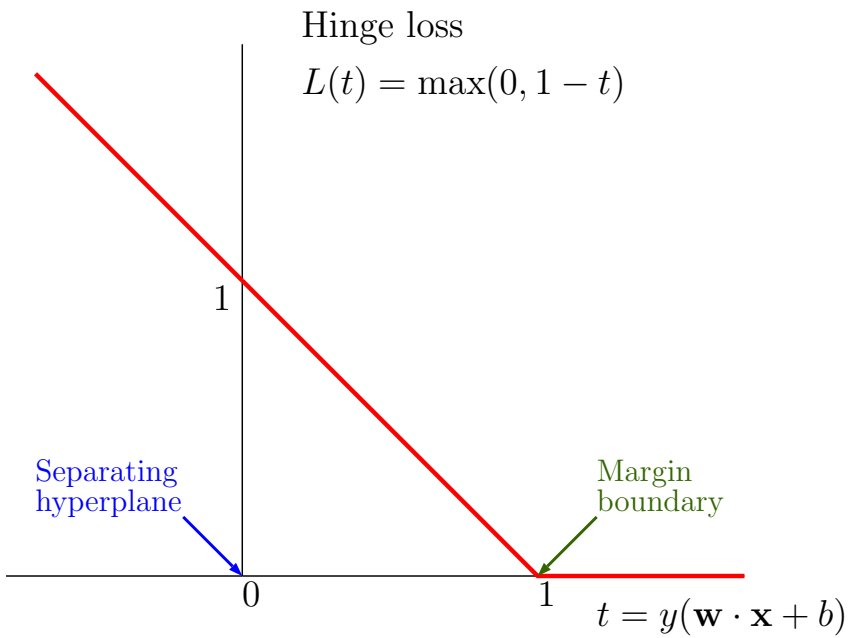
$$\min_{\mathbf{w}, b, \vec{\xi}} \ \frac{1}{2}\|\mathbf{w}\|_2^2 + C \cdot \sum_i \xi_i$$

$$\text{subject to} \quad y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0 \text{ for all } i.$$

Remarks:
(1) Also a quadratic program with linear ineq. constraints (just more variables): $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) + \xi_i \geq 1$.

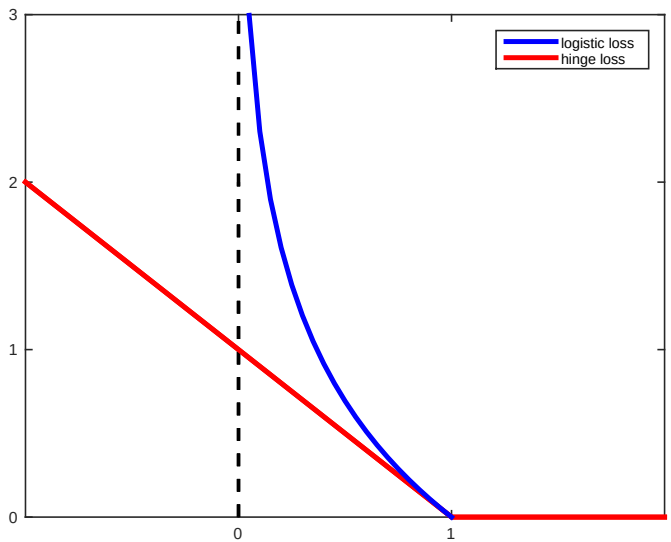
(2) The problem may be rewritten as an unconstrained optimization problem

$$\min_{\mathbf{w},b} \underbrace{\frac{1}{2}\|\mathbf{w}\|_2^2}_{\text{regularization}} + C \cdot \underbrace{\sum_{i=1}^{n} \max(0, 1 - y_i(\mathbf{w} \cdot \mathbf{x}_i + b))}_{\text{hinge loss}}$$



Remark. There is a close connection to the ℓ_2-regularized logistic regression:

$$\min_{\vec{\theta}} \quad \underbrace{C\|\vec{\theta}\|_2^2}_{\text{regularization}} \quad \underbrace{-\sum_{i=1}^{n} y_i \log p(\mathbf{x}_i;\vec{\theta}) + (1-y_i)\log(1-p(\mathbf{x}_i;\vec{\theta}))}_{\text{logistic loss}}$$



The Lagrange dual problem

The associated Lagrange function is

$$L(\mathbf{w}, b, \vec{\xi}, \vec{\lambda}, \vec{\mu}) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\lambda_i(y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \xi_i) - \sum_{i=1}^{n}\mu_i\xi_i$$

To find the dual problem we need to fix $\vec{\lambda}, \vec{\mu}$ and maximize over $\mathbf{w}, b, \vec{\xi}$:

$$\begin{aligned}
\frac{\partial L}{\partial \mathbf{w}} &= \mathbf{w} - \sum \lambda_i y_i \mathbf{x}_i = 0 \\
\frac{\partial L}{\partial b} &= \sum \lambda_i y_i = 0 \\
\frac{\partial L}{\partial \xi_i} &= C - \lambda_i - \mu_i = 0, \quad \forall\, i
\end{aligned}$$

This yields the Lagrange dual function

$$L^*(\vec{\lambda}, \vec{\mu}) = \sum \lambda_i - \frac{1}{2} \sum \lambda_i \lambda_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j, \qquad \text{where}$$
$$\lambda_i \geq 0,\ \mu_i \geq 0,\ \lambda_i + \mu_i = C,\ \text{and}\ \sum \lambda_i y_i = 0.$$

The dual problem would be to maximize L^* over $\vec{\lambda}, \vec{\mu}$ subject to the constraints.

