

**The  
Hundred-  
Page**

**Machine  
Learning**

**Book**

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*“All models are wrong, but some are useful.”*  
— *George Box*

The book is distributed on the “read first, buy later” principle.

## 3 Fundamental Algorithms

In this chapter, we describe five algorithms which are not just the most known but also either very effective on their own or are used as building blocks for the most effective learning algorithms out there.

### 3.1 Linear Regression

Linear regression is a popular regression learning algorithm that learns a model which is a linear combination of features of the input example.

#### 3.1.1 Problem Statement

We have a collection of labeled examples  $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$ , where  $N$  is the size of the collection,  $\mathbf{x}_i$  is the  $D$ -dimensional feature vector of the example  $i = 1 \dots N$ ,  $y_i$  is a real valued target ( $y_i \in \mathbb{R}$ ) and every feature  $x_i^{(j)}$ ,  $j = 1 \dots D$ , is also a real number.

We want to build a model  $f_{\mathbf{w},b}(\mathbf{x})$  as a linear combination of features of the example  $\mathbf{x}$ :

$$f_{\mathbf{w},b}(\mathbf{x}) = \mathbf{w}\mathbf{x} + b, \tag{1}$$

where  $\mathbf{w}$  is a  $D$ -dimensional vector of parameters,  $b$  is a real number and  $\mathbf{w}\mathbf{x}$  is a *dot-product*. The notation  $f_{\mathbf{w},b}$  means that the model  $f$  is parametrized by two values:  $\mathbf{w}$  and  $b$ .

We will use the model to predict the unknown  $y$  for a given  $\mathbf{x}$  like this:  $y = f_{\mathbf{w},b}(\mathbf{x})$ . Two models parametrized by two different pairs  $(\mathbf{w}, b)$  will likely produce two different predictions when applied to the same example. We want to find the optimal values  $(\mathbf{w}^*, b^*)$ . Obviously, the optimal values of parameters will define the model that makes more accurate predictions.

You can notice that the form of our linear model in eq. 1 is very similar to the form of the SVM model. The only difference is the missing *sign* operator. The two models are indeed similar. However, the hyperplane in the SVM plays the role of the decision boundary: it's used to separate two groups of examples from one another. As such, it has to be as far from each group as possible. On the other hand, the hyperplane in linear regression is chosen to be as close to all training examples as possible.

You can see why this latter requirement is important by looking at the below illustration in fig. 1. It displays the regression line (in light-blue) for the one-dimensional examples (dark-blue dots). We can use this line to predict the value of the target  $y_{new}$  for a new unlabeled input example  $x_{new}$  that wasn't used to build the model. If our examples are  $D$ -dimensional feature vectors, the only difference is that the regression model will be not a line but a plane (for two-dimensional feature vectors) or a hyperplane for  $D > 2$ .

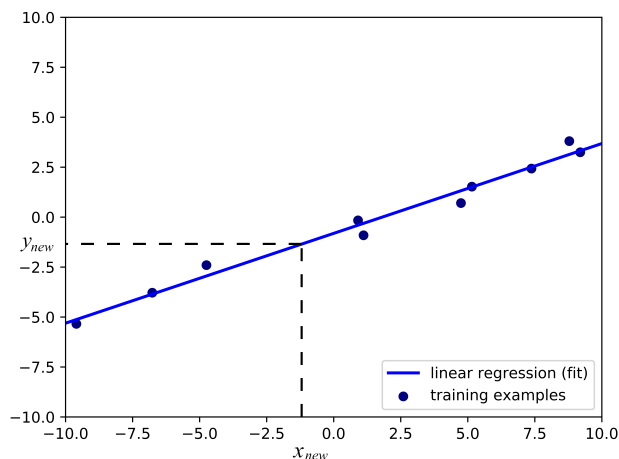


Figure 1: Linear Regression for one-dimensional examples.

Now you see why it's important to have the requirement that the regression hyperplane lies as close to the training examples as possible: if the blue line in fig. 1 was far from the blue dots, the prediction  $y_{new}$  would have fewer chances to be correct.

### 3.1.2 Solution

To get this latter requirement satisfied, in linear regression the optimization procedure which we use to find the optimal values for  $\mathbf{w}^*$  and  $b^*$  tries to minimize the following objective:

$$\min_{\mathbf{w}, b} \frac{1}{N} \sum_{i=1 \dots N} (f_{\mathbf{w}, b}(\mathbf{x}_i) - y_i)^2. \quad (2)$$

The expression  $(f(\mathbf{x}_i) - y_i)^2$  is called the **loss function**. It's a measure of penalty for misclassification of example  $i$ . This particular choice of the loss function is called **squared error loss**. All model-based learning algorithms have a loss function and what we do to find the best model is we try to minimize the **average loss** also called **empirical risk**. The average loss, or empirical risk, for a model, is the average of all penalties obtained by applying the model to the training data.

