Some notes from the book Hands On Machine Learning - OReilly created on: 2022-11-06 11:01:20

Hands On Machine Learning Notes

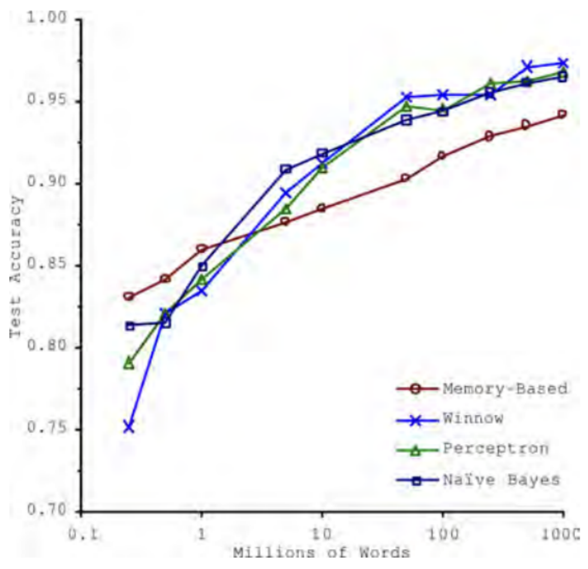
Chapter 1

how can we classify machine learning models:

1. how are they trained: supervised, unsupervised, semi-supervised, "self supervised", RL.
    1. **Supervised**: labeled data
    2. **Unsupervised**: unlabeled data; clustering, anomaly detection, dimensonality reduction
    3. **Semi-supervised**: semi-labeled data (non random).
    4. **Self-supervised**: non-labeled dataset and then is first classified with an unsupervised learning model and then we train a supervised model on top.
2. can they be updated ? Batch Learning vs Online Learning
    1. **Batch learning**. Train once (offline), and predict online. This models can suffer from **data drift** or **model rot** that means don't update the model enough for fitting new datasets.
    2. **Online learning or Incremental learning**. Instead of using a batch of data this model is trained with batches of data and then it has the capability to be re-trained with new batches but keeping the old weights from previous trainings. helpful for large datasets or fast-evolving problems. Learning rate: inertia of the model against new batches.
3. How they generalize: Instance base vs Model based.
    1. In a nutshell, **instance based** is an exact matching algorithm, i.e. we look for "closer" known instances and we "predict" based on that (ex `KNeighborRegressor`).
    2. **Model based** is a learning algorithm that can interpolate or extrapolate based on the previous samples (it assumes a "model").

The Unreasonable effectiveness of Data

> In a famous paper published in 2001, Microsoft researchers Michele Banko and Eric Brill showed that very different Machine Learning algorithms, including fairly simple ones, performed almost identically well on a complex problem of natural language disambiguation once they were given enough data.



Representativeness of data

Is important that the data used for training is a well representation for the test data. If the data is subject to **sampling bias** we will encounter an issue afterwards. **Irrelevant features**: adding noise features can damage the performance of the model. **regularization**: punish the amount of features used by the model adding a cost on the objective function.

Test and validation

we use always an **out-of-sample validation** that means that we calculate the score on a test set, different to the dataset that we use for training.

when doing hyperparameter optimization we usually split the dataset in three: **"train set", "validation set", "test set"**. we use the first one to train all the models and the second one to choose the best model (or the best hyperparameters). finally, we train the "best model" in the train-set+validation set and we evaluate it in the "test-set"

NFL theorem

The No-Free-Lunch (NFL) theorem is a concept in machine learning that essentially states there is no universally superior algorithm for all tasks. It suggests that the performance of any optimization algorithm, including machine learning models, is averaged out across all possible problems, meaning that **no single algorithm can be considered the best for every problem**. This theorem highlights the importance of choosing an algorithm based on the specifics of the problem at hand rather than relying on a one-size-fits-all solution. The theorem implies that the effectiveness of an algorithm is highly dependent on the problem space, and improvements in performance on one set of problems often come at the expense of reduced performance on other sets of problems. In simpler terms, there's no free lunch; every algorithm has its strengths and weaknesses, and what works well in one scenario might not work as well in another.

Chapter 2

Performance Metrics

to measure the performance of a model we have multiples metrics

$$ RMSE(X, h_0) = \sqrt{\frac{1}{m} \sum_{i \in m}{(\theta^{T}X^{(i)}-y^{i})^{2}}} $$

the RMSE is the $\ell_2$ norm (Also known as the euclidean norm), whereas the $MAE$ is equal to the norm $\ell_1$ (also known as the Manhattan distance)

$$ MAE(X, h_0) = \frac{1}{m} \sum_{i \in m}{ \lVert{\theta^{T}X^{(i)}-y^{i}} \rVert} $$

Given the nature of the norms, a higher value norm $\geq \ell_2$ will overweight larger distances higher, meaning it tends to be more sensitive to outliers. Whereas, lower norms tend to be less sensitive.

STD deviation: The standard deviation is generally denoted $\sigma$ (the Greek letter sigma), and it is the square root of the variance, which is the average of the squared deviation from the mean.

$$ \sigma = \sqrt{VAR} $$ $$ \text{VAR} = \sigma^2= \frac{1}{n}\sum_n{(x_i - \mu)^2} $$ When a feature has a bell-shaped normal distribution (also called a Gaussian distribution), which is very common, the "68-95-99.7" rule applies:about 68% of the values fall within $1\sigma$ of the mean, 95% within $2\sigma$, and 99.7% within $3\sigma$.

Stratified Sampling Split

> do stratified sampling based on the income category. For this you can use Scikit-Learn's `StratifiedShuffleSplit` class:

```
from sklearn.model_selection import StratifiedShuffleSplit

split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
#initialize splitter

#stratified sample that keeps the proportion of the categorical
# variable "income_cat" -in this case-
split_datasets_indexes= split.split(housing, housing["income_cat"])

for train_index, test_index in split_datasets_indexes:
    #n_splits (param on splitter)
    #it yield the indexes not the data
    strat_train_set = housing.loc[train_index]
    strat_test_set = housing.loc[test_index]
```

there's another way using sklearn `train_test_split()` and the argument `stratify`

```
strat_train_set, strat_test_set = train_test_split(housing_df,
                                                   test_size=0.2,

stratify=housing["income_cat"],
                                                   random_state=42)
```

Correlation (Pearson's r)

The correlation coefficient only measures linear correlations (“as x goes up, y generally goes up/down”). It may completely miss out on nonlinear relationships (e.g., “as x approaches 0, y generally goes up”). Figure 2-16 shows a variety of datasets along with their corre- lation coefficient. Note how all the plots of the bottom row have a correlation coefficient equal to 0, despite the fact that their axes are clearly not independent: these are examples of nonlinear relation- ships. Also, the second row shows examples where the correlation coefficient is equal to 1 or –1; notice that this has nothing to do with the slope. For example, your height in inches has a correlation coefficient of 1 with your height in feet or in nanometers.