Since L^* is constant with respect to the μ_i, we can eliminate them to obtain a reduced dual problem:

$$\max_{\lambda_1, \ldots, \lambda_n} \sum \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$
$$\text{subject to} \quad \underbrace{0 \leq \lambda_i \leq C}_{\text{box constraints}} \ \text{and} \ \sum \lambda_i y_i = 0.$$

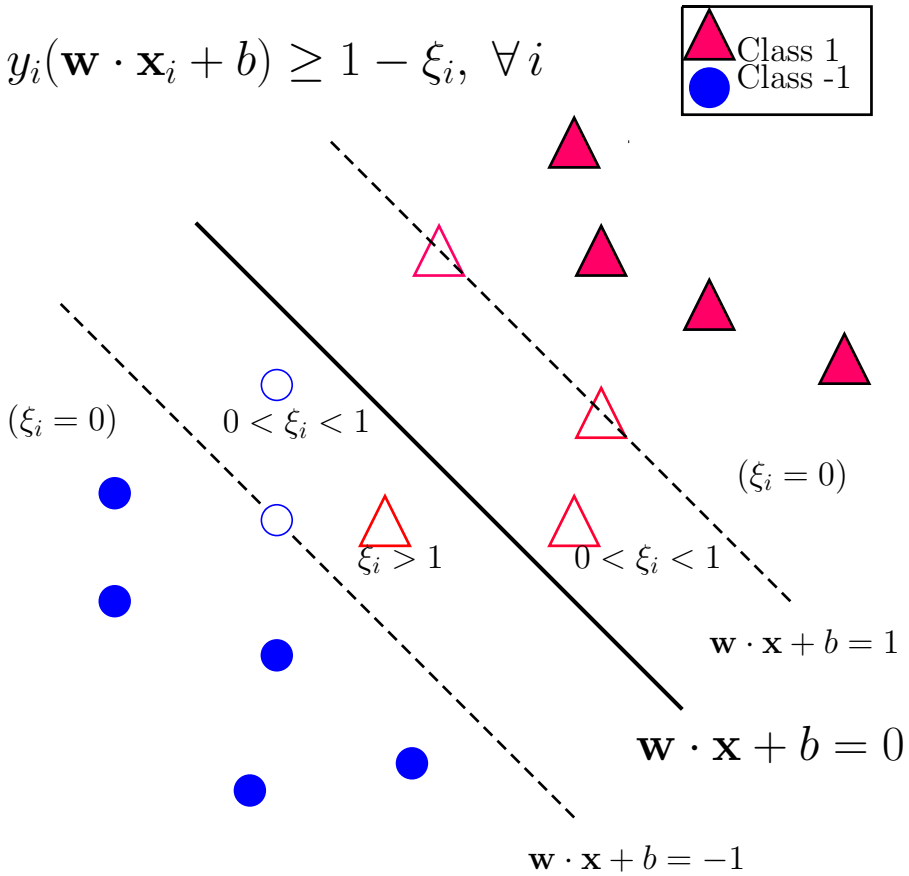
What about the KKT conditions?

The KKT conditions are the following

$$\mathbf{w} = \sum \lambda_i y_i \mathbf{x}_i, \quad \sum \lambda_i y_i = 0, \quad \lambda_i + \mu_i = C$$
$$\lambda_i (y_i (\mathbf{w} \cdot \mathbf{x}_i + b) - 1 + \xi_i) = 0, \quad \mu_i \xi_i = 0$$
$$\lambda_i \geq 0, \quad \mu_i \geq 0$$
$$y_i (\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

We see that

- The optimal $\mathbf{w}$ has the same formula: $\mathbf{w} = \sum \lambda_i y_i \mathbf{x}_i$.
- Any point with $\lambda_i > 0$ and correspondingly $y_i(\mathbf{w} \cdot \mathbf{x} + b) = 1 - \xi_i$ is a support vector (not just those on the margin boundary $\mathbf{w} \cdot \mathbf{x} + b = \pm 1$).



- To find b, choose any support vector $\mathbf{x}_i$ with $0 < \lambda_i < C$ (which implies that $\mu_i > 0$ and $\xi_i = 0$), and use the formula $b = \frac{1}{y_i} - \mathbf{w} \cdot \mathbf{x}_i$.

Binary SVM via quadratic programming

Again, we first need to transform the previous formulation to the standard form

$$\min_{\lambda_1,\ldots,\lambda_n} \ \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x}_i\cdot\mathbf{x}_j - \sum\lambda_i$$

$$\text{subject to} \quad -\lambda_i \le 0,\ \lambda_i \le C,\ \text{and}\ \sum\lambda_i y_i = 0$$

