Download from finelybook www.finelybook.com Once you find the vector $\hat{\alpha}$ that minimizes this equation (using a QP solver), you can compute $\widehat{\mathbf{w}}$ and \widehat{b} that minimize the primal problem by using Equation 5-7.

Equation 5-7. From the dual solution to the primal solution

$$\widehat{\mathbf{w}} = \sum_{i=1}^{m} \widehat{\alpha}^{(i)} t^{(i)} \mathbf{x}^{(i)}$$

$$\widehat{b} = \frac{1}{n_s} \sum_{\substack{i=1 \ \widehat{\alpha}^{(i)} > 0}}^{m} \left(1 - t^{(i)} \left(\widehat{\mathbf{w}}^T \cdot \mathbf{x}^{(i)} \right) \right)$$

The dual problem is faster to solve than the primal when the number of training instances is smaller than the number of features. More importantly, it makes the kernel trick possible, while the primal does not. So what is this kernel trick anyway?

Kernelized SVM

Suppose you want to apply a 2nd-degree polynomial transformation to a twodimensional training set (such as the moons training set), then train a linear SVM classifier on the transformed training set. Equation 5-8 shows the 2nd-degree polynomial mapping function ϕ that you want to apply.

Equation 5-8. Second-degree polynomial mapping

$$\phi(\mathbf{x}) = \phi \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1^2 \\ \sqrt{2} x_1 x_2 \\ x_2^2 \end{pmatrix}$$

Notice that the transformed vector is three-dimensional instead of two-dimensional. Now let's look at what happens to a couple of two-dimensional vectors, a and b, if we apply this 2nd-degree polynomial mapping and then compute the dot product of the transformed vectors (See Equation 5-9).

Download from finelybook www.finelybook.com Equation 5-9. Kernel trick for a 2^{nd} -degree polynomial mapping

$$\phi(\mathbf{a})^{T} \cdot \phi(\mathbf{b}) = \begin{pmatrix} a_{1}^{2} \\ \sqrt{2} a_{1} a_{2} \\ a_{2}^{2} \end{pmatrix}^{T} \cdot \begin{pmatrix} b_{1}^{2} \\ \sqrt{2} b_{1} b_{2} \\ b_{2}^{2} \end{pmatrix} = a_{1}^{2} b_{1}^{2} + 2a_{1} b_{1} a_{2} b_{2} + a_{2}^{2} b_{2}^{2}$$
$$= (a_{1} b_{1} + a_{2} b_{2})^{2} = \begin{pmatrix} a_{1} \\ a_{2} \end{pmatrix}^{T} \cdot \begin{pmatrix} b_{1} \\ b_{2} \end{pmatrix}^{2} = (\mathbf{a}^{T} \cdot \mathbf{b})^{2}$$

How about that? The dot product of the transformed vectors is equal to the square of the dot product of the original vectors: $\phi(\mathbf{a})^T \cdot \phi(\mathbf{b}) = (\mathbf{a}^T \cdot \mathbf{b})^2$.

Now here is the key insight: if you apply the transformation ϕ to all training instances, then the dual problem (see Equation 5-6) will contain the dot product $\phi(\mathbf{x}^{(i)})^T \cdot \phi(\mathbf{x}^{(j)})$. But if ϕ is the 2nd-degree polynomial transformation defined in Equation 5-8, then you can replace this dot product of transformed vectors simply by $(\mathbf{x}^{(i)^T} \cdot \mathbf{x}^{(j)})^2$. So you don't actually need to transform the training instances at all: just replace the dot product by its square in Equation 5-6. The result will be strictly the same as if you went through the trouble of actually transforming the training set then fitting a linear SVM algorithm, but this trick makes the whole process much more computationally efficient. This is the essence of the kernel trick.

The function $K(\mathbf{a}, \mathbf{b}) = (\mathbf{a}^T \cdot \mathbf{b})^2$ is called a 2nd-degree *polynomial kernel*. In Machine Learning, a *kernel* is a function capable of computing the dot product $\phi(\mathbf{a})^T \cdot \phi(\mathbf{b})$ based only on the original vectors \mathbf{a} and \mathbf{b} , without having to compute (or even to know about) the transformation ϕ . Equation 5-10 lists some of the most commonly used kernels.

Equation 5-10. Common kernels

Linear:
$$K(\mathbf{a}, \mathbf{b}) = \mathbf{a}^T \cdot \mathbf{b}$$

Polynomial: $K(\mathbf{a}, \mathbf{b}) = (\gamma \mathbf{a}^T \cdot \mathbf{b} + r)^d$
Gaussian RBF: $K(\mathbf{a}, \mathbf{b}) = \exp(-\gamma \| \mathbf{a} - \mathbf{b} \|^2)$
Sigmoid: $K(\mathbf{a}, \mathbf{b}) = \tanh(\gamma \mathbf{a}^T \cdot \mathbf{b} + r)$

Mercer's Theorem

According to *Mercer's theorem*, if a function $K(\mathbf{a}, \mathbf{b})$ respects a few mathematical conditions called *Mercer's conditions* (K must be continuous, symmetric in its arguments so $K(\mathbf{a}, \mathbf{b}) = K(\mathbf{b}, \mathbf{a})$, etc.), then there exists a function ϕ that maps \mathbf{a} and \mathbf{b} into another space (possibly with much higher dimensions) such that $K(\mathbf{a}, \mathbf{b}) = \phi(\mathbf{a})^T \cdot \phi(\mathbf{b})$. So you can use K as a kernel since you know ϕ exists, even if you don't know what ϕ is. In the case of the Gaussian RBF kernel, it can be shown that ϕ actually maps each training instance to an infinite-dimensional space, so it's a good thing you don't need to actually perform the mapping!