Why is the loss in linear regression a quadratic function? Why couldn't we just get the absolute value of the difference between the true target  $y_i$  and the predicted value  $f(\mathbf{x}_i)$  and use it as a penalty? We could. And we also could use a cube instead of a square.

Now you probably start realizing how many seemingly arbitrary decisions are made when we design a machine learning algorithm: we decided to use the linear combination of features to predict the target. But we could use a square or some other polynomial to combine the values of features. We could also use some other loss function that makes sense: the absolute difference between  $f(\mathbf{x}_i)$  and  $y_i$  makes sense, the cube of the difference too; the **binary loss** (1 when  $f(\mathbf{x}_i)$  and  $y_i$  are different and 0 when they are the same) also makes sense, right?

If we made different decisions about the form of the model, the form of the loss function, and about the choice of the algorithm that minimizes the average loss to find the best values of parameters, we would end up inventing a different machine learning algorithm. Sounds easy, doesn't it? But do not rush to invent a new learning algorithm. The fact that it's different doesn't mean that it will work better in practice.

People invent new learning algorithms for one of the two main reasons:

1. The new algorithm solves a specific practical problem better than the existing algorithms.
2. The new algorithm has better theoretical guarantees on the quality of the model it produces.

One practical justification of the choice of the linear form for the model is that it's simple. Why use a complex model when you can use a simple one? Another consideration is that linear models rarely overfit. **Overfitting** is the property of a model such that the model predicts very well labels of the examples used during training but frequently makes errors when applied to examples that weren't seen by the learning algorithm during training.

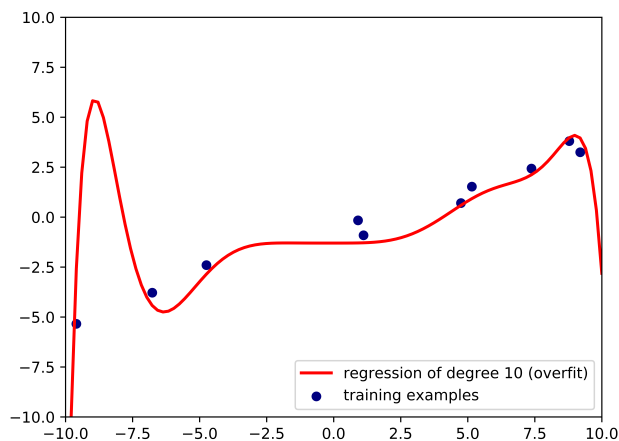


Figure 2: Overfitting.

An example of overfitting in regression is shown in fig. 2. The data used to build the red regression line is the same as in fig. 1. The difference is that this time, this is the polynomial

regression with a polynomial of degree 10. The regression line predicts almost perfectly the targets almost all training examples, but will likely make significant errors on new data. We will talk more about overfitting and how to avoid it Chapter 5.

Now we know why linear regression can be useful: it doesn't overfit much. But what about the quadratic loss? Why did we decide that it should be quadratic? In 1705, the French mathematician Adrien-Marie Legendre, who first published the sum of squares method for gauging the quality of the model stated that squaring the error before summing is *convenient*. Why did he say that? The absolute value is not convenient, because it doesn't have a continuous derivative, which makes the function not smooth. Functions that are not smooth create unnecessary difficulties when employing linear algebra to find closed form solutions to optimization problems. Closed form solutions to finding an optimum of a function are simple algebraic expressions and are often preferable to using complex numerical optimization methods, such as **gradient descent**.

Intuitively, quadratic penalties are also advantageous because they exaggerate the difference between the true target and the predicted one according to the value of this difference. We might also use the powers 3 or 4, but their derivatives are more complex to work with.

Finally, why we care about the derivative of the average loss? Remember from algebra that if we can calculate the gradient of the function in eq. 2, we can then equal this gradient to zero<sup>1</sup> and find the solution to a system of equations that will give us the optimal values  $\mathbf{w}^*$  and  $b^*$ . You can spend several minutes and check it yourself.

## 3.2 Logistic Regression

The first thing to say is that logistic regression is not a regression, but a classification learning algorithm. The name comes from statistics and is due to the fact that the mathematical formulation of logistic regression is similar to that of linear regression.

We will explain logistic regression in the case of binary classification. However, it can naturally be extended to multiclass classification.

### 3.2.1 Problem Statement

In logistic regression, we still want to model  $y_i$  as a linear function of  $\mathbf{x}_i$ , however with a binary  $y_i$  this is not straightforward. The linear combination of features such as  $\mathbf{w}\mathbf{x}_i + b$  is a function that spans from minus infinity to plus infinity, while  $y_i$  has only two possible values.

