CS 474/574 Machine Learning
4 . Support Vector Machines (SVMs)

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Agenda

- Perceptron algorithm – Its model differs from SVMs a lot. But it shows that the weight vector is a linear combination of some samples – it resembles SVMs in that sense.
- The intuition of SVMs: separate similar samples of both classes apart as far as possible.
- Deriving the primal form of SVMs, and solving it in KKT conditions
- Dual forms of SVMs and the kernel tricks
- Soft-margin SVMs

All samples are equal. But some samplers are equaler.

- Let's first see a demo of a linear classifier for linearly separable cases. Pay attention to the prediction outcome.
- Think about the error-based loss function for a classifier: $\sum_i (\hat{y} - y)^2$ where y is the ground truth label and $\hat{y}$ is the prediction.
- If $y = +1$ and $\hat{y} = +1.5$, should the error be 0.25 or 0 (because properly classified)?

The perceptron algorithm

- Recall earlier that a sample $(\mathbf{x}_i, y_i)$ is correctly classified if $\mathbf{w}^T\mathbf{x}_i y_i > 0$ and $y_i \in \{1, -1\}$.
- Let's define a new cost function to be minimized: $J(\mathbf{w}) = \sum_{x_i \in \mathcal{M}} -\mathbf{w}^T\mathbf{x}_i y_i$ where $\mathcal{M}$ is the set of all samples misclassified ($\mathbf{w}^T\mathbf{x}_i y_i < 0$).
- Then, $\nabla J(\mathbf{w}) = \sum_{\mathbf{x}_i \in \mathcal{M}} -\mathbf{x}_i y_i$ (because $\mathbf{w}$ is the coefficients.)
- Only those misclassified matter!
- Batch perceptron algorithm: In each batch, computer $\nabla J(\mathbf{w})$ for all samples misclassified using the same current $\mathbf{w}$ and then update.

Single-sample perceptron algorithm

- Another common type of perceptron algorithm is called single-sample perceptron algorithm.
- Update $\mathbf{w}$ whenever a sample is misclassified.
  1. Initially, $\mathbf{w}$ has arbitrary values. Timestep (or iteration) $t = 1$.
  2. In the t-th iteration, use sample $\mathbf{x}_j$ such that $j = t \mod n$ to update the $\mathbf{w}$ by:

$$\mathbf{w}_{t+1} = \begin{cases} \mathbf{w}_t + \rho \mathbf{x}_j y_j & \text{, if } \mathbf{w}_j^T \mathbf{x_j} y_j \leq 0, \text{ (wrong prediction)} \\ \mathbf{w}_t & \text{, if } \mathbf{w}_j^T \mathbf{x_j} y_j > 0 \text{ (correct classification)} \end{cases}$$

     where ρ is a constant called **learning rate**.
  3. The algorithm terminates when all samples are classified correctly.

An example of single-sample preceptron algorithm

- Feature vectors **not augmented** and corresponding labels:
  - $\mathbf{x}'_1 = (0,0)^T$, $y_1 = 1$
  - $\mathbf{x}'_2 = (0,1)^T$, $y_2 = 1$
  - $\mathbf{x}'_3 = (1,0)^T$, $y_3 = -1$
  - $\mathbf{x}'_4 = (1,1)^T$, $y_4 = -1$
- First, let's augment them and multiply with the labels:
  - $\mathbf{x}_1 y_1 = (0,0,1)^T$,
  - $\mathbf{x}_2 y_2 = (0,1,1)^T$,
  - $\mathbf{x}_3 y_3 = (-1,0,-1)^T$
  - $\mathbf{x}_4 y_4 = (-1,-1,-1)^T$

0. Begin our iteration. Let $\mathbf{w}_1 = (0,0,0)^T$ and $\rho = 1$.
1. $\mathbf{w}_1^T \cdot \mathbf{x}_1 y_1 = \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0 \leq 0$.