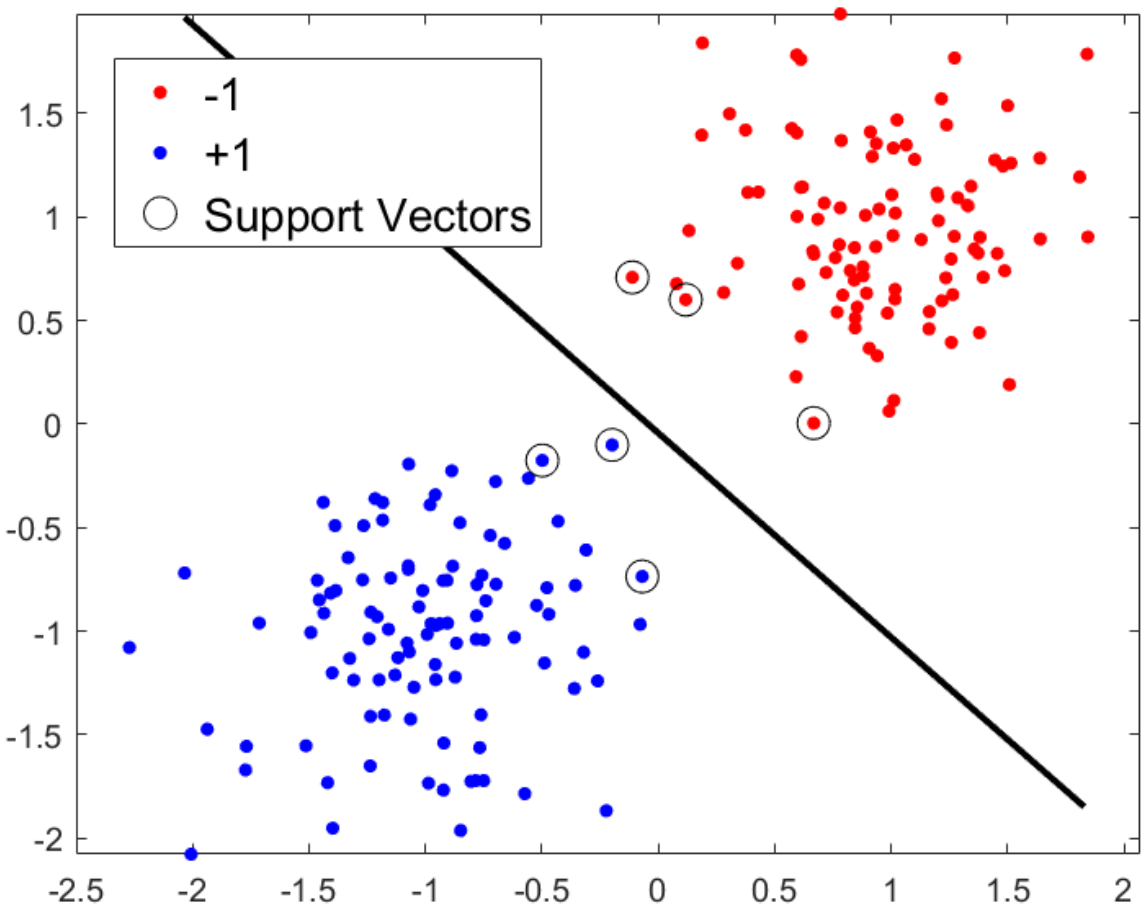
and then matrice/vectorize it:

$$\min_{\vec{\lambda}} \ \frac{1}{2}\vec{\lambda}^T\mathbf{H}\vec{\lambda} + \mathbf{f}^T\vec{\lambda}$$

$$\text{subject to} \quad \mathbf{A}\vec{\lambda} \le \mathbf{b}\ \text{and}\ \mathbf{A}_{\text{eq}}\vec{\lambda} = \mathbf{b}_{\text{eq}}$$

Note. Both $\mathbf{A}, \mathbf{b}$ are twice as tall as before (the other variables remain the same).

Support Vector Machine



Binary SVM: Nonlinearly separable, with outliers

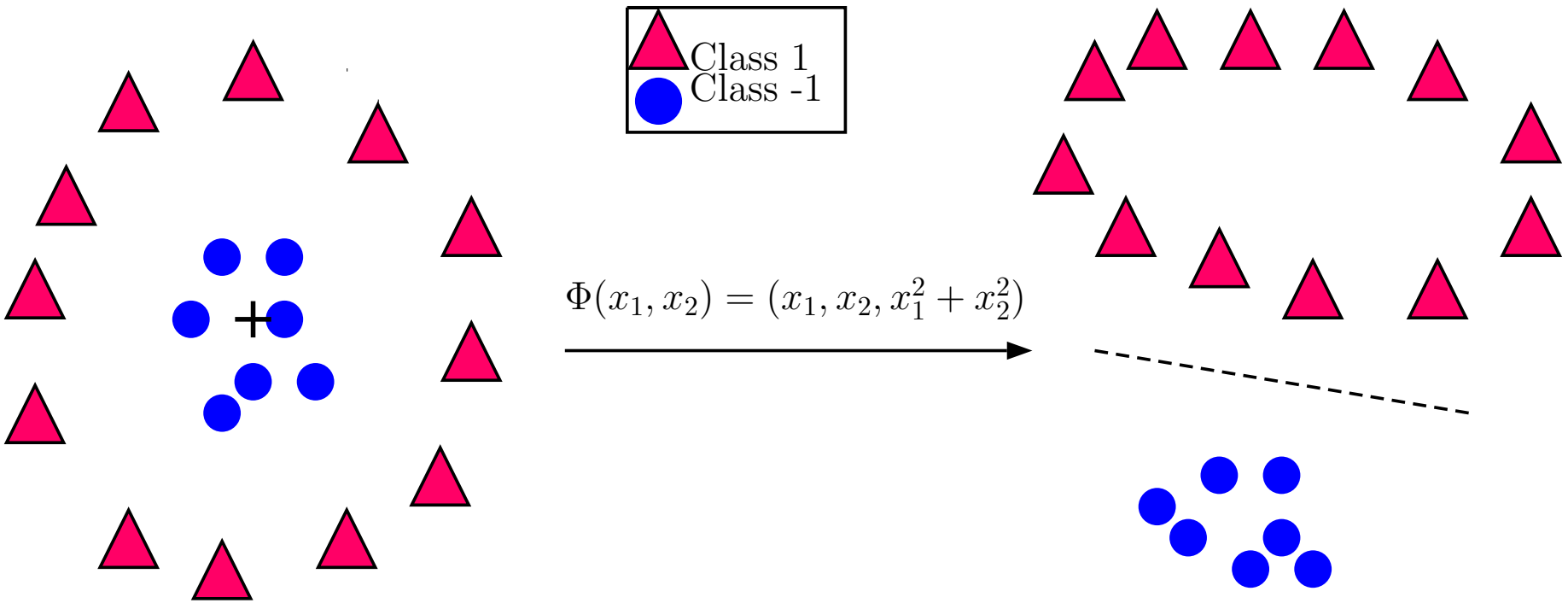
Feature map

When the classes are nonlinearly separable, a transformation of the data (both training and test) is often used (so that the training classes in the new space becomes linearly separable):

$$\Phi: \ \mathbf{x}_i \in \mathbb{R}^d \mapsto \Phi(\mathbf{x}_i) \in \mathbb{R}^\ell$$

where often $\ell \gg d$, and sometimes $\ell = \infty$.