In the absence of computers, forced to do calculations manually, the scientists in the past wanted to find a linear classification model very much. They figured out that if we define a negative label as 0 and the positive label as 1, we would just need to find a simple continuous

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<sup>1</sup>To find the minimum or the maximum of a function, we set the gradient to zero because the value of the gradient at extrema of a function is always zero. In 2D, the gradient at an extremum is a horizontal line.

function whose codomain is  $(0, 1)$ . In such a case, if the value returned by the model for input  $\mathbf{x}$  is closer to 0, then we assign a negative label to  $\mathbf{x}$ , otherwise, the example will be labeled as positive. One function that has such a property is the **standard logistic function** (also known as the **sigmoid function**):

$$f(x) = \frac{1}{1 + e^{-x}},$$

where  $e$  is the base of the natural logarithm (also called *Euler's number* or the *exp* function in Excel and many programming languages). Its graph is depicted in fig. 3.

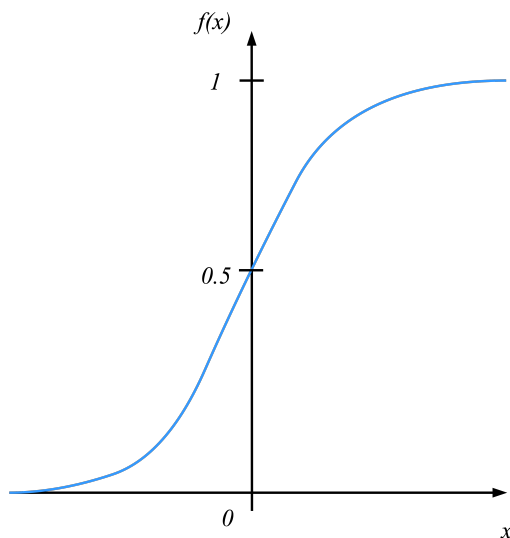


Figure 3: Standard logistic function.

By looking at the standard logistic function graph, we can see how well it fits our classification purpose: if we optimize the values of  $\mathbf{x}$  and  $b$  in an appropriate way, we could interpret the output of  $f(\mathbf{x})$  as the probability of  $y_i$  being positive. For example, if it's higher than or equal to 0.5 we would say that the class of  $\mathbf{x}$  is positive, otherwise it's negative. In practice, the choice of the threshold, 0.5, could be different depending on the problem. We will return to this discussion in Chapter 5 when we will talk about model performance assessment.

So our logistic regression model will look like this:

$$f_{\mathbf{w},b}(\mathbf{x}) \stackrel{\text{def}}{=} \frac{1}{1 + e^{-(\mathbf{w}\mathbf{x}+b)}}. \quad (3)$$

You can see the familiar term  $\mathbf{w}\mathbf{x} + b$  from linear regression. Now, how do we find the best values  $\mathbf{w}^*$  and  $b^*$  for our model? In linear regression, we minimized the empirical risk which

was defined as the average squared error loss.

### 3.2.2 Solution

In logistic regression, instead of using a quadratic loss and trying to minimize the empirical risk, we maximize the *likelihood function*. The likelihood function in statistics defines how likely is the observation (an example) according to our model.

For instance, assume that we have a labeled example  $(\mathbf{x}_i, y_i)$  in our training data. Assume also that we have found (guessed) some specific values  $\hat{\mathbf{w}}$  and  $\hat{b}$  of our parameters. If we now apply our model  $f_{\hat{\mathbf{w}}, \hat{b}}$  to  $\mathbf{x}_i$  using eq. 3 we will get some value  $0 < p < 1$  as output. If  $y_i$  is the positive class, the likelihood of  $y_i$  being the positive class, according to our model, is given by  $p$ . Similarly, if  $y_i$  is the negative class, the likelihood of it being the negative class is given by  $1 - p$ .

The optimization criterion in logistic regression is called **maximum likelihood**. Instead of minimizing the average loss, like in linear regression, we now maximize the likelihood of the training data according to our model:

$$\max_{\mathbf{w}, b} L_{\mathbf{w}, b},$$

where,

$$L_{\mathbf{w}, b} \stackrel{\text{def}}{=} \prod_{i=1 \dots N} f_{\mathbf{w}, b}(\mathbf{x})^{y_i} (1 - f_{\mathbf{w}, b}(\mathbf{x}))^{(1 - y_i)}, \quad (4)$$

and  $f_{\mathbf{w}, b}(\mathbf{x})^{y_i} (1 - f_{\mathbf{w}, b}(\mathbf{x}))^{(1 - y_i)}$  is a fancy mathematical way of saying “ $f_{\mathbf{w}, b}(\mathbf{x})$  when  $y_i = 1$  and  $(1 - f_{\mathbf{w}, b}(\mathbf{x}))$  otherwise”.