   Need to update $\mathbf{w}$: $\mathbf{w}_2 =$

   $\mathbf{w}_1 + \rho \cdot \mathbf{x}_1 y_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$
2. $\mathbf{w}_2^T \cdot \mathbf{x}_2 y_2 = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = 1 > 0$. No updated need. But since $\mathbf{w}$ so far does not classify all samples correctly, we need to keep going. Just let $\mathbf{w}_3 = \mathbf{w}_2$.

An example of preceptron algorithm (cond.)

Continue in perceptron.ipynb

14. In the end, we have $\mathbf{w}_{14} = \begin{pmatrix} -3 \\ 0 \\ 2 \end{pmatrix}$, let's verify how well it works

- $$\begin{cases} \mathbf{w}_{14} \cdot \mathbf{x}_1 y_1 & = 2 > 0 \\ \mathbf{w}_{14} \cdot \mathbf{x}_2 y_2 & = 2 > 0 \\ \mathbf{w}_{14} \cdot \mathbf{x}_3 y_3 & = 1 > 0 \\ \mathbf{w}_{14} \cdot \mathbf{x}_4 y_4 & = 1 > 0 \end{cases}$$

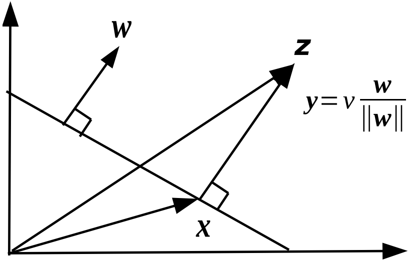
- Mission accomplished!
- Note that the perceptron algorithm will not *converge* unless the data is linearly separable.
- What is $\mathbf{w}$ exactly? A linear composition of all training samples!
- Do all samples contribute to $\mathbf{w}$? Not really!

Now let's begin the SVM journey.

Getting ready for SVMs

- Earlier our discussion used the augmented definition of linear binary classifier: the feature vector $\mathbf{x} = (x_1, \ldots, x_n, 1)^T$ and the weight vector $\mathbf{w} = (w_1, \ldots, w_n, w_b)^T$. The hyperplane is an equation $\mathbf{w}^T\mathbf{x} = 0$. If $\mathbf{w}^T\mathbf{x} > 0$, then the sample belongs to one class. If $\mathbf{w}^T\mathbf{x} < 0$, the other class.
- Let's go back to the un-augmented version. Let $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$ and $\mathbf{w} = [w_1, w_2, \ldots, w_n]^T$. If $\mathbf{w}^T\mathbf{x} + w_b > 0$ then $\mathbf{x} \in C_1$. If $\mathbf{w}^T\mathbf{x} + w_b < 0$ then $\mathbf{x} \in C_2$. The equation $\mathbf{w}^T\mathbf{x} + w_b = 0$ is the hyperplane, where $\mathbf{w}$ only determines the direction of the hyperplane. To build a classifier is to search for the values for $w_1, \ldots, w_n$ and w_b, the bias/threshold.
- For convenience, we denote $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$.
- We have proved that $\mathbf{w}$, augmented or not, is perpendicular to the hyperlane.

What is the distance from a sample $\mathbf{z}$ to the hyperplane?