- The function Φ is called a *feature map*,
- The target space $\mathbb{R}^\ell$ is called a *feature space*, and
- The images $\Phi(\mathbf{x}_i)$ are called *feature vectors*.


Class 1
Class -1
$\Phi(x_1, x_2) = (x_1, x_2, x_1^2 + x_2^2)$

The kernel trick

In principle, once we find a good feature map $\Phi : \mathbb{R}^d \to \mathbb{R}^\ell$ we just need to work in the new space to build a binary SVM model and classify test data (after being transformed in the same way):

- SVM in feature space

$$\min_{\mathbf{w},b,\vec{\xi}} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum \xi_i \quad \text{subject to}$$
$$y_i(\mathbf{w}\cdot\Phi(\mathbf{x}_i)+b) \geq 1-\xi_i, \text{ and } \xi_i \geq 0 \text{ for all } i.$$

- Decision rule for test data $\mathbf{x}$

$$y = \text{sgn}(\mathbf{w}\cdot\Phi(\mathbf{x})+b)$$

However, in many cases the feature space is very high dimensional, making computing intensive.

We can apply a **kernel trick** thanks to the Lagrange dual formulation of SVM:

$$\max_{\lambda_1,\ldots,\lambda_n} \sum \lambda_i - \frac{1}{2}\sum_{i,j} \lambda_i \lambda_j y_i y_j \underbrace{\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_j)}_{:=\kappa(\mathbf{x}_i,\mathbf{x}_j)}$$

$$\text{subject to} \quad 0 \le \lambda_i \le C \text{ and } \sum \lambda_i y_i = 0$$

That is to specify only the dot product function κ of the feature space, called a **kernel function** and avoid explicitly using the feature map Φ.

In the toy example, $\Phi(\mathbf{x}) = (\mathbf{x}, \|\mathbf{x}\|_2^2)$, and $\kappa(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}\cdot\tilde{\mathbf{x}} + \|\mathbf{x}\|_2^2 \cdot \|\tilde{\mathbf{x}}\|_2^2$.

Can the decision rule also avoid the explicit use of Φ?

$$y = \operatorname{sgn}(\mathbf{w} \cdot \Phi(\mathbf{x}) + b)$$

The answer is yes, because $\mathbf{w}$ is a linear combination of the support vectors in the feature space:

$$\mathbf{w} = \sum \lambda_i y_i \Phi(\mathbf{x}_i)$$

and so is b (for any support vector $\Phi(\mathbf{x}_{i_0})$ with $0 < \lambda_{i_0} < C$):

$$b = y_{i_0} - \mathbf{w} \cdot \Phi(\mathbf{x}_{i_0})$$

Consequently,

$$y = \operatorname{sgn}\left(\sum \lambda_i y_i \kappa(\mathbf{x}_i, \mathbf{x}) + b\right), \qquad \text{where} \quad b = y_{i_0} - \sum \lambda_i y_i \kappa(\mathbf{x}_i, \mathbf{x}_{i_0})$$

Steps of kernel SVM

- Pick a kernel function κ (which corresponds to some feature map Φ)
- Solve the following quadratic program

$$\max_{\lambda_1,\ldots,\lambda_n} \sum_i \lambda_i - \frac{1}{2}\sum_{i,j} \lambda_i \lambda_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)$$
$$\text{subject to} \quad 0 \le \lambda_i \le C \text{ and } \sum \lambda_i y_i = 0$$

- Classify new data $\mathbf{x}$ based on the following decision rule:

$$y = \operatorname{sgn}\left(\sum \lambda_i y_i \kappa(\mathbf{x}_i, \mathbf{x}) + b\right)$$

where b can be determined from any support vector with $0 < \lambda_i < C$.

What are good kernel functions?

- **Linear** (= no kernel, just regular SVM)

$$\kappa(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x} \cdot \tilde{\mathbf{x}}$$

- **Polynomial** (of degree $p \geq 1$)

$$\kappa(\mathbf{x}, \tilde{\mathbf{x}}) = (1 + \mathbf{x} \cdot \tilde{\mathbf{x}})^p$$

- **Gaussian** (also called Radial Basis Function, or RBF)

$$\kappa(\mathbf{x}, \tilde{\mathbf{x}}) = e^{-\|\mathbf{x}-\tilde{\mathbf{x}}\|_2^2/(2\sigma^2)} = e^{-\gamma\|\mathbf{x}-\tilde{\mathbf{x}}\|_2^2}$$

- **Sigmoid** (also called Hyperbolic Tangent)

$$\kappa(\mathbf{x}, \tilde{\mathbf{x}}) = \tanh(\gamma \mathbf{x} \cdot \tilde{\mathbf{x}} + r)$$

The MATLAB 'fitcsvm' function for binary SVM

% SVM training with different kernels

SVMModel = fitcsvm(trainX, Y, 'BoxConstraint', 1, 'KernelFunction', 'linear') % both are default values

SVMModel = fitcsvm(trainX, Y, 'BoxConstraint', 1, 'KernelFunction', 'gaussian', 'KernelScale', 1) % 'KernelFunction' may be set to 'rbf'. 'KernelScale' is the sigma parameter (default = 1)