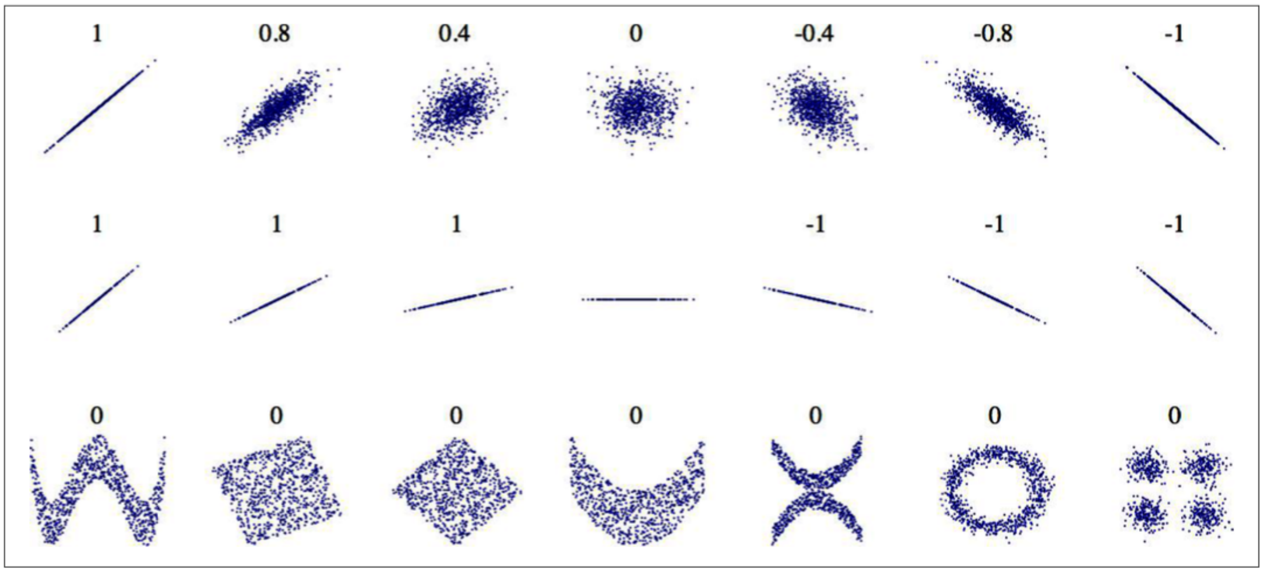


Figure 2-16. Standard correlation coefficient of various datasets (source: Wikipedia; public domain image)

Data Imputation

you will use a handy Scikit-Learn class: `SimpleImputer`. The benefit is that it will store the median value of each feature: this will make it possible to impute missing values not only on the training set, but also on the validation set, the test set, and any new data fed to the mode

```
from sklearn.impute import SimpleImputer imputer =
SimpleImputer(strategy="median")
housing_num = housing.select_dtypes(include=[np.number])
imputer.fit(housing_num)
# median per numeric feature
>>> imputer.statistics_
array([-118.51 , 34.26 , 29. , 2125. , 434. , 1167. , 408. , 3.5385])
# add imputation
X = imputer.transform(housing_num)
```

some other imputers:

1. `KNNImputer` replaces each missing value with the mean of the k-nearest neighbors’ values for that feature. The distance is based on all the available features.
2. `IterativeImputer` trains a regression model per feature to predict the missing values based on all the other available features. It then trains the model again on the updated data, and repeats the process several times, improving the models and the replacement values at each iteration.

Value Normalization

Min-max scaling (many people call this normalization) is the simplest: for each attribute, the values are shifted and rescaled so that they end up ranging from 0 to 1. This is performed by subtracting the min value and dividing by the difference between the min and the max. Scikit-Learn provides a transformer called `MinMaxScaler` for this. It has a feature_range hyperparameter that lets you change the range if, for some reason, you don’t want 0–1 (e.g., neural networks work best with zero-mean inputs, so a range of –1 to 1 is preferable). It’s quite easy to use:

```
from sklearn.preprocessing import MinMaxScaler min_max_scaler =
MinMaxScaler(feature_range=(-1, 1))
    housing_num_min_max_scaled = min_max_scaler.fit_transform(housing_num)
```

Standardization is different: first it subtracts the mean value (so standardized values have a zero mean), then it divides the result by the standard deviation (so standardized values have a standard deviation equal to 1). Unlike min-max scaling, standardization does not restrict values to a specific range. However, standardization is much less affected by outliers. For example, suppose a district has a median income equal to 100 (by mistake), instead of the usual 0–15. Min-max scaling to the 0–1 range would map this outlier down to 1 and it would crush all the other values down to 0–0.15, whereas standardization would not be much affected. Scikit-Learn provides a transformer called `StandardScaler` for standardization:

```
from sklearn.preprocessing import StandardScaler std_scaler =
StandardScaler()
    housing_num_std_scaled = std_scaler.fit_transform(housing_num)
```

A way of Normalizing and transforming multimodal distributions is to add a feature for each of the modes (at least the main ones), using for example a similarity to the kernel value. The similarity measure is typically computed using a radial basis function (RBF)—any function that depends only on the distance between the input value and a fixed point. The most commonly used RBF is the `Gaussian RBF`, whose output value decays exponentially as the input value moves away from the fixed point. For example, the Gaussian RBF similarity between the housing age x and 35 is given by the equation $exp(–\gamma(x – 35)^2)$. The hyperparameter γ (gamma) determines how quickly the similarity measure decays as x moves away from 35. Using Scikit-Learn’s `rbf_kernel()` function, you can create a new Gaussian RBF feature measuring the similarity between the housing median age and 35:

```
from sklearn.metrics.pairwise import rbf_kernel
age_simil_35 = rbf_kernel(housing[["housing_median_age"]], [[35]],
gamma=0.1)
```

Figure 2-18 shows this new feature as a function of the housing median age (solid line). It also shows what the feature would look like if you used a smaller gamma value. As the chart shows, the new age similarity feature peaks at 35, right around the spike in the housing median age distribution: if this particular age group is well correlated with lower prices, there's a good chance that this new feature will help.

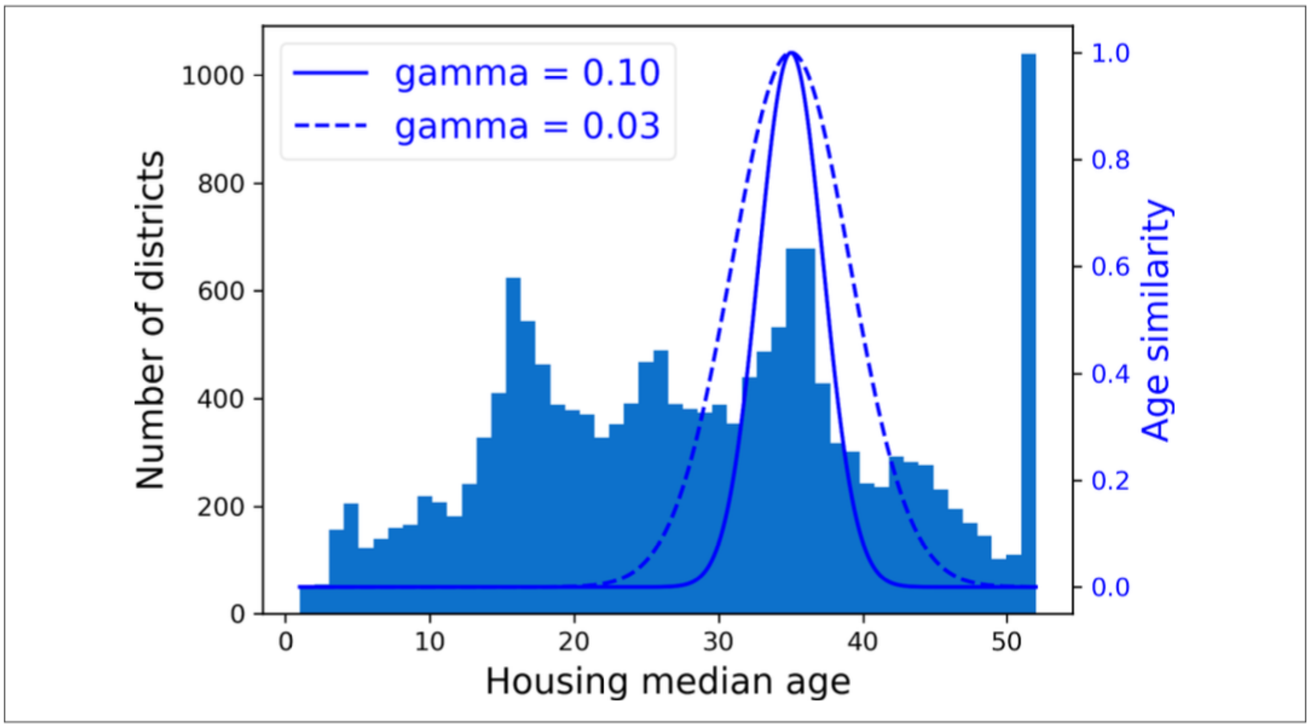


Figure 2-18. Gaussian RBF feature measuring the similarity between the housing median age and 35

Randomized Search

The grid search approach is fine when you are exploring relatively few combinations, like in the previous example, but when the hyperparameter search space is large, it is often preferable to use `RandomizedSearchCV` instead. This class can be used in much the same way as the `GridSearchCV` class, but instead of trying out all possible combinations, it evaluates a given number of random combinations by selecting a random value for each hyperparameter at every iteration.