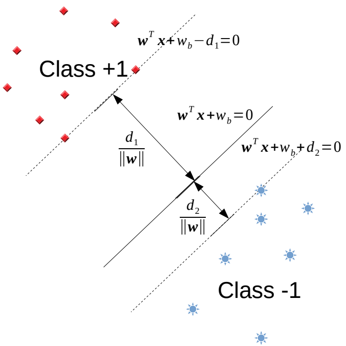


1. Let the point on the hyperplane closest to $\mathbf{z}$ be $\mathbf{x}$. Define $\mathbf{z} = \mathbf{x} + \mathbf{y}$.
2. Because both $\mathbf{y}$ and $\mathbf{w}$ are perpendicular to the hyperplane, we can rewrite $\mathbf{y} = v\frac{\mathbf{w}}{||\mathbf{w}||}$, where v is the Euclidean distance from $\mathbf{z}$ to $\mathbf{x}$ (what we are trying to get), $\frac{\mathbf{w}}{||\mathbf{w}||}$ is the unit vector pointing at the direction of $\mathbf{w}$, $||\mathbf{w}||$ is the l^2 norm of $\mathbf{w}$.
3. Therefore, $\mathbf{z} = \mathbf{x} + v\frac{\mathbf{w}}{||\mathbf{w}||}$.
4. The prediction for $\mathbf{z}$ is then (subsituting into linear classifier equation):

$$
\begin{aligned}
& \mathbf{w}^T\mathbf{z} + w_b \\
= \quad & \mathbf{w}^T\left(\mathbf{x} + v\frac{\mathbf{w}}{||\mathbf{w}||}\right) + w_b \\
= \quad & \mathbf{w}^T\mathbf{x} + v\frac{\mathbf{w}^T\mathbf{w}}{||\mathbf{w}||} + w_b = \underbrace{\mathbf{w}^T\mathbf{x} + w_b}_{=0,\text{by definition}} + v\frac{\mathbf{w}^T\mathbf{w}}{||\mathbf{w}||} \\
= \quad & v\frac{\mathbf{w}^T\mathbf{w}}{||\mathbf{w}||} = v\frac{||\mathbf{w}||^2}{||\mathbf{w}||} = v||\mathbf{w}||.
\end{aligned}
$$

5. Finally, $v = \overbrace{(\mathbf{w}^T\mathbf{z} + w_b)}^{prediction=d}/||\mathbf{w}||$.
6. **Conclusion**: a sample $\mathbf{z}$'s distance to a hyperplane $\mathbf{w}^T\mathbf{x} + w_b = 0$ is $d/||\mathbf{w}||$ **if and only if** the prediction for it $\mathbf{w}^T\mathbf{z} + w_b$ is $\pm d$. (The sign ahead of d depends on which side the sample is on.)

Hard margin linear SVM (for two linearly separable classes)



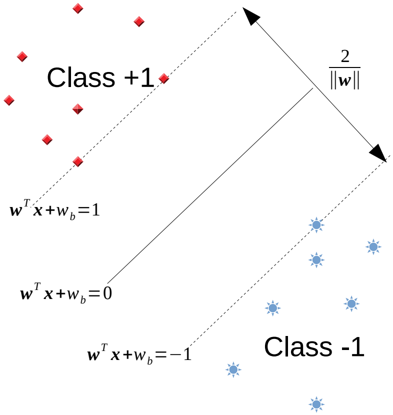
- All samples of Classes $+1$ and -1 are above and below the hyperplane, respectively.
- For Class $+1$, denote the distance from the sample(s) closest to the hyperplane as $d_1/||\mathbf{w}||$ $(d_1 > 0)$.
- Using the conclusion from previous slide, the prediction $\mathbf{w}^T\mathbf{x} + w_b$ for any sample $\mathbf{x}$ of Class $+1$ is thus at least d_1: $\mathbf{w}^T\mathbf{x} + w_b \geq d_1$.
- Similary, for Class -1, we have $\mathbf{w}^T\mathbf{x} + w_b \leq -d_2$, where d_2 is the minimal distance. (Changes: $-$ and $\leq$)

- The idea of an SVM is to find a direction (defined by $\mathbf{w}$) along which closest samples of both classes are apart the most.
- **margin**: the strip between $\mathbf{w}^T\mathbf{x} + w_b = d_1$ and $\mathbf{w}^T\mathbf{x} + w_b = -d_2$ where no sample falls into.