You may have noticed that we used the product operator  $\prod$  in the objective function instead of the sum operator  $\sum$  which was used in linear regression. This is because the likelihood of observing  $N$  labels for  $N$  examples is the product of likelihoods of each observation (assuming that all observations are independent of one another, which is the case). You can draw a parallel with the multiplication of probabilities of outcomes in a series of independent experiments in the probability theory.

Because of the *exp* function used in the model, in practice it's more convenient to maximize the *log-likelihood* instead of likelihood. The log-likelihood is defined like follows:

$$\text{Log}L_{\mathbf{w}, b} \stackrel{\text{def}}{=} \ln(L_{\mathbf{w}, b}(\mathbf{x})) = \sum_{i=1}^N y_i \ln f_{\mathbf{w}, b}(\mathbf{x}) + (1 - y_i) \ln (1 - f_{\mathbf{w}, b}(\mathbf{x})).$$



The solution of this new optimization problem will be the same as the solution to the original problem because *log* is a *strictly increasing function*. The latter property means that if we maximize the log of some function we maximize the function itself too.

Contrary to linear regression, there's no closed form solution to the above optimization problem. A common numerical optimization procedure used in such cases is **gradient descent**. We will talk about it in the next chapter.

### 3.3 Decision Tree Learning

A decision tree is an acyclic graph that can be used to make decisions. In each branching node of the graph, a specific feature  $j$  of the feature vector is examined. If the value of the feature is below a specific threshold, then the left branch is followed, otherwise, the right branch is followed. As the leaf node is reached, the decision is made about the class the example belongs to.

As the title of the section suggests, a decision tree can be learned from data.

#### 3.3.1 Problem Statement

Like previously, we have a collection of labeled examples; labels belong to the set  $\{0, 1\}$ . We want to build a decision tree that would allow us to predict the class of an example given a feature vector.

#### 3.3.2 Solution

There are various formulations of the decision tree learning algorithm. In this book, we consider just one, called **ID3**.

The optimization criterion in this case is the average log-likelihood:

$$\frac{1}{N} \sum_{i=1}^N y_i \ln f_{ID3}(\mathbf{x}) + (1 - y_i) \ln (1 - f_{ID3}(\mathbf{x})), \quad (5)$$

where  $f_{ID3}$  is a decision tree.

By now, it looks very similar to logistic regression. However, contrary to the logistic regression learning algorithm which builds a **parametric model**  $f_{\mathbf{w}^*, b^*}$  by finding an *optimal solution* to the optimization criterion, the ID3 algorithm optimizes it *approximately* by greedily constructing a **non-parametric model**  $f_{ID3}(\mathbf{x}) \stackrel{\text{def}}{=} \Pr(y_i = 1 | \mathbf{x})$ .

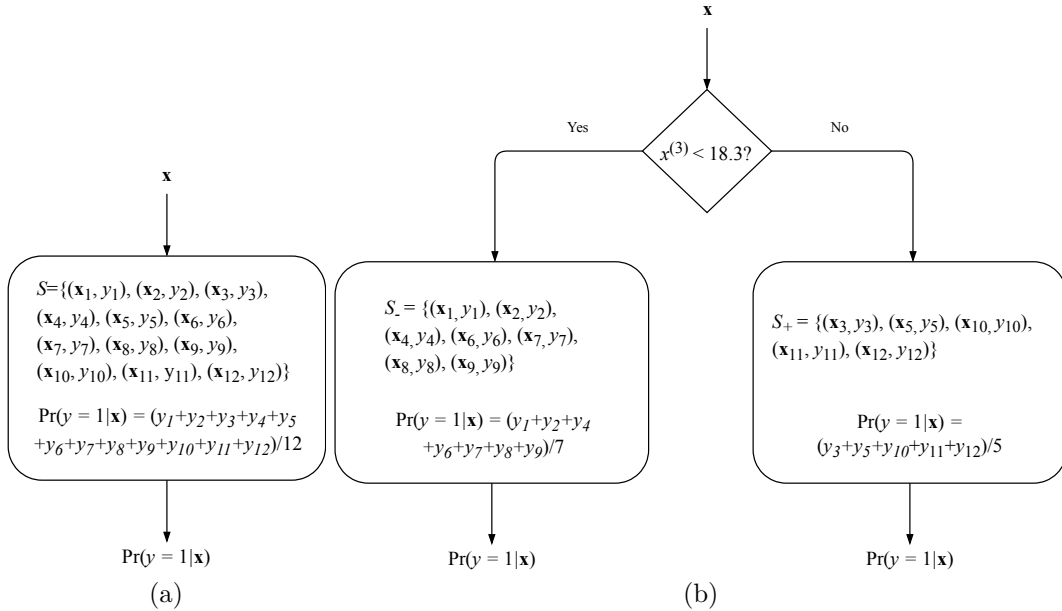


Figure 4: An illustration of a decision tree building algorithm. The set  $\mathcal{S}$  contains 12 labeled examples. (a) In the beginning, the decision tree only contains the start node; it makes the same prediction for any input. (b) The decision tree after the first split; it tests whether feature 3 is less than 18.3 and, depending on the result, the prediction is made in one of the two leaf nodes.