Comparing two errors samples from CV

In some examples using the mean error of a number of CVsamples might be missing some variance of the error, to compare more effectively use a `scipy.stats.t.interval()` test. (a t-test confidence interval)

```
from scipy import stats
squared_errors =  (final_predictions -  y_test)**2
ic = np.sqrt(stats.t.interval(
        confidence=0.95,
        len(squared_errors)-1, # sample size
        loc=squared_errors.mean(), # mean distr
        scale=stats.sem(squared_errors) # SE of the mean
    ))
```

Chapter 3

Classification Metrics - Confusion Matrix

predicted	values
TN	FP
FN	TP

$$Precision = \frac{TP}{FP+TP}$$

$$Recall = \frac{TP}{FN+TP}$$

$F1$ is the harmonic mean. Whereas the regular mean treats all values equally, the harmonic mean gives much more weight to low values. As a result, the classifier will only get a high F1 score if both recall and precision are high.

$$F1 = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}} = \frac{Precision*Recall}{Precision + Recall}$$

Precision Recall Trade-off

Scikit-Learn does not let you set the threshold directly, but it does give you access to the decision scores that it uses to make predictions. Instead of calling the classifier's `predict()` method, you can call its `decision_function()` method, which returns a score for each instance, and then use any threshold you want to make predictions based on those scores.

```
y_scores = cross_val_predict(sgd_clf, X_train, y_train_5, cv=3,
                             method="decision_function")
from sklearn.metrics import precision_recall_curve
precisions, recalls, thresholds = precision_recall_curve(y_train_5,
y_scores)



#plot
import matplotlib.pyplot as plt
plt.plot(thresholds, precisions[:-1], "b--", label="Precision",
linewidth=2)
plt.plot(thresholds, recalls[:-1], "g-", label="Recall", linewidth=2)
plt.vlines(threshold, 0, 1.0, "k", "dotted", label="threshold")
plt.show()
```

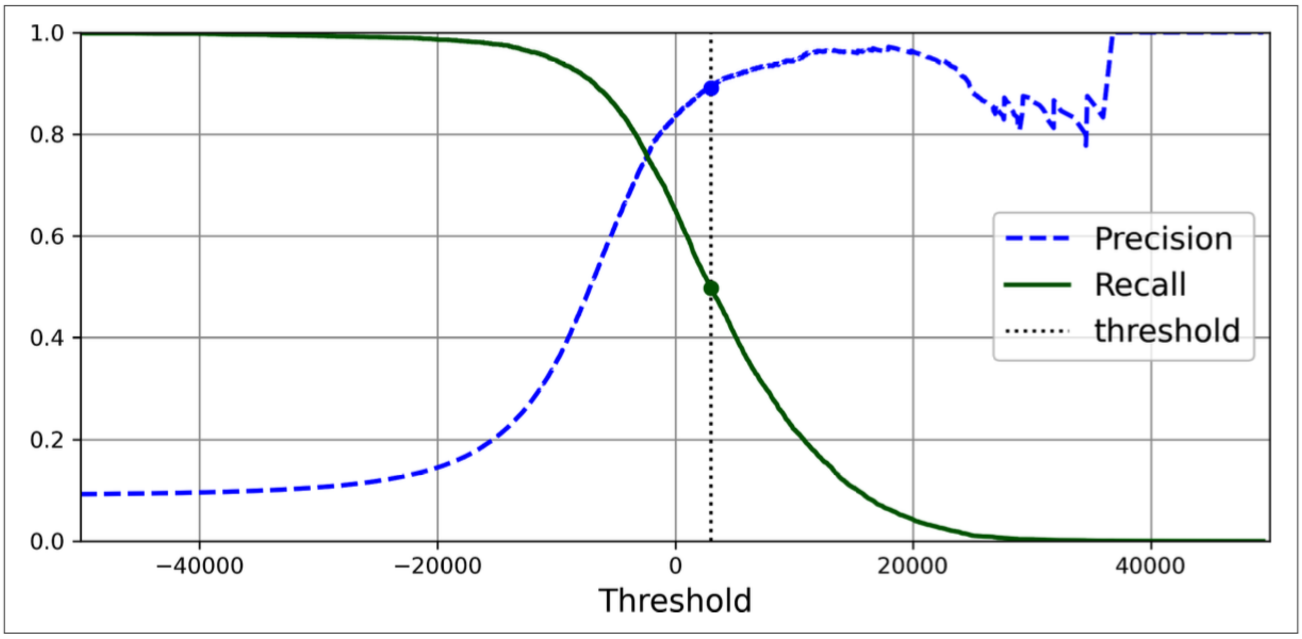


Figure 3-5. Precision and recall versus the decision threshold

You may wonder why the precision curve is bumpier than the recall curve in Figure 3-5. The reason is that precision may sometimes go down when you raise the threshold (although in general it will go up). To understand why, notice what happens when you start from the central threshold and move it just one digit to the right: precision goes from 4/5 (80%) down to 3/4 (75%). On the other hand, recall can only go down when the threshold is increased, which explains why its curve looks smooth.

Another way to select a good precision/recall trade-off is to plot precision directly against recall, as shown in Figure 3-6 (the same threshold is shown)