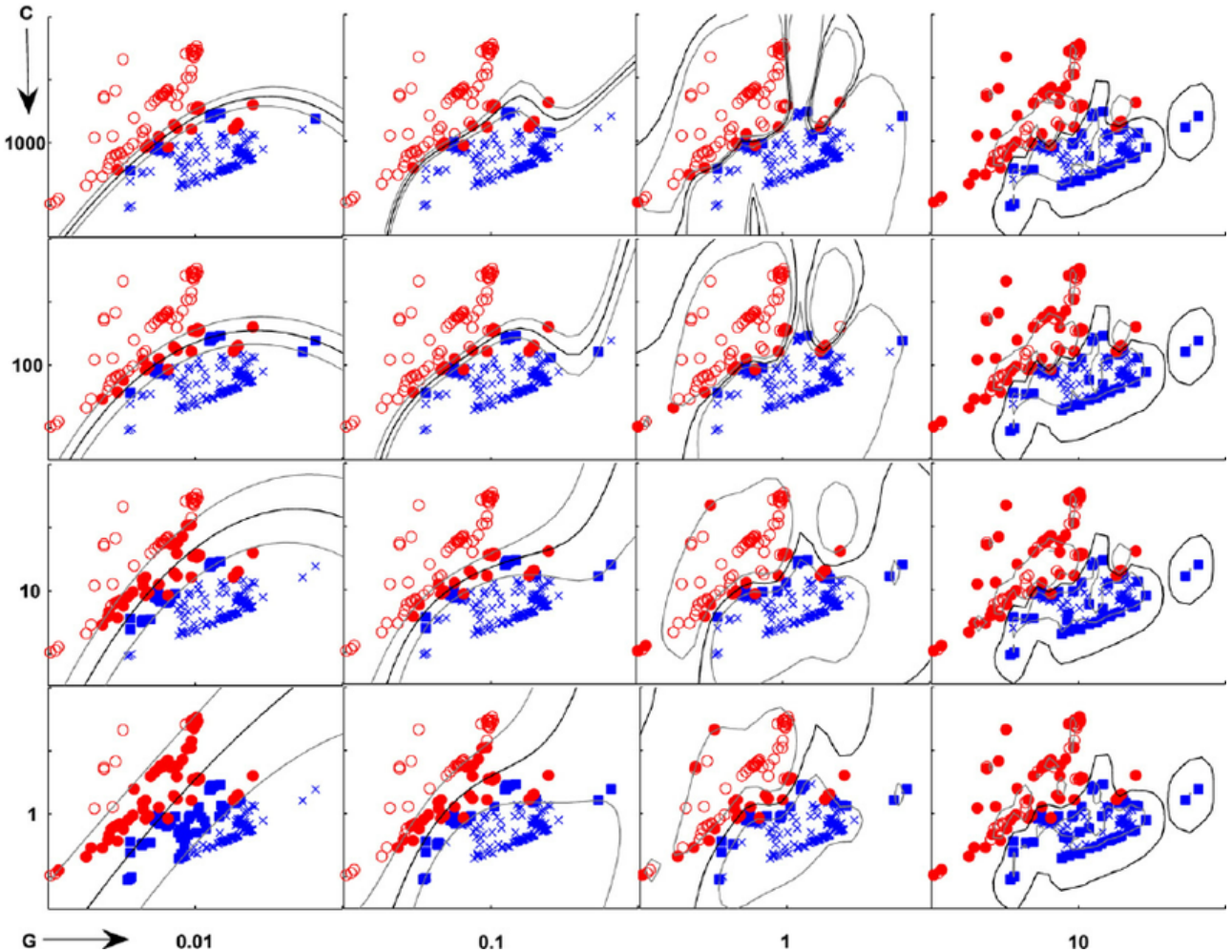
SVMModel = fitcsvm(trainX, Y, 'BoxConstraint', 1, 'KernelFunction', 'polynomial', 'PolynomialOrder', 3) % default order = 3

```
% SVM validation (important for parameter tuning)

CVSVMModel = crossval(SVMModel); % 10-fold by default

kloss = kfoldLoss(CVSVMModel);


% SVM testing

pred = predict(SVMModel, testX);
```

Experiments

- The polynomial kernel
  - C: margin parameter
  - p: degree of polynomial (shape parameter)
- The Gaussian kernel (see plot on next slide)
  - C: margin parameter
  - σ (or γ): smoothness parameter

Support Vector Machine



Practical issues

- **Scaling**: SVM often requires to rescale each dimension (pixel in our case) linearly to an interval [0,1] or [-1,1], or instead standardizes it to zero mean, unit variance.
- **High dimensional data**: Training is expensive and tends to overfit the data when using flexible kernel SVMs (such as Gaussian or polynomial). Dimensionality reduction by PCA is often needed.
- **Hyper-parameter tuning**
  - The tradeoff parameter C (for general SVM)
  - Kernel parameter: $\gamma = \frac{1}{2\sigma^2}$ (Gaussian), p (polynomial)