The ID3 learning algorithm works like follows. Let  $\mathcal{S}$  denote a set of labeled examples. In the beginning, the decision tree only has a start node that contains all examples:  $\mathcal{S} \stackrel{\text{def}}{=} \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ . Start with a totally constant model  $f_{ID3}^{\mathcal{S}}$ :

$$f_{ID3}^{\mathcal{S}} = \frac{1}{|\mathcal{S}|} \sum_{(\mathbf{x}, y) \in \mathcal{S}} y, \quad (6)$$

where  $|\mathcal{S}|$  denotes the size of  $\mathcal{S}$ . The prediction given by the above model,  $f_{ID3}^{\mathcal{S}}(\mathbf{x})$ , would be the same for any input  $\mathbf{x}$ . The corresponding decision tree is shown in fig 4 (a).

Then you search through all features  $j = 1 \dots D$  and all thresholds  $t$ , and split the set  $\mathcal{S}$  into two subsets:  $\mathcal{S}_- \stackrel{\text{def}}{=} \{(\mathbf{x}, y) \mid (\mathbf{x}, y) \in \mathcal{S}, x^{(j)} < t\}$  and  $\mathcal{S}_+ = \{(\mathbf{x}, y) \mid (\mathbf{x}, y) \in \mathcal{S}, x^{(j)} \geq t\}$ . The two new subsets would go to two new leaf nodes, and we evaluate, for all possible pairs  $(j, t)$ , how good the split with pieces  $\mathcal{S}_-$  and  $\mathcal{S}_+$  is. Finally, we pick the best such values  $(j, t)$ , split  $\mathcal{S}$  into  $\mathcal{S}_+$  and  $\mathcal{S}_-$ , form two new leaf nodes, and continue recursively on  $\mathcal{S}_+$  and  $\mathcal{S}_-$  (or quit if no split produces a model that's sufficiently better). A decision tree after one split is

illustrated in fig 4 (b).

Now you should wonder what the words “evaluate how good the split is” mean. In *ID3*, the goodness of a split is estimated by using the criterion called *entropy*. The entropy of a set of examples  $S$  is given by:

$$H(S) = -f_{ID3}^S \log f_{ID3}^S - (1 - f_{ID3}^S) \log(1 - f_{ID3}^S).$$

When we split a set of examples by a certain attribute  $j$  and a threshold  $t$ , the entropy of a split,  $H(\mathcal{S}_-, \mathcal{S}_+)$ , is simply a weighted sum of two entropies:

$$H(\mathcal{S}_-, \mathcal{S}_+) = \frac{|\mathcal{S}_-|}{|\mathcal{S}|} H(\mathcal{S}_-) + \frac{|\mathcal{S}_+|}{|\mathcal{S}|} H(\mathcal{S}_+). \quad (7)$$

So, in *ID3*, at each step, at each leaf node, we find a split that minimizes the entropy given by eq. 7 or we stop at this leaf node.

The algorithm stops at a leaf node in any of the below situations:

- All examples in the leaf node are classified correctly by the one-piece model (eq. 6).
- We cannot find an attribute to split upon.
- The split reduces the entropy less than some  $\epsilon$  (the value for which has to be found experimentally<sup>2</sup>).
- The tree reaches some maximum depth  $d$  (also has to be found experimentally).

Because in *ID3*, the decision to split the dataset on each iteration is local (doesn't depend on future splits), the algorithm doesn't guarantee an optimal solution. The model can be improved by using techniques like *backtracking* during the search for the optimal decision tree at the cost of possibly taking longer to build a model.



The entropy-based split criterion intuitively makes sense: entropy reaches its minimum of 0 when all examples in  $\mathcal{S}$  have the same label; on the other hand, the entropy is at its maximum of 1 when exactly one half of examples in  $\mathcal{S}$  is labeled with 1, making such a leaf useless for classification. The only remaining question is how this algorithm approximately maximizes the average log-likelihood criterion. We leave it for further reading.

### 3.4 Support Vector Machine

We already considered SVM in the introduction, so this section will only fill a couple of blanks. There are two important questions that need to be answered:

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<sup>2</sup>We will show how in Chapter 5 when we will talk about hyperparameter tuning.