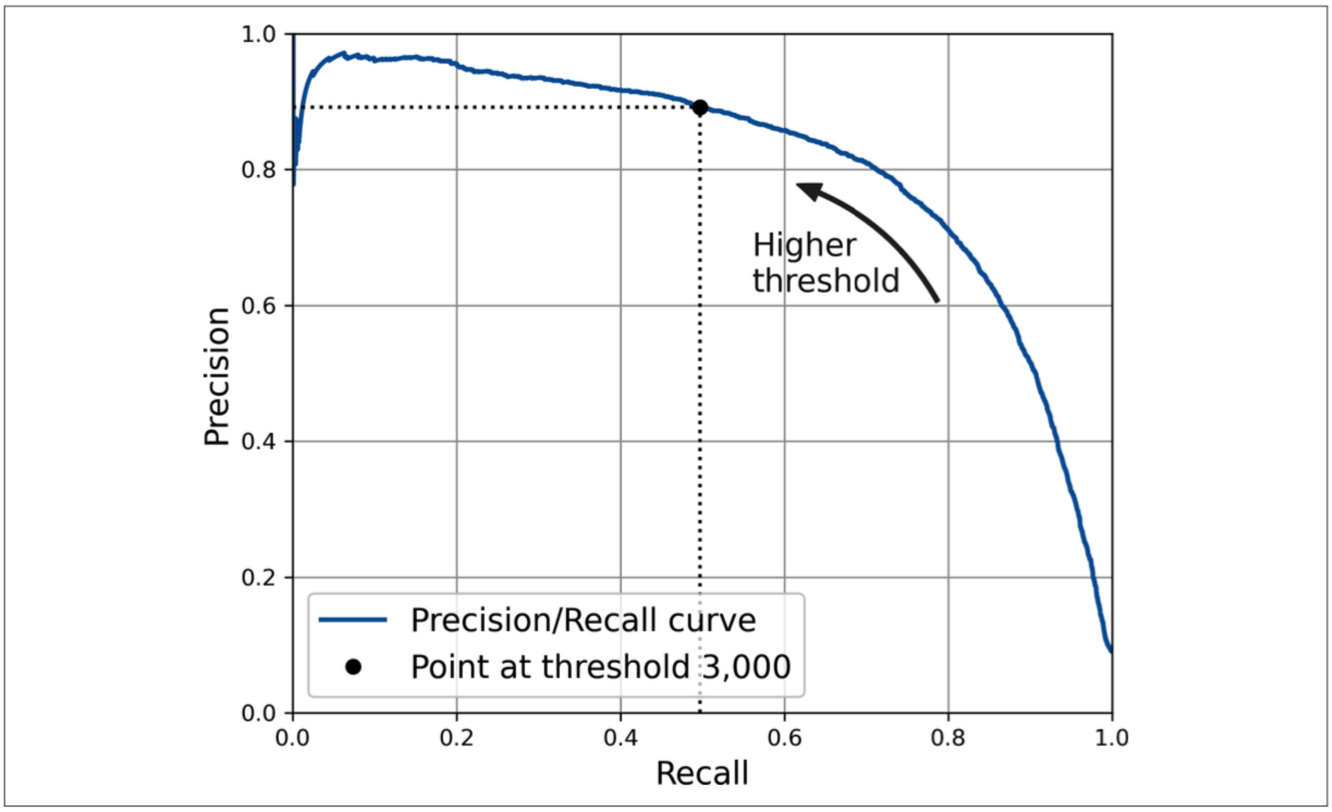


Figure 3-6. Precision versus recall

ROC curve

Is a plot with the `recall (TPR)` against the `false positive rate (FPR)` (this is equal to `1-TNR` also called `"specificity"`). We said than the ROC curve is the plot between `Recall/1-Specificity`.

Once again there is a trade-off: the higher the recall (TPR), the more false positives (FPR) the classifier produces. The dotted line represents the ROC curve of a purely random classifier; a good classifier stays as far away from that line as possible (toward the top-left corner).

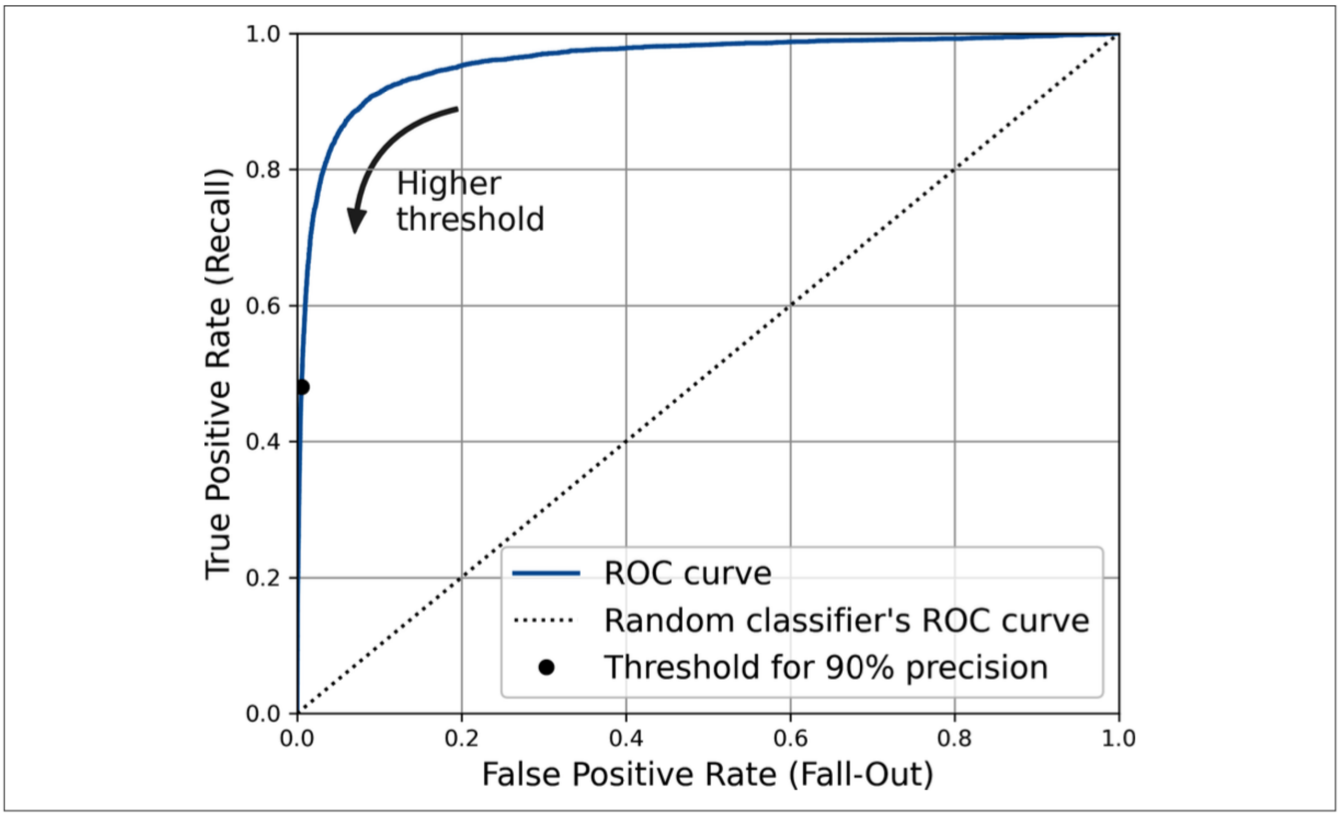


Figure 3-7. A ROC curve plotting the false positive rate against the true positive rate for all possible thresholds; the black circle highlights the chosen ratio (at 90% precision and 48% recall)

Since the ROC curve is so similar to the precision/recall (or PR) curve, you may wonder how to decide which one to use. As a rule of thumb, **you should prefer the PR curve whenever the positive class is rare** or when you care more about the false positives than the false negatives, and the ROC curve otherwise.

Multiclass Classificator

one-versus-the-rest (OvR)

One way to create a system that can classify the digit images into 10 classes (from 0 to 9) is to train 10 binary classifiers, one for each digit (a 0-detector, a 1-detector, a 2-detector, and so on). Then when you want to classify an image, you get the decision score from each classifier for that image and you select the class whose classifier outputs the highest score. This is called the **one-versus-the-rest (OvR)** strategy

one-versus-one (OvO) strategy

Another strategy is to train a binary classifier for every pair of digits: one to distinguish 0s and 1s, another to distinguish 0s and 2s, another for 1s and 2s, and so on. This is called the **one-versus-one (OvO) strategy**. If there are N classes, you need to train N × (N – 1) / 2 classifiers. For the MNIST problem, this means training 45 binary classifiers! When you want to classify an image, you have to run the image through all 45 classifiers and see which class wins the most duels.

OvO vs OvA?

Some algorithms (such as support vector machine classifiers) scale poorly with the size of the training set. For these algorithms OvO is preferred because it is faster to train many classifiers on small training sets than to train few classifiers on large training sets. For most binary classification algorithms, however, OvR is preferred.

MultiLabel/Multioutput Classification

Some models in SKlearn provide the possibility to generate many labels for the same sample. Also you can create multioutput Models than generate from multiples samples multiples outputs (but one output per sample)

This might be useful for example to clean images in a `MultiOutput-Classification` problem

```
stateDiagram-v2
direction LR
    img_noise --> Model
    Model --> img_clean
```

each pixel will be one prediction with a number between `[0,255]`

Chapter 4

fitting models

Linear Regression

$$ \min \quad MSE(X, h_0) = \frac{1}{m} \sum_{i \in m}{(\theta^{T}X^{(i)}-y^{i})^{2}} $$ $$ \text{solution: } \hat{\theta} = (X^{t}X)^{-1}X^{t}Y $$

The complexity of this estimation (pseudo inversion), which consist on inverting X^tX, is between $O(n^{2.4})$ and $O(n^{3})$ depending on the matrix to invert $(X^{t}X)^{-1}$. There is a pseudo inversion using SVD that can lead to a reduction in complexity of $O(n^{2})$. Regardless, when the number of samples is too big, the approach is to use gradient descent.