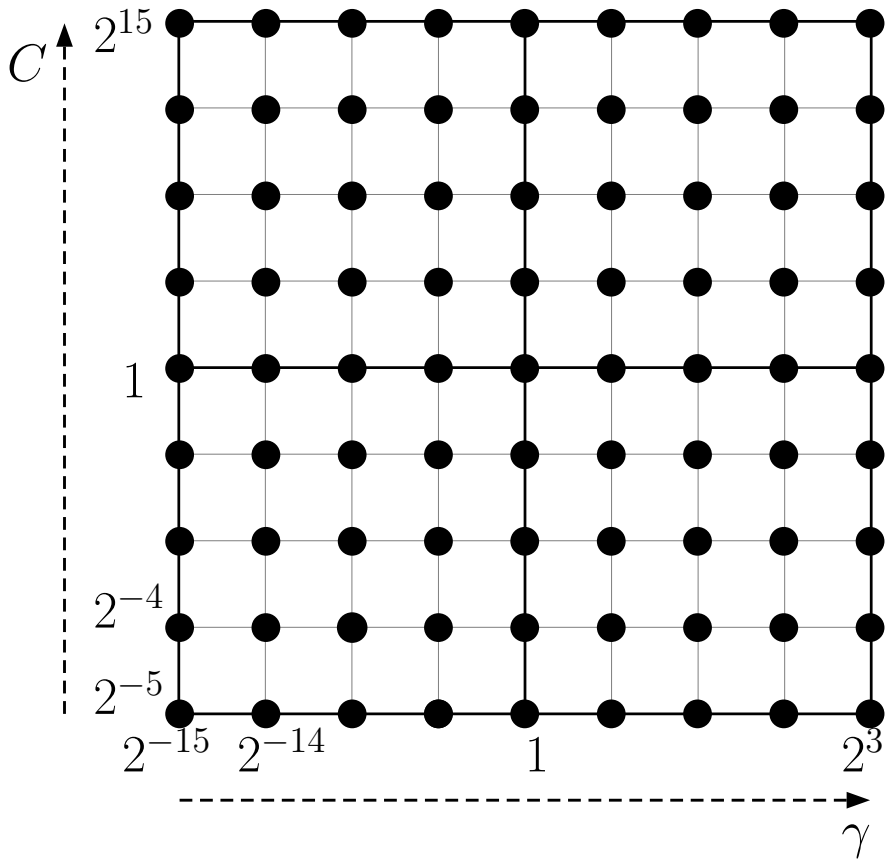
Parameter estimation for Gaussian-kernel SVM

GkSVM is a powerful, general-purpose kernel, but there is a practical difficulty in tuning γ (or σ) and C.

Typically, it is tuned by cross validation in a grid search fashion:

$$\gamma = 2^{-15}, 2^{-14}, \ldots, 2^{3}, \text{ and}$$
$$C = 2^{-5}, 2^{-4}, \ldots, 2^{15}$$

One popular, efficient implementation is LIBSVM: `https://www.csie.ntu.edu.tw/~cjlin/libsvm/`



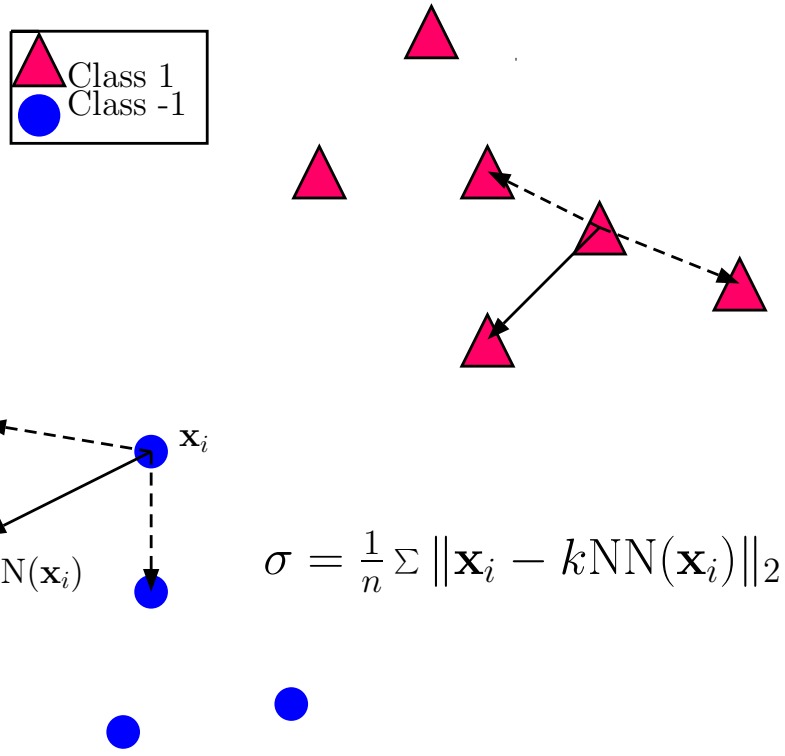
We[a] set the parameter σ in the Gaussian kernel

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2\sigma^2}}$$

directly based on training data:

$$\sigma = \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{x}_i - k\mathrm{NN}(\mathbf{x}_i)\|_2$$

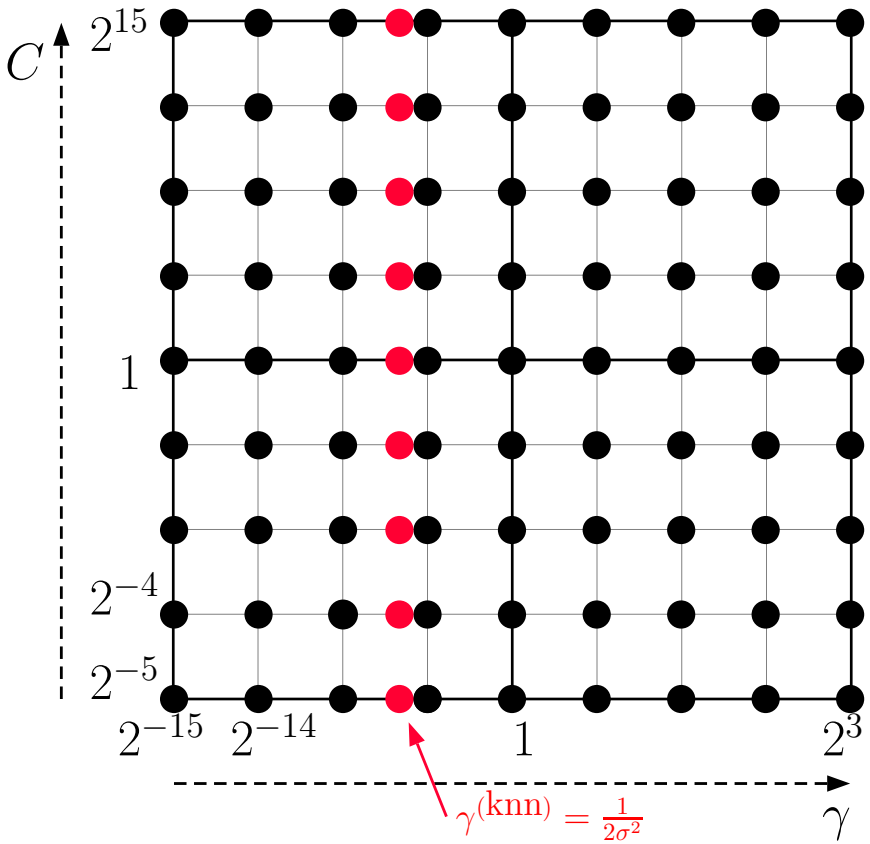
where $k\mathrm{NN}(\mathbf{x}_i)$ is the kth nearest neighbor of $\mathbf{x}_i$ within its own training class.[b]