1. What if there's noise in the data and no hyperplane can perfectly separate positive examples from negative ones?
2. What if the data cannot be separated using a plane, but could be separated by a higher-order polynomial?

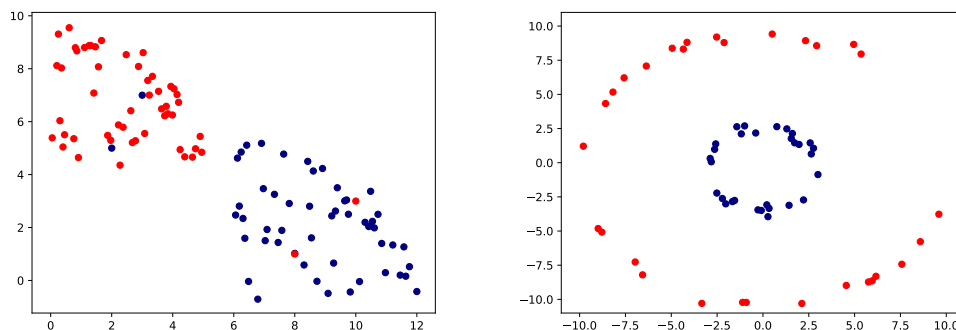


Figure 5: Linearly non-separable cases. Left: the presence of noise. Right: inherent nonlinearity.

You can see both situations depicted in fig 5. In the left case, the data could be separated by a straight line if not for the noise (outliers or examples with wrong labels). In the right case, the decision boundary is a circle and not a straight line.

Remember that in SVM, we want to satisfy the following constraints:

- a)  $\mathbf{w}\mathbf{x}_i - b \geq 1$  if  $y_i = +1$ , and
- b)  $\mathbf{w}\mathbf{x}_i - b \leq -1$  if  $y_i = -1$

We also want to minimize  $\mathbf{w}$  so that the hyperplane was equally distant from the closest examples of each class. Minimizing  $\mathbf{w}$  is equivalent to minimizing  $\frac{1}{2}\|\mathbf{w}\|^2$  and the use of this term makes it possible to perform quadratic programming optimization later on. The optimization problem for SVM therefore looks like this:

$$\min \frac{1}{2}\|\mathbf{w}\|^2 \text{ s.t. } y_i(\mathbf{x}_i\mathbf{w} + b) - 1 \geq 0, i = 1 \dots N. \quad (8)$$

### 3.4.1 Dealing With Noise

To extend SVM to cases in which the data is not linearly separable, we introduce the **hinge loss** function:

$$\max(0, 1 - y_i(\mathbf{w}\mathbf{x}_i - b)).$$

Hinge loss function is zero if the constraints a) and b) are satisfied, in other words, if  $\mathbf{w}\mathbf{x}_i$  lies on the correct side of the decision boundary. For data on the wrong side of the decision boundary, the function's value is proportional to the distance from the decision boundary.

We then wish to minimize,

$$C\|\mathbf{w}\|^2 + \frac{1}{N} \sum_{i=1}^N \max(0, 1 - y_i(\mathbf{w}\mathbf{x}_i - b)),$$

where the hyperparameter  $C$  determines the tradeoff between increasing the size of the decision boundary and ensuring that each  $\mathbf{x}_i$  lie on the correct side of the decision boundary. The value of  $C$  is usually chosen experimentally, just like ID3's hyperparameters  $\epsilon$  and  $d$ . SVMs that optimize hinge loss are called *soft-margin* SVMs, while the original formulation is referred to as a *hard-margin* SVM.

As you can see, for sufficiently high values of  $C$ , the second term in the loss function will become negligible, so the SVM algorithm will try to find the highest margin by completely ignoring misclassification. As we decrease the value of  $C$ , making classification errors is becoming more costly, so the SVM algorithm will try to make fewer mistakes by sacrificing the margin size. As we have already discussed, a larger margin is better for generalization. Therefore,  $C$  regulates the tradeoff between classifying well the training data well (minimizing empirical risk) and classifying well future examples well (generalization).

### 3.4.2 Dealing With Inherent Non-Linearity

SVM can be adapted to work with datasets that cannot be separated by a hyperplane in its original space. However, if we manage to transform the original space into a space of higher dimensionality, we could hope that the examples will become linearly separable in this transformed, higher dimensional space. In SVMs, using a function to *implicitly* transform the original space into a higher dimensional space during the loss function optimization is called the **kernel trick**.