- Width of the margin $\frac{d_1}{||\mathbf{w}||} + \frac{d_2}{||\mathbf{w}||}$.
- We want to maximize margin width:

$$\begin{cases} \max & \frac{d_1}{||\mathbf{w}||} + \frac{d_2}{||\mathbf{w}||} \\ s.t. & \mathbf{w}^T\mathbf{x} + w_b - d_1 \geq 0, \forall \mathbf{x} \in C_{+1} \\ & \mathbf{w}^T\mathbf{x} + w_b + d_2 \leq 0, \forall \mathbf{x} \in C_{-1} \end{cases}$$

Hard margin linear SVM (cond.)



- We prefer $d_1 = d_2$: both classes are equal.
- Since d_1 and d_2 are constants, we can let them be 1.
- Leveraging the label $y_k \in \{+1, -1\}$, we have a consise form:
$$\begin{cases} \max & \frac{2}{||\mathbf{w}||} \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1, \forall \mathbf{x}_k \in C_{+1} \cup C_{-1}. \end{cases}$$
- Maximizing $\frac{2}{||\mathbf{w}||}$ is equivalent to minimizing $\frac{||\mathbf{w}||}{2}$.
- Finally, we transform it into a quadratic programming problem (**the primal form of SVMs**):
$$\begin{cases} \min & \frac{1}{2}||\mathbf{w}||^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1, \forall \mathbf{x}_k. \end{cases}$$
- Why square $||\mathbf{w}||$?

Recap: the Karush-Kuhn-Tucker (KKT) conditions

- Given a nonlinear optimization problem

$$\begin{cases} \min & f(\mathbf{x}) \\ s.t. & h_k(\mathbf{x}) \geq 0, \forall k \in [1..K], \end{cases}$$

where $\mathbf{x}$ is a vector, and $h_k(\cdot)$ is linear, its Lagrangian function is:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{k=1}^{K} \lambda_k h_k(\mathbf{x})$$

- The necessary conditions that the problem above has a solution are KKT conditions:

$$\begin{cases} \frac{\partial L}{\partial \mathbf{x}} = \mathbf{0}, & \\ \lambda_k \geq 0, & \forall k \in [1..K] \\ \lambda_k h_k(\mathbf{x}) = 0, & \forall k \in [1..K] \end{cases}$$

The last condition is sometimes written in the equivalent form $\sum_k \lambda_k h_k(\mathbf{x}) = 0$.

The Lagrangian function of a hard-margin linear SVM

- Given a nonlinear optimization problem $\begin{cases} \min & f(\mathbf{x}) \\ s.t. & h_k(\mathbf{x}) \geq 0, \forall k \in [1..K], \end{cases}$ where $\mathbf{x}$ is a vector, and $h_k(\cdot)$ is linear, its Lagrangian function is:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{k=1}^{K} \lambda_k h_k(\mathbf{x})$$

- Thus, given the primal form of SVMs: $\begin{cases} \min & \frac{1}{2}||\mathbf{w}||^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1, \forall \mathbf{x}_k. \end{cases}$ its Lagrangian function is:

$$L(\mathbf{w}, w_b, \lambda) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{k=1}^{K} \lambda_k [y_k(\mathbf{w}^T\mathbf{x}_k + w_b) - 1]$$

where K is the total number of samples.

The KKT conditions and properties of hard margin linear SVM

For an SVM problem, the KKT conditions thus are:

$$\begin{cases} A : \frac{\partial L}{\partial w} = \mathbf{0}, & \\ B : \frac{\partial L}{\partial w_b} = 0, & \\ C : \lambda_k \geq 0, & \forall k \in [1..K] \\ D : \lambda_k [y_k(\mathbf{w}^T \mathbf{x_k} + w_b) - 1] = 0, & \forall k \in [1..K] \end{cases}$$