Gradient Descent

Direction of descent:

$$ \nabla_{\theta}MSE(\Theta) = \frac{2}{m}X^t(X\theta-y) $$

Step calculation. Where η is the learning rate.

$$ \theta^{(next step)} = \theta - \eta\nabla_{\theta}MSE(\Theta) $$

We usually use a stopping criteria such as $\theta^{next} - \theta<\epsilon $. We call ϵ the `"tolerance"`

While the cost function has the shape of a bowl, it can be an elongated bowl if the features have very different scales.Figure 4-7 shows gradient descent on a training set where features 1 and 2 have the same scale (on the left), and on a training set where feature 1 has much smaller values than feature 2 (on the right)

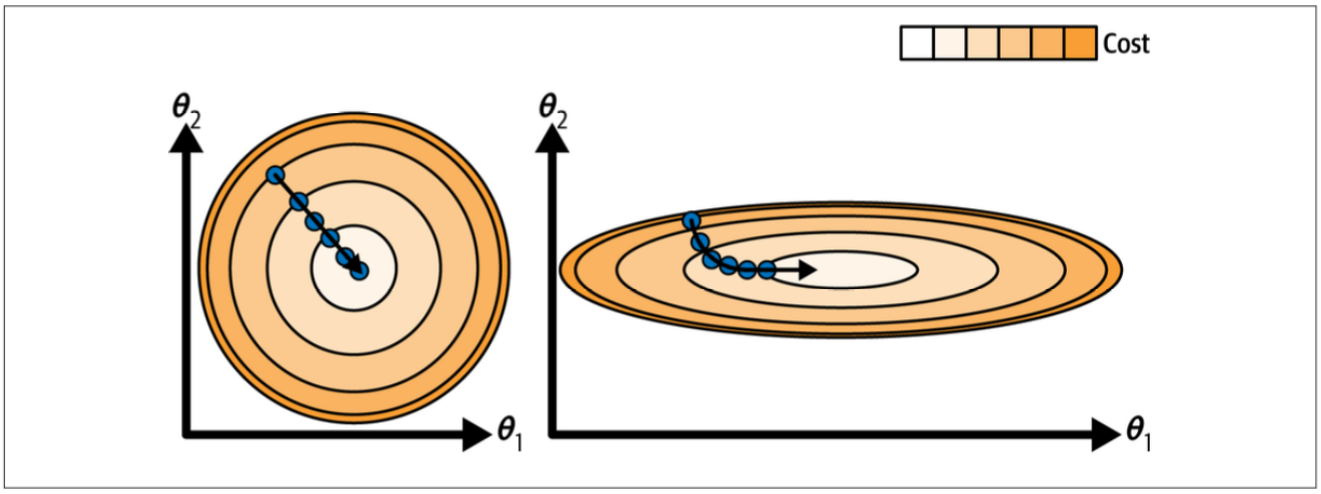


Figure 4-7. Gradient descent with (left) and without (right) feature scaling

When using gradient descent, you should ensure that all features have a similar scale (e.g., using Scikit-Learn's StandardScaler class), or else it will take much longer to converge.

Each iteration over the training set is called an epoch. You may wonder how to set the number of epochs. If it is too low, you will still be far away from the optimal solution when the algorithm stops; but if it is too high, you will waste time while the model parameters do not change anymore. A simple solution is to set a very large number of epochs but to interrupt the algorithm when the gradient vector becomes tiny that is, when its norm becomes smaller than a tiny number ϵ (called the tolerance)

Stochastic Gradient Descent

we can perform the same Gradient Descent methodology but using just a sample from the entire dataset (to improve speed). It only uses one sample, therefore the convergence is very noisy. Because this algorithm is super noise it hardly converges to a minimum and stays there, therefore we could iteratively reduce the learning rate η this is call **Simulated Annealing**. The reduction rate function is called *learning schedule*.

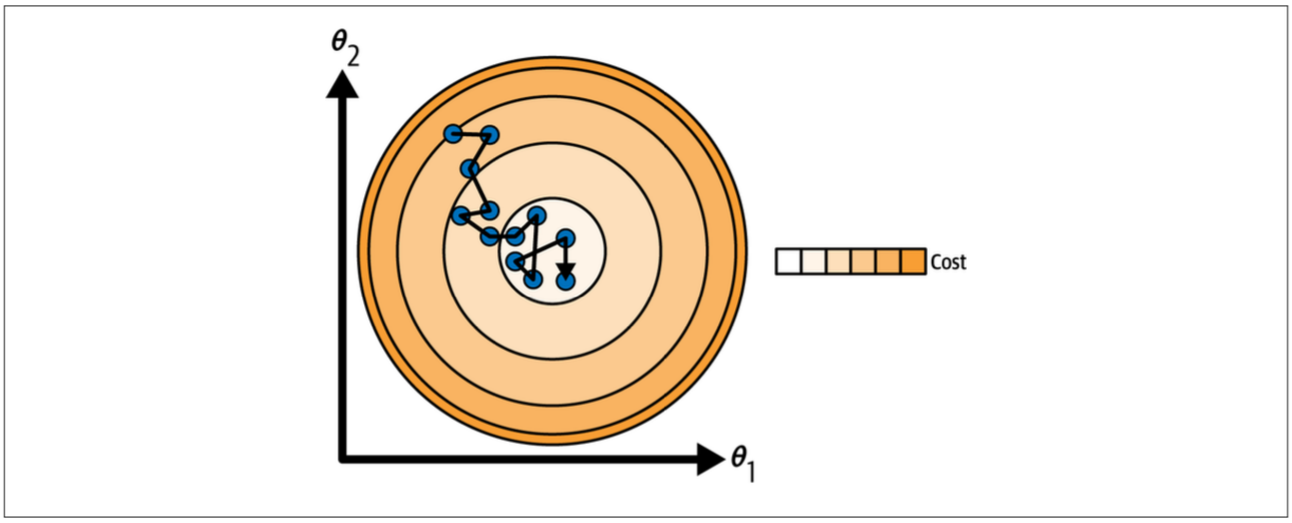


Figure 4-9. With stochastic gradient descent, each training step is much faster but also much more stochastic than when using batch gradient descent

MiniBatch Gradient Descent: Minibatch Is the same as Stochastic Gradient Descent, but, instead of adding one sample at the time, it adds a batch of `n_samples` therefore making the computation harder, but increasing the stability of the convergence.

Table 4-1. Comparison of algorithms for linear regression

Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal equation	Fast	No	Slow	0	No	N/A
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	N/A
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	N/A

Learning Curves

Another way to tell is to look at the learning curves, which are plots of the model's training error and validation error as a function of the training iteration: just evaluate the model at regular intervals during training on both the training set and the validation set, and plot the results. If the model cannot be trained incrementally (i.e., if it does not support `partial_fit()` or `warm_start`), then you must train it several times on gradually larger subsets of the training set.

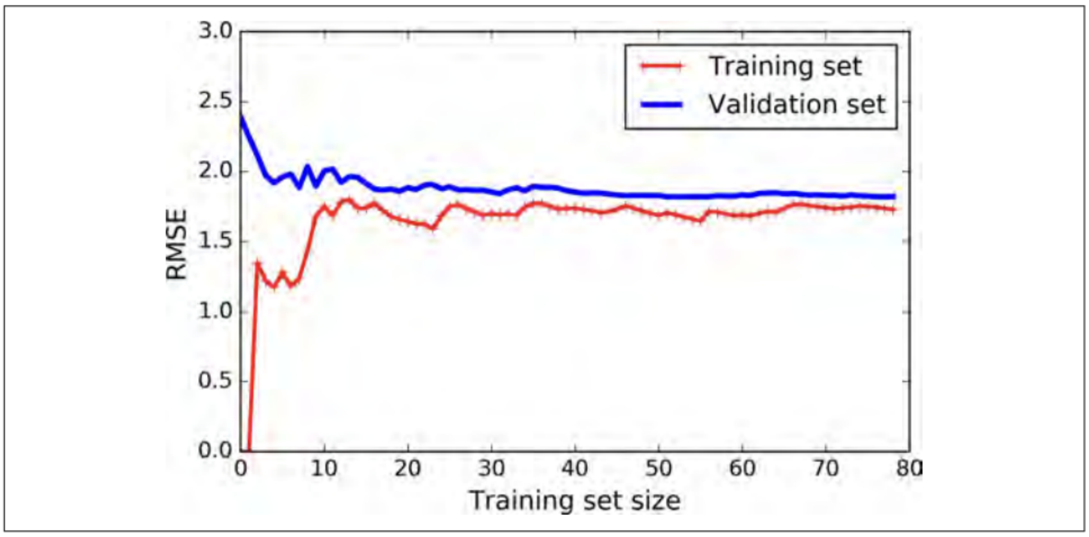


Figure 4-15. Learning curves

if the two curves have a gap is a sign of overfitting, but if they both overlap and they have no gap it can mean that we are underfitting