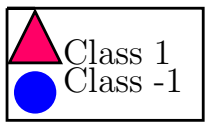


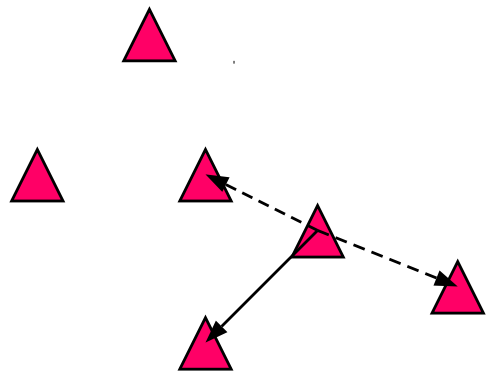
[a] G. Chen, W. Florero-Salinas, and D. Li (2017), "Simple, Fast and Accurate Hyper-parameter Tuning in Gaussian-kernel SVM", Intl. Joint Conf. on Neural Networks

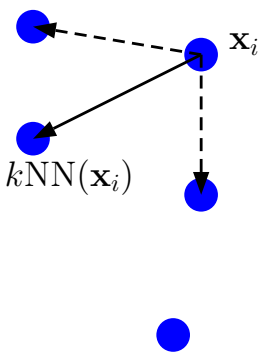
[b] When n is large, we may use only a small, randomly selected subset of training data to estimate σ, leading to a stochastic algorithm.

Grid search method vs. kNN tuning (for $k = 3$)







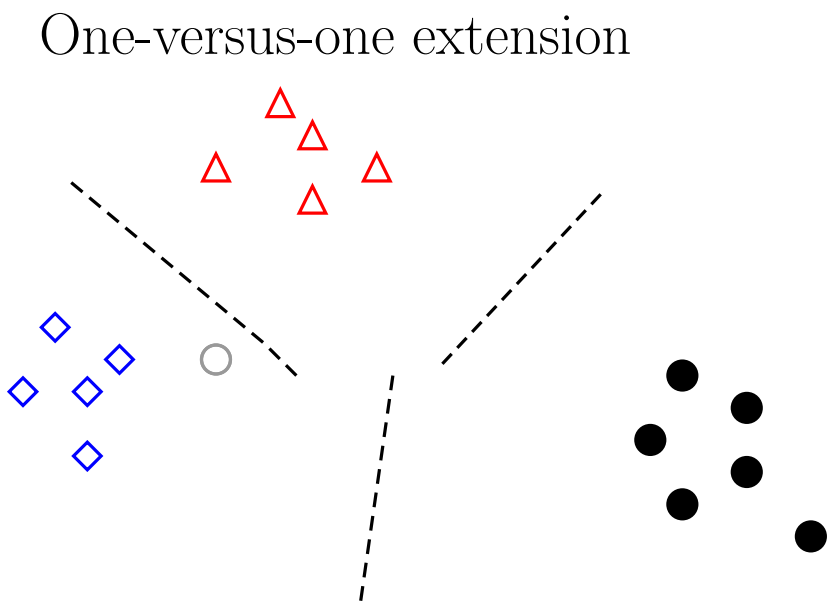


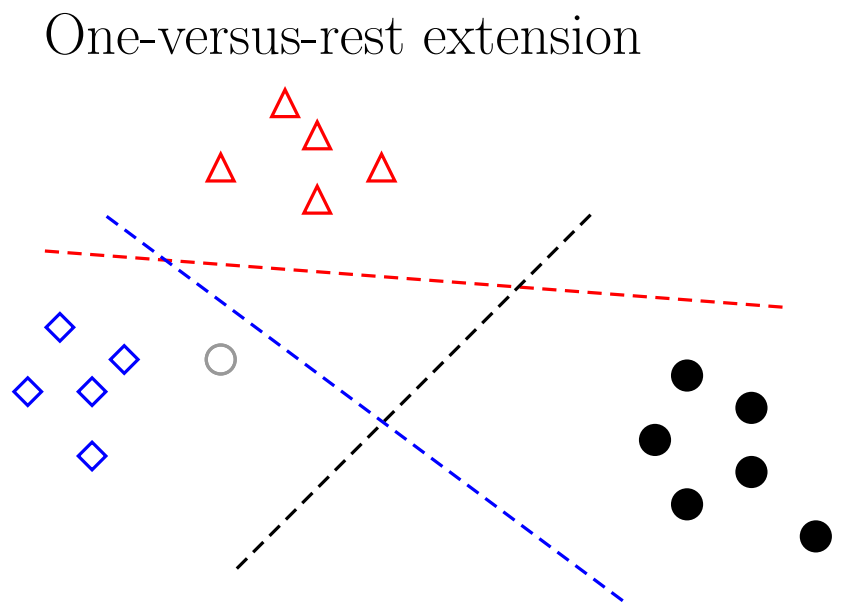
$$\sigma = \frac{1}{n} \Sigma \, \|\mathbf{x}_i - k\text{NN}(\mathbf{x}_i)\|_2$$