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From Eqs. A and B,

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{k=1}^{K} \lambda_k y_k \mathbf{x_k} = \mathbf{0} \Rightarrow \mathbf{w} = \sum_{k=1}^{K} \lambda_k y_k \mathbf{x_k}$$

$$\frac{\partial L}{\partial w_b} = \sum_{k=1}^{K} \lambda_k y_k = 0$$

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$$\frac{\partial L}{\partial w_b} = \sum_{k=1}^{K} \lambda_k y_k = 0$$

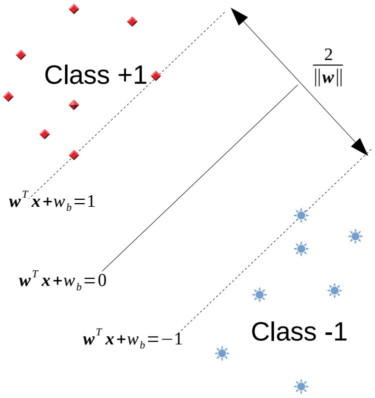
Because λ_k is either positive or 0, the solution of the SVM problem is only associated with samples whose $\lambda_k \neq 0$. Denote them as $N_s = \{\mathbf{x}_k | \lambda_k \neq 0, k \in [1..K]\}$.

Properties of hard margin linear SVM (cont.)

- Therefore, Eq. A can be rewritten into

$$\mathbf{w} = \sum_{\mathbf{x}_k \in N_s} \lambda_k y_k \mathbf{x_k}$$

- The samples $\mathbf{x}_k \in N_s$ collectively determine the $\mathbf{w}$, and thus called **support vectors**, supporting the solution.
- The support vectors also have an interesting "visual" properties. From Eq. D, we have $\lambda_k[y_k(\mathbf{w}^T\mathbf{x_k} + w_b) - 1] = 0$. Because for $\mathbf{x}_k \in N_s$, $\lambda_k > 0$, then $y_k(\mathbf{w}^T\mathbf{x_k} + w_b) = 1$.
- Given that $y_k \in \{+1, -1\}$, we have $\mathbf{w}^T\mathbf{x_k} + w_b = \pm 1$. They support the **gutters**.



The dual form of an SVM

1. Given a nonlinear optimization problem in the **primal** form

$$
\begin{cases}
\min & f(\mathbf{x}) \\
s.t. & h_k(\mathbf{x}) \geq 0, \forall k \in [1..K],
\end{cases}
$$

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2. its **dual form** is

$$\begin{cases} \max & L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{k=1}^{K} \lambda_k h_k(\mathbf{x}) \\ s.t. & \lambda_k \geq 0, \forall k \in [1..K], \\ & \nabla L = \mathbf{0} \end{cases}$$

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3. Thus for a **primal** SVM problem

$$\begin{cases} \min & \frac{1}{2}||\mathbf{w}||^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1, \forall \mathbf{x}_k. \end{cases}$$

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4. its **dual form** is

$$\begin{cases} \max & \frac{1}{2}||\mathbf{w}||^2 - \sum\limits_{k=1}^{K} \lambda_k(y_k(\mathbf{w}^T\mathbf{x_k} + w_b) - 1) \\ s.t. & \lambda_k \geq 0, \forall k \in [1..K], \\ & \mathbf{w} = \sum\limits_{k=1}^{K} \lambda_k y_k x_k \quad (from \quad \frac{\partial L}{\partial \mathbf{w}} = 0), \\ & \sum\limits_{k=1}^{K} \lambda_k y_k = 0 \quad (from \quad \frac{\partial L}{\partial w_b} = 0) \end{cases}$$

The dual form of an SVM (cond.)

$$\begin{cases} \max & \frac{1}{2}||\mathbf{w}||^2 - \sum_{k=1}^{K} \lambda_k (y_k(\mathbf{w}^T \mathbf{x_k} + w_b) - 1) \\ s.t. & \lambda_k \geq 0, \forall k \in [1..K], \\ & \mathbf{w} = \sum_{k=1}^{K} \lambda_k y_k x_k \;\; (from \;\; \frac{\partial L}{\partial \mathbf{w}} = 0), \\ & \sum_{k=1}^{K} \lambda_k y_k = 0 \;\; (from \;\; \frac{\partial L}{\partial w_b} = 0) \end{cases}$$