Bias Variance Trade-off

An important theoretical result of statistics and Machine Learning is the fact that a model's generalization error can be expressed as the sum of three very different errors:

$$ \text{Model Generalization Error} = \text{Bias} + \text{Variance} + \text{Irreductible Error} $$

Bias: Wrong assumptions on the data $f(X)$ is not a good fit to the data (**underfit**)

Variance: Too much sensitivity to data variance (**overfit**)

Irreductible Error: Error in the data acquisition method/instrument, underlying noise.

1. More Model Complexity => Less Bias, More Variance
2. Less Model Complexity => More Bias, Less Variance
3. Adding Regularization => More Bias, Less Variance

Regularization

with regularization we basically add a penalty term to the objective function to punish based on the number of features used, there are two common norms to use here $|\theta|$ (Lasso) and $|\theta|_2$ (Ridge). Also known as L1 and L2 norms. θ is a vector with the coefficients, therefore we will try to make the β coefficients `0` ($\beta=\theta$ in this context).

Note that the regularization terms use θ on the cost function, that means that **the cost is sensible to the scale of the parameters, always normalize before using regularization**.

$$ \text{Ridge Regression} = MSE(\theta)+\alpha\frac{1}{2}\sum_{i}{\theta_i^2} $$ $$ \text{Lasso Regression} = MSE(\theta)+\alpha\sum_{i}|{\theta_i}| $$

An important characteristic of lasso regression is that it tends to eliminate the weights of the least important features (i.e., set them to zero).

There is a third way that is called **Elastic Net** that is basically a convex combination of the L1 and L2 Norms, using a mix ratio called $r \in [0,1]$

$$ \text{Elastic Net Regression} = MSE(\theta)+(r)\alpha\frac{1}{2}\sum_{i}{\theta_i^2}+(1-r)\alpha\sum_{i}|{\theta_i}| $$

> So when should you use Linear Regression, Ridge, Lasso, or Elastic Net? It is almost always preferable to have at least a little bit of regularization, so generally you should avoid plain Linear Regression. Ridge is a good default, but if you suspect that only a few features are actually useful, you should prefer Lasso or Elastic Net since they tend to reduce the useless features' weights down to zero as we have discussed. In general, Elastic Net is preferred over Lasso since Lasso may behave erratically when the number of features is greater than the number of training instances or when several features are strongly correlated.

Early Stopping

Another way to add regularization to a model (that uses gradient descent or other iterative optimization technique) is to stop the iterations whenever the test score reaches a minimum. To detect that you wait for a few iterations where the score haven't improve and you go back to the point were you have the highest score (or the lowest error).

Logistic Regression

Is the same as a regular regression but the output is transformed before using the sigmoid function Therefore we have a better estimator for probabilities.

$$ \hat{\mathbb{P}} = \sigma(X^t\theta)= \frac{1}{1+exp(X^t\theta)} $$

The cost function for the Logit will be called `log-loss`. This is basically the average of the errors, the errors will depend if the sample is positive (`y=1`) or negative (`y=0`), then one of the log probabilities will be summed to the cost total

$$ J(\theta) = -\frac{1}{m}\sum_{i \in m}{[y^{(i)} log(\hat{p}^{(i)}) + (1-y^{(i)}) log(1-\hat{p}^{(i)})]} $$

The bad news is that there is no known closed-form equation to compute the value of θ that minimizes this cost function (there is no equivalent of the Normal equation). But the good news is that this cost function is convex, so gradient descent (or any other optimization algorithm) is guaranteed to find the global minimum (if the learning rate is not too large and you wait long enough).

The Softmax Regression is nothing more than the extension of the Logit function to be used in a multiclass setup. The importance is that is not necessary to train multiples models because we can just extend the logit.

$$ \hat{\mathbb{P}}k = |frac{exp(X^t|theta_k)}{|sum{j \in k}{exp(X^t\theta_j)}} $$

Chapter 5

Classification and Regression Equivalence

1. Regression models can be transformed into classification models by applying the sigmoid function. (or other transformation function - $arctan(y_r)$)
2. Classification models can be adapted into regression models through the use of a continuous probability estimator. Some classification models output probabilities, while others provide scores, which can be more discrete and fluctuating. These scores can be converted into probabilities using Platt scaling or logistic regression based on the score, a method attributed to Vladimir Vapnik, the inventor of the Support Vector Machine. Platt Scaling consist on fitting this model (A, B params) using the true labels y. It also recommends a transformation before the fitting.

$$\mathrm{P}(y=1 | x) = \frac{1}{1 + \exp(Af(x) + B)}$$

Support Vector Machine

based on: The Hundred-Page Machine Learning Book

support vector machine is a linear separation algorithm that fits a linear curve and two wider bounds (determinate by $\propto \frac{1}{c}$)

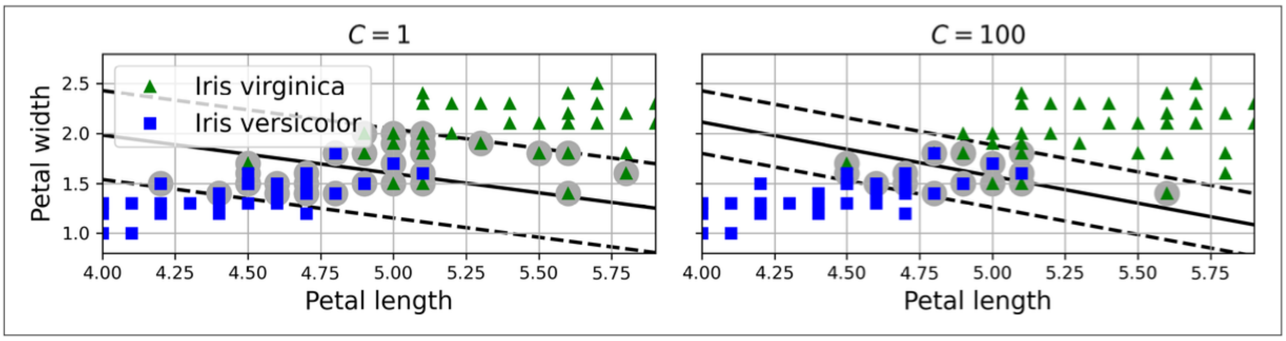


Figure 5-4. Large margin (left) versus fewer margin violations (right)

Given that SVM is a linear separation -and not all feature spaces can be separated by linear separators- we do transformations on the space to fit a linear separator, the most common one being kernel transformations.

the prediction function for SVM is equal to:

$$f(x)= sign(wx-b^)$$

The output of this function is ${+1,-1}$ that can easily be mapped to ${1,0}$ the binary output -in this case $y_i = {+1,-1}$. In the "hard" version of the algorithm we solve the following optimization problem

$$\min ||w||_2$$

$$s.t. \quad y_i (w*x_i-b)\ge 1$$

In simple terms we have two hyperplanes $(wx-b=-1)$ and $(wx-b=1)$ and we want to maximize the "margin" $= \frac{2}{||w||_2}$. which is equal to minimize the norm of the weights $||w||_2$ while keeping all the samples separated (guaranteed by the constraint)