Multiclass extensions

Multiclass SVM

Like logistic regression, binary SVM can be extended to a multiclass setting in one of the following ways:





In either case, the "maximally winning" class is adopted as the final prediction:

- For one-versus-one multiclass SVM, the final prediction for a test point is the most frequent label predicted;
- For one-versus-rest multiclass SVM,
  - The reference classes are assigned label 1 (the rest with label -1)
  - For each binary model, record the 'score': $\mathbf{w}^{(i)} \cdot \mathbf{x} + b^{(i)}$ (not the predicted label)
  - The final prediction is the reference class with the largest (positive) score

$$y = \arg\max_i \ \mathbf{w}^{(i)} \cdot \mathbf{x} + b^{(i)}$$

Matlab implementation for Multiclass SVM

The previously mentioned function, 'fitcsvm', is designed only for binary classification. To use multiclass SVM, you have the following options:

- Implement one-versus-one and one-versus-rest on your own (note that you have already done this for logistic regression)
- Use the Matlab function 'fitcecoc':
  temp = templateSVM('BoxConstraint', 1, 'KernelFunction', 'gaussian', 'KernelScale', 1); % Gaussian kernel SVM
  temp = templateSVM('BoxConstraint', 1, 'KernelFunction', 'polynomial', 'PolynomialOrder', 3); % polynomial kernel SVM
  Mdl = fitcecoc(trainX,Y,'Coding','onevsone','learners',temp);
  Mdl = fitcecoc(trainX,Y,'Coding','onevsall','learners',temp);

Python functions for SVM

See documentation at

- **scikit-learn** (`http://scikit-learn.org/stable/modules/svm.html`)
- **LibSVM** (`http://www.csie.ntu.edu.tw/~cjlin/libsvm/`)

Remarks:

- scikit-learn uses LibSVM to handle all computations, so the two should be the same thing.
- LibSVM contains an efficient, grid-search based Matlab implementation for SVM (including the multiclass extensions).

Summary

- Binary SVM (hard/soft margin, and kernel) and multiclass extensions
- **Advantages**:
  - Based on nice theory
  - Excellent generalization properties
  - Globally optimal solution
  - Can handle outliers and nonlinear boundary simultaneously
- **Disadvantage**: SVM might be slower than some other methods due to parameter tuning and quadratic programming

HW6 (due Nov 15, Thursday noon)

1. This question concerns the application of the binary linear soft-margin SVM classifier to the data used in HW4-Q5. Do the following:

   (1a) Use 5-fold cross validation to select the optimal value of C from $\{2^{-6}, 2^{-5}, \ldots, 2^{4}\}$

   (1b) Apply the binary classifier with the value of C determined in part (a) to the data and compare with LDA and Logistic Regression in terms of decision boundary and test accuracy.

2. Repeat Question 1 with the quadratic polynomial kernel SVM by comparing it with the QDA classifier using the same criteria.

3. Apply each of the three binary kernel SVM classifiers - linear, quadratic polynomial, and cubic polynomial - with all values of $C = 2^{-6}, 2^{-5}, \ldots, 2^{4}$ directly to the following subsets of the USPS data set separately:
(a) 0, 1 (b) 1, 7 (c) 4, 9.

   For each subset, plot three test error curves (against C), one for each classifier. Because of the high dimensionality of the data, you may want to perform PCA (95% or a better choice) on each subset of digits before you apply the SVM classifiers.

4. Apply the binary Gaussian kernel SVM classifier to the same three subsets of USPS digits above (after PCA) with your own choices of σ and C. Try different combinations of values of the two parameters so as to get a "low" test error for each subset. Report your parameter values and corresponding test error rates.

5. (Extra credit questions). You must type your work.

   (5a) Solve the following constrained optimization problem by hand:

$$\min_{x,y} \; y - x^2 \qquad \text{subject to} \quad 4 - x^2 - y^2 \geq 0$$

   (5b) First find the Lagrange dual of the following (primal) problem

$$\min_{x} \; \frac{1}{2}x^2 \qquad \text{subject to} \quad 2x - 1 \geq 0$$

   and then verify that the two problems have the same solution.

HW7 (due Wed noon, Nov 21)

This is a group assignment (meaning you can collaborate with a partner and hand in just one submission).

This homework focuses on the multiclass SVM classifier. In all questions below try different values of $C = 2^{-4}, 2^{-3}, \ldots, 2^{5}$ (no validation is needed).

1. Apply the one-vs-one multiclass linear SVM classifier to the USPS digits (after PCA 95%). Plot the test errors against the different values of C. How does it compare with the one-vs-one extension of the logistic regression classifier?

2. Implement the one-versus-one extension of the third-degree polynomial kernel SVM classifier and apply it to the USPS digits (after PCA 95%). Plot the test errors against C.

3. Repeat Question 2 with the one-versus-rest extension instead. Which extension is better?

4. Implement the one-versus-one extension of the Gaussian kernel SVM classifier and apply it to the USPS digits (after PCA 95%). To set the kernel parameter σ, use a random sample of 100 points with $k = 7$ (or a better choice). Report the value of σ you got and plot the corresponding test errors against C. How does it compare with weighted kNN classifier with Gaussian weights using the same σ and various k between 3 and 10?

5. Repeat Question 4 with the one-versus-rest extension instead. Which extension is better?