Note that some frequently used kernels (such as the Sigmoid kernel) don't respect all of Mercer's conditions, yet they generally work well in practice.

There is still one loose end we must tie. Equation 5-7 shows how to go from the dual solution to the primal solution in the case of a linear SVM classifier, but if you apply the kernel trick you end up with equations that include $\phi(x^{(i)})$. In fact, $\widehat{\mathbf{w}}$ must have the same number of dimensions as $\phi(x^{(i)})$, which may be huge or even infinite, so you can't compute it. But how can you make predictions without knowing $\widehat{\mathbf{w}}$? Well, the good news is that you can plug in the formula for $\widehat{\mathbf{w}}$ from Equation 5-7 into the decision function for a new instance $\mathbf{x}^{(n)}$, and you get an equation with only dot products between input vectors. This makes it possible to use the kernel trick, once again (Equation 5-11).

Equation 5-11. Making predictions with a kernelized SVM

$$\begin{split} h_{\widehat{\mathbf{w}},\,\hat{b}}\big(\phi\big(\mathbf{x}^{(n)}\big)\big) &= \widehat{\mathbf{w}}^T \cdot \phi\big(\mathbf{x}^{(n)}\big) + \hat{b} = \left(\sum_{i=1}^m \widehat{\alpha}^{(i)} t^{(i)} \phi\big(\mathbf{x}^{(i)}\big)\right)^T \cdot \phi\big(\mathbf{x}^{(n)}\big) + \hat{b} \\ &= \sum_{i=1}^m \widehat{\alpha}^{(i)} t^{(i)} \Big(\phi\big(\mathbf{x}^{(i)}\big)^T \cdot \phi\big(\mathbf{x}^{(n)}\big)\Big) + \hat{b} \\ &= \sum_{i=1}^m \widehat{\alpha}^{(i)} t^{(i)} K\Big(\mathbf{x}^{(i)}, \mathbf{x}^{(n)}\big) + \hat{b} \\ &= \widehat{\alpha}^{(i)} > 0 \end{split}$$

Note that since $\alpha^{(i)} \neq 0$ only for support vectors, making predictions involves computing the dot product of the new input vector $\mathbf{x}^{(n)}$ with only the support vectors, not all the training instances. Of course, you also need to compute the bias term \hat{b} , using the same trick (Equation 5-12).

Download from finelybook www.finelybook.com Equation 5-12. Computing the bias term using the kernel trick

$$\begin{split} \hat{b} &= \frac{1}{n_s} \sum_{\substack{i=1\\ \hat{\alpha}^{(i)} > 0}}^{m} \left(1 - t^{(i)} \widehat{\mathbf{w}}^T \cdot \phi \left(\mathbf{x}^{(i)} \right) \right) = \frac{1}{n_s} \sum_{\substack{i=1\\ \hat{\alpha}^{(i)} > 0}}^{m} \left(1 - t^{(i)} \left(\sum_{j=1}^{m} \widehat{\alpha}^{(j)} t^{(j)} \phi \left(\mathbf{x}^{(j)} \right) \right)^T \cdot \phi \left(\mathbf{x}^{(i)} \right) \right) \\ &= \frac{1}{n_s} \sum_{\substack{i=1\\ \hat{\alpha}^{(i)} > 0}}^{m} \left(1 - t^{(i)} \sum_{\substack{j=1\\ \hat{\alpha}^{(j)} > 0}}^{m} \widehat{\alpha}^{(j)} t^{(j)} K \left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right) \right) \end{split}$$

If you are starting to get a headache, it's perfectly normal: it's an unfortunate side effects of the kernel trick.

Online SVMs

Before concluding this chapter, let's take a quick look at online SVM classifiers (recall that online learning means learning incrementally, typically as new instances arrive).

For linear SVM classifiers, one method is to use Gradient Descent (e.g., using SGDClassifier) to minimize the cost function in Equation 5-13, which is derived from the primal problem. Unfortunately it converges much more slowly than the methods based on QP.

Equation 5-13. Linear SVM classifier cost function

$$J(\mathbf{w}, b) = \frac{1}{2} \mathbf{w}^T \cdot \mathbf{w} + C \sum_{i=1}^{m} max(0, 1 - t^{(i)} (\mathbf{w}^T \cdot \mathbf{x}^{(i)} + b))$$

The first sum in the cost function will push the model to have a small weight vector **w**, leading to a larger margin. The second sum computes the total of all margin violations. An instance's margin violation is equal to 0 if it is located off the street and on the correct side, or else it is proportional to the distance to the correct side of the street. Minimizing this term ensures that the model makes the margin violations as small and as few as possible

Hinge Loss

The function max(0, 1 - t) is called the *hinge loss* function (represented below). It is equal to 0 when $t \ge 1$. Its derivative (slope) is equal to -1 if t < 1 and 0 if t > 1. It is not differentiable at t = 1, but just like for Lasso Regression (see "Lasso Regression" on page 130) you can still use Gradient Descent using any *subderivative* at t = 0 (i.e., any value between -1 and 0).