Subsituting $\mathbf{w}$ with $\sum_{k=1}^{K} \lambda_k y_k x_k$, the objective function becomes:

$$L = -\frac{1}{2} \sum_{i=1}^{K} \sum_{j=1}^{K} \lambda_i \lambda_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{k=1}^{K} \lambda_k$$

Thus, the new **dual form** is:

$$\begin{cases} \max & -\frac{1}{2} \sum_{i=1}^{K} \sum_{j=1}^{K} \lambda_i \lambda_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{k=1}^{K} \lambda_k \\ s.t. & \lambda_k \geq 0, \forall k \in [1..K], \\ & \sum_{k=1}^{K} \lambda_k y_k = 0 \end{cases}$$

- The number of unknowns to solve drops from n features to K samples.
- Instead of finding $\mathbf{w}$, find K λ_k's. (Is an SVM really non-parametric?)
- The new SVM: $g(\mathbf{x}) + w_b = \mathbf{w}^T \mathbf{x} + w_b = \sum_{k=1}^{K} \lambda_k y_k (\mathbf{x}^T \mathbf{x_k}) + w_b$.
- To store an SVM model, just store the support vectors $\mathbf{x}_i$'s, their labels y_i's and weights λ_i's, and the bias w_b.

SVMs are similarity-based classifiers

- The prediction for a sample $\mathbf{x}$:

$$\sum_{k=1}^{K} \lambda_k y_k (\mathbf{x}^T \mathbf{x_k}) + w_b$$

- Recall that $y_k = +1$ if a sample $\mathbf{x}_k$ belongs to class $+1$ (the set C_{+1}), while $y_k = -1$ if class -1 (the set C_{-1}).
- Thus the prediction can be rewritten into three terms:

$$\underbrace{\sum_{\mathbf{x_k} \in C_{+1}} \lambda_k (\mathbf{x}^T \mathbf{x_k})}_{\text{weighted similarity to positive samples}} - \underbrace{\sum_{\mathbf{x_k} \in C_{-1}} \lambda_k (\mathbf{x}^T \mathbf{x_k})}_{\text{weighted similarity to negative samples}} + w_b$$

- The expression above basically says: whether the sample $\mathbf{x}$ is more like the negative (-1) samples or the positive ($+1$) samples.
- Similarities are weighted by sample weights λ_i. Samples whose $\lambda_i = 0$ have no "voting power." Only support vectors, i.e., those whose $\lambda_i > 0$, have.

Kernel tricks: achieving non-linearity on SVMs

- In the previous slides, any two samples "interact" with each other thru dot product, e.g., $\mathbf{x_i}^T\mathbf{x}_j$ (in training, between two samples) or $\mathbf{x}^T\mathbf{x_k}$ (in prediction, between a sample to be predicted and a support vector).
- Note that dot product is about measuring similarity between two vectors.
- It can be expanded to any function, denoted as $\mathcal{K}(\mathbf{x},\mathbf{y})$ ($\mathbf{x}$ and $\mathbf{y}$ are any two vectors of same dimension. Not the input and output of an estimator), between two vectors, known as the **kernel function** or **kernel tricks**.
- SVM dual form using the kernel function $\mathcal{K}$ (to solve, not for prediction):