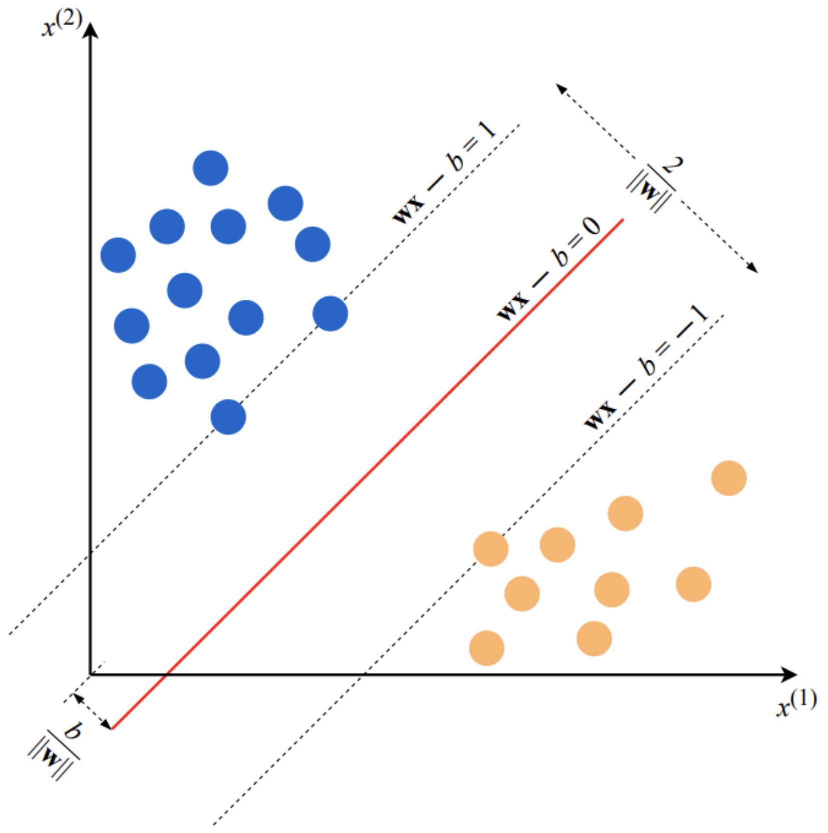


Figure 1.1: An example of an SVM model for two-dimensional feature vectors.

The separation problem

To extend SVM for **non hyperplane separable problems** we introduce **hinge loss**:

$$\max (0, 1 – y_i(wx_i – b))$$

The hinge loss function is zero if the constraints in the "hard" optimization problem are satisfied. but increases in size proportional to the distance violated from the hyperplane to the sample misclassified. Or in other words, it represents the slack value of the relaxation of the constraint when positive.

We then wish to minimize the following cost function. Which is nothing more than the original minimization function plus the hinge loss

$$\min C||w||^2 + \frac{1}{N}\sum_{i=1}^{N} \max (0, 1 – y_i(wx_i – b))$$

There's an interesting property given by this optimization problem and the kernel transformations. The optimization problem solved by SVM is a QP, given that minimizing the norm is equivalent to minimize the square of the norm. QP's are often solved using lagrange multipliers.

Kernels are transformations from n-spaces to higher-n-spaces. solving the QP in a higher dimensional space tends to be more expensive -if solved directly-. however, kernel transformations (usually denoted as $\phi(a,b)$) have an interesting property, you can compute $\phi(a)*\phi(b)$ only knowing a and b. Using this property + the use of lagrangian multipliers on the solver you can "cheaply" apply kernels on top of SVM.

Chapter 6

Decision Trees - CART algorithm

We first define `"Gini Impurity"`. Given a particular leaf of a tree $i$ we estimate the ratio of the $k$ class on that leaf $p_{i,k}$. Therefore we can estimate the "Impurity" of a leaf using the following formula:

$$ \text{Gini Impurity}: \quad G_i = 1 - \sum_{k = 1}^{n}{p_{i,k}^{2}} $$

A Gini coefficient of 0 will represent a leaf with only one class, while a Gini of anything positive will have more than one class. The Gini coefficient is `1 - sum((ratios)**2)` the only clear scenario is when one ratio is 1 and the others are 0 (pure node), the other distances are weirder to explain, but probably a more impure node is when the ratios are equal (same number of samples of all classes). In the case of 2 classes, the Gini coefficient will have numbers between `0` to `0.5` (50%/50%) any other proportion e.g.: (70%/30%) will have something less than `<0.5`.

Finally, the CART algorithm will operate by iterating over this. Given a feature $k$ and a split-threshold $t_k$ we will choose those values minimizing the following cost function:

$$ \min_{k, t_k} J(k,t_k) = \frac{m_{left}}{m} G_{left} + \frac{m_{right}}{m}G_{right} $$

This algorithm stops when a hyperparameter stopping criteria is reached, such as, `max_depth`, `max_leafs_nodes`, `min_samples_leaf` etc.

There is a second metric that we can use in CART called `entropy`. Entropy is similar to Gini Impurity, in the sense that is 0 when there's only one class in the node and positive otherwise.

$$ \text{Entropy:} \quad H_i = \sum_{k \in n}{p_{i,k}log_2(p_{i,k})} $$ Both Entropy and Gini can be used exchangeable on the CART algorithm, they produce similar results, Gini is faster to compute. As you can observe the CART algorithm is a greedy algorithm and will not guarantee optimality, however the full problem is known to be NP-Complete $O(exp(n))$

We can regularize the Decision Trees using the hyperparameters but also using **Pruning**. Pruning is a technique that will reduce the amount of leafs using certain criteria, usually we use a chi-squared test $\chi^2$ to validate that certain leaf is statistical insignificant using a p-value criteria, such as 5%, if is higher, then remove that leaf and their children's.

Decision Trees - CART for Regression

We can use CART for regression as well just changing the Gini or Entropy error for the MSE to use it in a regression context

$$ \min_{k, t_k} J(k,t_k) = \frac{m_{left}}{m} MSE_{left} + \frac{m_{right}}{m}MSE_{right} $$

Chapter 7

Ensemble Methods

--aggregated method categories--

1. **Hard Voting Classifier**: Ensemble a List of models a predict certain sample, **The Most Voted Class** will be the prediction of the ensemble. This method often gets a performance that is better than the best model in the ensemble.

2. **Soft Voting Classifier**: Ensemble a List of models a predict certain sample, we average the probability of each class k: $\mathbb{P^i_k}$ where i is the prediction of the i model, then we choose the highest probability as the prediction of the ensemble. This method usually outperforms the Hard Voting One.

--fitting categories--

1. **Bagging**: (or Bootstrap Aggregating) We split the training set `X` in `m` subsets **with replacement**. We train a model on every subset. Then we use a voting system like the ones described before. If we also sample features we call this method **Random Patches**, if we only sample features and not samples we call this **Random Subspaces**.

2. **Pasting**: same as bagging but we split the training set **without replacement** Generarly, the **Bagging** and **Pasting** methods effectively reduced variance while keeping the bias similar to a simple model trained on the dataset. Usually **bagging** outperforms **pasting** with a slightly higher computational cost.

3. **Random Patches**: you could also sample the features, with or without replacement. if you sample both, features and instances this is known as Random Patches.

4. **Random Subspaces**: if you only sample features but all training samples are given to all learners, we call this "Random Subspaces"

Out of Bag Evaluation

by default when we do bagging, on average, each learner is trained using 63% of the samples (each sample size is `m` samples, where m is the size of the original dataset). that means that we could evaluate each learner using the 37% of samples not using on his training, also known as "out of bag samples" (**OOB**). in Sklearn we can use the parameter `oob_score =True` to get the score of the OOB samples on the learners.

```
bag_clf = BaggingClassifier(DecisionTreeClassifier(), n_estimators=500,
                            oob_score=True, n_jobs=-1, random_state=42)
bag_clf.fit(X_train, y_train)
bag_clf.oob_score_
> 0.896
```

Random Forest

A random forest is a bagging of decision trees that also introduces randomness in the splits. This extra randomness is added **choosing the best split within a random subset of the available features on each tree** $\sqrt{n}$ features out of n. Remember that the CART algorithm is greedy,therefore it always choose the feature with the lower cost for each split, so we control that via sampling set of features- This increases the tree diversity among the forest. This increase in randomness trades a slightly increase in bias to an expected higher reduction in variance.