The effect of applying the kernel trick is illustrated in fig. 6. As you can see, it's possible to transform a two-dimensional non-linearly-separable data into a linearly-separable three-dimensional data using a specific mapping  $\phi : \mathbf{x} \rightarrow \phi(\mathbf{x})$ , where  $\phi(\mathbf{x})$  is a vector of higher dimensionality than  $\mathbf{x}$ . For the example of 2D data in fig. 6 (left), the mapping  $\phi$  for example  $\mathbf{x} = [q, p]$  that projects this example into a 3D space (right) would look like this  $\phi([q, p]) = (q^2, \sqrt{2}qp, p^2)$ , where  $q^2$  means  $q$  squared. You see now that the data becomes linearly separable in the transformed space.

However, we don't know a priori which mapping  $\phi$  would work for our data. If we first transform all our input examples using some mapping into very high dimensional vectors and then apply SVM to this data, and we try all possible mapping functions, the computation could become very inefficient and we would never solve our classification problem.

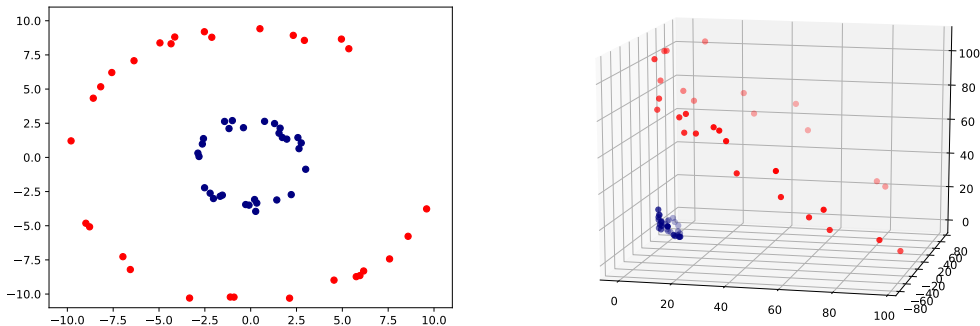


Figure 6: Left: the original non-linearly separable two-dimensional data. Right: the same data is linearly separable after a transformation into a three-dimensional space.

Fortunately, scientists figured out how to use **kernel functions** (or, simply, **kernels**) to easily work in higher-dimensional spaces while looking for an SVM model *without doing this transformation explicitly*. To understand how kernels work, we have to show first how the optimization algorithm for SVM finds the optimal values for  $\|\mathbf{w}\|$  and  $b$ .

The method traditionally used to solve the optimization problem in eq. 8 is the *method of Lagrange multipliers*. Instead of solving the original problem from eq. 8, it is convenient to solve an equivalent problem formulated like this:

$$\max_{\alpha_1 \dots \alpha_N} \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{k=1}^N y_i \alpha_i (\mathbf{x}_i \mathbf{x}_k) y_k \alpha_k \text{ subject to } \sum_{i=1}^N \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0, i = 1 \dots N,$$

where  $\alpha_i$  are Lagrange multipliers. Formulated like this, the optimization problem becomes a convex quadratic optimization problem, efficiently solvable by quadratic programming algorithms.

Now, you could have noticed that in the above formulation, there is a term  $\mathbf{x}_i \mathbf{x}_k$ , and this is the only place where the feature vectors are used. If we want to transform our vector space into a higher dimensional space, we need to transform  $\mathbf{x}_i$  into  $\phi(\mathbf{x}_i)$  and  $\mathbf{x}_j$  into  $\phi(\mathbf{x}_j)$  and then multiply  $\phi(\mathbf{x}_i)$  and  $\phi(\mathbf{x}_j)$ . It would be very costly to do so.

On the other hand, we are only interested in the result of this multiplication, which is a real number. We don't care how this number was obtained as long as it's correct. By using the kernel trick we can get rid of a costly transformation of original feature vectors into higher-dimensional vectors and avoid computing the dot-product of them. We replace that by a simple operation on the original feature vectors that gives the same result. For example, instead of transforming  $(q_1, p_1)$  into  $(q_1^2, \sqrt{2}q_1p_1, p_1^2)$  and  $(q_2, p_2)$  into  $(q_2^2, \sqrt{2}q_2p_2, p_2^2)$  and

then computing the dot-product of  $(q_1^2, \sqrt{2}q_1p_1, p_1^2)$  and  $(q_2^2, \sqrt{2}q_2p_2, p_2^2)$  to obtain  $(q_1^2q_2^2 + 2q_1q_2p_1p_2 + p_1^2p_2^2)$  we could find the dot-product between  $(q_1, p_1)$  and  $(q_2, p_2)$  to get  $(q_1q_2 + p_1p_2)$  and then square it to get exactly the same result  $(q_1^2q_2^2 + 2q_1q_2p_1p_2 + p_1^2p_2^2)$ .