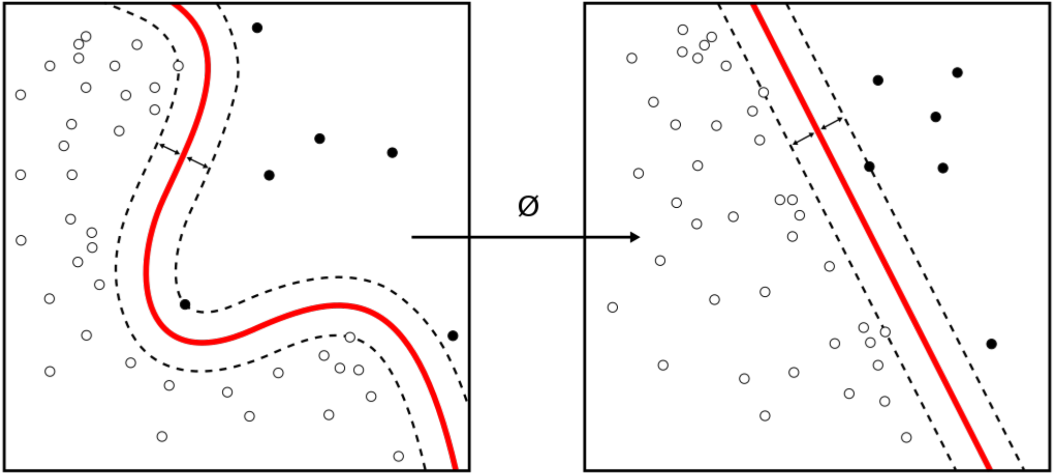
$$\begin{cases} \max & -\frac{1}{2}\sum_{i=1}^{K}\sum_{j=1}^{K}\lambda_i\lambda_j y_i y_j \mathcal{K}(\mathbf{x}_i,\mathbf{x}_j) + \sum_{k=1}^{K}\lambda_k \\ s.t. & \lambda_k \geq 0, \forall k \in [1..K], \sum_{k=1}^{K}\lambda_k y_k = 0 \end{cases}$$

- An SVM using the kernel function (predicting): $\sum_{k=1}^{K}\lambda_k y_k \mathcal{K}(\mathbf{x},\mathbf{x_k}) + w_b$

Types of kernels

- Linear kernels: what we have seen so far in SVMs.
- Polynomial kernels: $\mathcal{K}(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y} + b)^p$ where $p \in \mathbb{Z}^+$ and $b \in \mathbb{R}$.
- Gaussian (radial basis function, RBF) kernels (that build contours around support vectors when $\mathbf{y}$ is a support vector): $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/\sigma)$
- A Gaussian kernel amplifies the influence of close samples and attenuates that of distant samples.
- Usually linear and Gaussian are good enough. A Gaussian kernel can be decomposed into many polynomial terms.

Transforming a nonlinearly separable problem to a linearly separable one



Source: Wikipedia/SVM.

How to get the w_b?

- The optimization problem itself, in either the dual or primal form, ignores the bias term w_b.
- So how?

Generalized Linear Classifier

- Let $f_1(\cdot)$, $f_2(\cdot)$, ..., $f_P(\cdot)$ be P nonlinear functions where $f_p : \mathbb{R}^n \mapsto \mathbb{R}, \forall p \in [1..P]$.
- Then we can define a mapping from a feature vector $\mathbf{x} \in \mathbb{R}^n$ (the **input space**) to a vector in another space $\mathbf{z} = [f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_P(\mathbf{x})]^T \in \mathbb{R}^P$, which is called the **feature space**.
- The problem then becomes finding the value P and the functions $f_p(\cdot)$ such that the two classes are linearly separable.
- Once the space transform is done, we wanna find a weight vector $\mathbf{w} \in \mathbb{R}^P$ such that

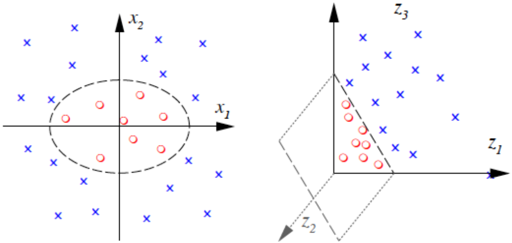
$$\begin{cases} \mathbf{w}^T\mathbf{z} + w_b > 0 & \text{if } \mathbf{z} \in C_1 \\ \mathbf{w}^T\mathbf{z} + w_b < 0 & \text{if } \mathbf{z} \in C_2. \end{cases}$$