This was an example of the kernel trick and we used the quadratic kernel  $k(\mathbf{x}_i, \mathbf{x}_k) = (\mathbf{x}_i \mathbf{x}_k)^2$ . Multiple kernel functions exist, the most widely used of which is the **RBF kernel**:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right),$$

where  $\|\mathbf{x} - \mathbf{x}'\|^2$  is the squared **Euclidean distance** between two feature vectors. The Euclidean distance is given by the following equation:

$$d(\mathbf{x}_i, \mathbf{x}_k) = \sqrt{(x_i^{(1)} - x_k^{(1)})^2 + (x_i^{(2)} - x_k^{(2)})^2 + \dots + (x_i^{(N)} - x_k^{(N)})^2} = \sqrt{\sum_{j=1}^D (x_i^{(j)} - x_k^{(j)})^2}.$$

It can be shown that the feature space of the RBF kernel has an infinite number of dimensions. By varying the hyperparameter  $\sigma$ , the data analyst can choose between getting a smooth or curvy decision boundary in the original space.

### 3.5 k-Nearest Neighbors

**k-Nearest Neighbors** (kNN) is a non-parametric learning algorithm. Contrary to other learning algorithms that discard the training data after the model is built, kNN keeps all training examples in memory. Once a new, previously unseen example comes in, the kNN algorithm finds  $k$  most close examples in the  $D$ -dimensional space and returns the majority label (in case of classification) or the average label (in case of regression).

The closeness of two points is given by a distance function. For example, Euclidean distance seen above is frequently used in practice. Another popular choice of the distance function is the negative **cosine similarity**. Cosine similarity, defined like this,

$$s(\mathbf{x}_i, \mathbf{x}_k) = \cos(\angle(\mathbf{x}_i, \mathbf{x}_k)) = \frac{\sum_{j=1}^D x_i^{(j)} x_k^{(j)}}{\sqrt{\sum_{j=1}^D (x_i^{(j)})^2} \sqrt{\sum_{j=1}^D (x_k^{(j)})^2}},$$

is a measure of similarity of the directions of two vectors. If the angle between two vectors is 0 degrees, then two vectors point to the same direction and cosine similarity is equal to 1. If the vectors are orthogonal, the cosine similarity is 0. For vectors pointing in opposite directions, the cosine similarity is  $-1$ . If we want to use cosine similarity as a distance metric, we need to multiply it by  $-1$ . Other popular distance metrics include Chebychev distance,

Mahalanobis distance, and Hamming distance. The choice of the distance metric, as well as the value for  $k$ , are the choices the analyst makes before running the algorithm. So these are hyperparameters. The distance metric could also be learned from data (as opposed to guessing it). We will talk about that in one of the future chapters.

Now we know how the model building algorithm works and how the prediction is made. A reasonable question is what is the loss function here? Surprisingly, this question has not been well studied in the literature, despite the algorithm’s popularity since the earlier 1960s. The only attempt to analyze the loss function of kNN we aware of was undertaken by Li and Yang in 2003<sup>3</sup>. Below, we outline their considerations.

For simplicity, we make our derivation under the assumptions of binary classification ( $y \in \{0, 1\}$ ) with cosine similarity and **normalized** feature vectors<sup>4</sup>. Under these assumptions, kNN does a locally linear classification with the vector of coefficients,

$$\mathbf{w}_{\mathbf{x}} = \sum_{(\mathbf{x}', y') \in \mathcal{R}_k(\mathbf{x})} y' \mathbf{x}', \quad (9)$$

where  $\mathcal{R}_k(\mathbf{x})$  is the set of  $k$  nearest neighbors to the input example  $\mathbf{x}$ . The above equation says that we take the sum of all nearest neighbor feature vectors to some input vector  $\mathbf{x}$  by ignoring those that have label 0. The classification decision is obtained by defining a threshold on the dot-product  $\mathbf{w}_{\mathbf{x}} \mathbf{x}$  which, in the case of normalized feature vectors, is equal to the cosine similarity between  $\mathbf{w}_{\mathbf{x}}$  and  $\mathbf{x}$ .

Now, defining the loss function like this:

$$L = - \sum_{(\mathbf{x}', y') \in \mathcal{R}_k(\mathbf{x})} y' \mathbf{x}' \mathbf{w}_{\mathbf{x}} + \frac{1}{2} \|\mathbf{w}\|^2$$

and setting the first order derivative of the right-hand side to zero yields the formula for the coefficient vector in eq. 9.

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<sup>3</sup>F. Li and Y. Yang, “A loss function analysis for classification methods in text categorization,” in ICML 2003, pp. 472–479, 2003.

<sup>4</sup>We discuss normalization later in this book, but for the moment assume that all features of feature vectors were squeezed into the range  $[0, 1]$ .