- Essentially, we are building a new hyperplane $g(\mathbf{x}) = 0$ such that $g(\mathbf{x}) = w_b + \sum_{p=1}^{P} w_p f_p(\mathbf{x})$. Instead of computing the weighted sum of elements of feature vector, we compute that of elements of the transformed vector.

Creating features from input features

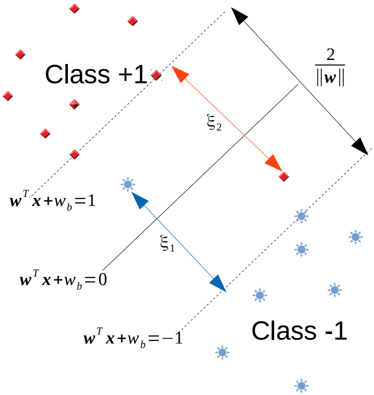
- For example, $g(\mathbf{x}) = w_b + w_1 x_1 + w_2 x_2 + w_{12} x_1 x_2 + w_{11} x_1^2 + w_{22} x_2^2$
- Here is another example,

$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2) x_1 x_2, x_2^2)$$



- A good explanation on StackOverflow: https://stats.stackexchange.com/questions/46425/what-is-feature-space

Soft margin linear SVM



- We could allow some samples to fall into the margin in exchange for wider margin on the remaining samples.
- Therefore, we have a new optimization problem:

$$\begin{cases} \min & \frac{1}{2}||\mathbf{w}||^2 + C\sum_{k=1}^{K}\xi_k \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1 - \xi_k, \forall \mathbf{x}_k \\ & \xi_k \geq 0. \end{cases}$$

  where C is a constant, and ξ_k is called a **slack** variable defined as $\max(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_k + w_b))$.
- Such SVM is called *soft-margin*.
- The constant C provides a balance between maximizing the margin and minimizing the quality, instead of quantity, of misclassification.
- How to find C? Grid search using cross-validation.

Hyperparameters of SVMs

- C: the trade-off between the margin and the misclassification error. For soft-margin SVMs only. The larger the C, the less tolerant the SVM is to misclassification errors.
- γ (also denoted as σ as in $\exp\left(\frac{||\mathbf{x}-\mathbf{y}||^2}{\sigma}\right)$): the kernel coefficient. For Gaussian kernels only. The larger the γ, the more influence the samples have on the decision boundary.

The slack variable and hinge loss

- What is the $\xi = \max(0, 1 - y_i(\mathbf{w}^T\mathbf{x} + w_b))$ when a sample $\mathbf{x}$ is correctly classified?
- It's zero.
- In that case, the constraint is the same as that for hard margin linear SVMs: $y_k(\mathbf{w}^T\mathbf{x} + w_b) \geq 0$.
- The expression $\max(0, 1 - y \cdot \hat{y})$ where $y \in \{+1, -1\}$ is the ground truth label and $\hat{y}$ is prediction for a classifier, is called a **hinge loss**. It's "hinge" because as long as the classification is correct, the loss/error is (capped at) 0.

Recap

- Intution: making the most similar samples of two classes (the support vectors) as different as possible, e.g., banana-looking apples vs apple-looking bananas.
- The support vectors are the closest samples to the decision hyperplane.
- Only support vectors determine the decision hyperplane.
- Soft-margin SVMs: allow some samples to fall into the margin in exchange for a wider margin.
- Non-linear SVMs: transform the input space to a feature space where the two classes are linearly separable.
- Future reading: A Gentle Introduction to Support Vector Machines in Biomedicine, Statnikov et al., AIMA 2019