Feature Importance

Given a fitted random forest we can estimate the feature importance looking into how much each feature is used to split the dataset in all the trees. The importance will be given by the amount of samples w_i that are in the node i where the feature f is being used to split (a proxy to the highness of a node).

$$\text{feature_score}*f = \frac{\sum*{i \in nodes} w_i}{|nodes|}$$

The score then is normalized across all features $score_f = \frac{score_f}{\sum_j{score_j}}$

Boosting

Ada Boosting (Adaptive Boosting)

The boosting methodology consists of consecutively updating the models training the samples that are more misclassified by the previous models. To do that we basically train and predict a dataset with a week-learner, using a weighted sample where all the weights are equal, then we train a second classifier based on the misclassified samples from the first learner, we will overweight this misclassified samples and train a second algorithm (using this new weights), and we will do that with a third one too, the algorithm is described next:

Train a learner using all samples with the same weight w_i

1. $$w_i = \frac{1}{m}$$

Then we estimated the **error rate** of the model j : r_j over the train set using the following formula:

2. $$r_{j} = \frac{\sum_{i \in m : \hat{y}*{j}^{(i)} \neq y*{j}^{(i)}}{w^{(i)}}}{\sum_{i \in m}w^{(i)}}$$

Basically the error rate will be sum the weights of the sample if it was misclassified. Then we estimate the **predictor weight** for the model j: α_j this number will be used to ensemble the predictions:

3. $$\alpha_{j} = \eta log(\frac{1-r_j}{r_j})$$

Finally, we update the weights for all the samples and iterate

$$ w^{(i)} \leftarrow \begin{cases} w^{(i)} & \text{if} ; \hat{y}_{j}^{(i)}=y^{(i)} \

w^{(i)}exp(\alpha_{j}) & \text{if} ; \hat{y}_{j}^{(i)} \neq y^{(i)} \end{cases} $$

the weights are normalized before feeding into the new learner. it's called "boosting" because we "boost" the weights of the misclassified samples each iteration. To make predictions we do with a soft voting but weighting each learner prediction based on their α_{j} score.

Gradient Boosting

Gradient boosting on the other hand is different from `ADABost` in the sense that it actually predicts the residuals from the previous models' ensemble. Each new tree will try to **predict the error**, Then the final prediction will be nothing more than the sum of all predictions.

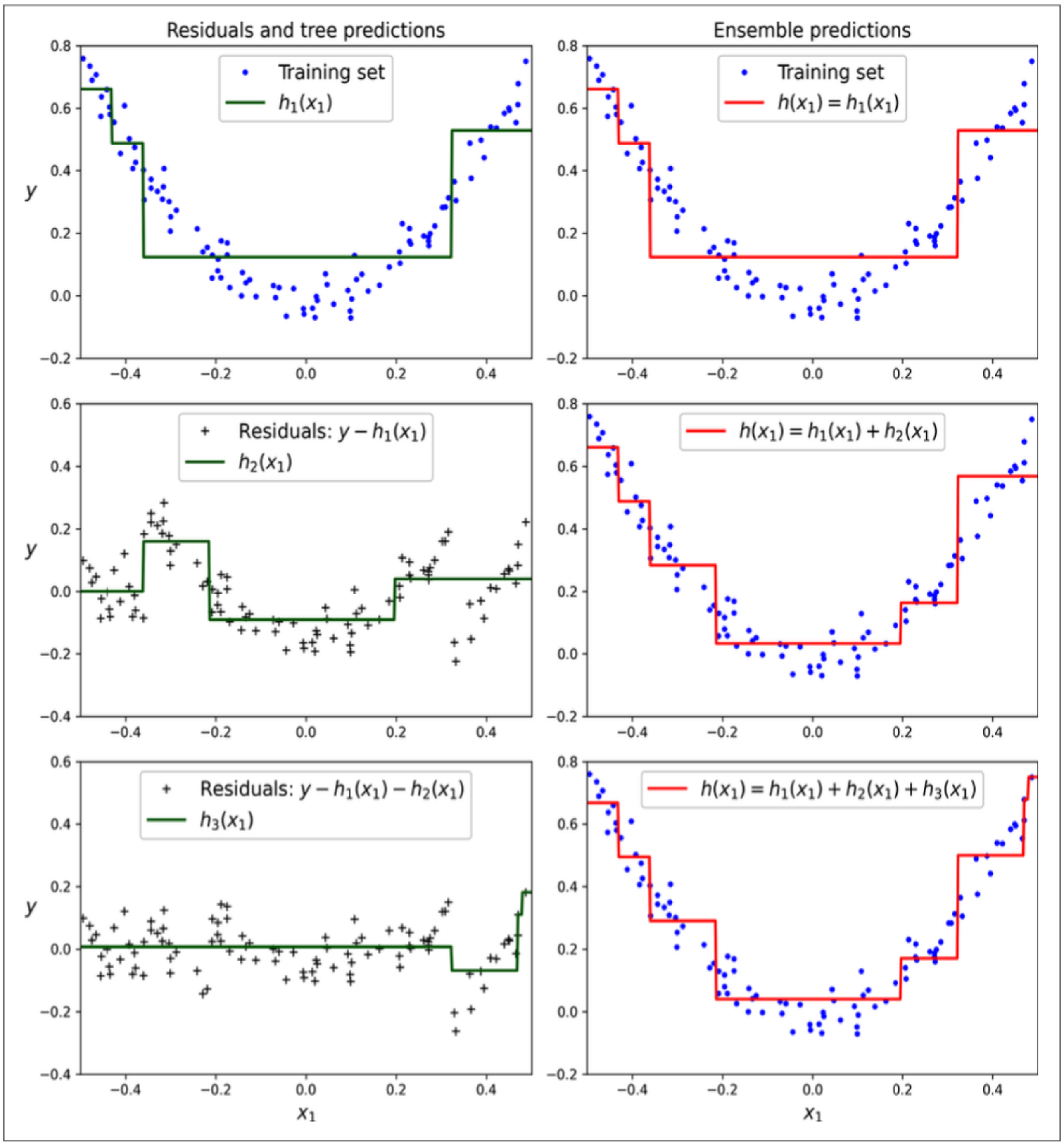


Figure 7-9. In this depiction of gradient boosting, the first predictor (top left) is trained normally, then each consecutive predictor (middle left and lower left) is trained on the previous predictor's residuals; the right column shows the resulting ensemble's predictions

The `learning_rate` hyperparameter scales the contribution of each tree. If you set it to a low value, such as 0.05, you will need more trees in the ensemble to fit the training set, but the predictions will usually generalize better. This is a regularization technique called *shrinkage*

$$ h(x_1) = h_1(x_1) +lr*h_2(x_1)+lr*h_3(x_1) $$

or something like that. You can use the parameter `n_iter_no_change` to do "early stopping" and set a threshold of number of new trees that don't improve the score on the `validation_fraction` set (inner CV from the algorithm) to apply gradient in a classification problem is not that straightforward, we estimate the error based on the observed value ${0,1}$ and the "predicted probability" (the ratio from the leaf). this will be called "residual", the residual of the tree needs to be transformed given that each leaf starts from a node with different proportions. This is not very easy to understand, but in simple we try to fit that "new residual" with a transformation into probability. Hard to understand

Histogram-Based Gradient Boosting

Scikit-Learn also provides another GBRT implementation, optimized for large data- sets: histogram-based gradient boosting (HGB). It works by binning the input features, replacing them with integers. The number of bins is controlled by the max_bins hyperparameter, which defaults to 255 and cannot be set any higher than this.

Stacking

Stacking is an improved voting system, whereas instead of using a hard or soft voting system we train a meta-learner that will try to predict the train-set using the predictions of all models as features. **We usually train the meta-learner in a hold-out group** not used by the train of the other models.

Chatpter 8

The curse of dimensionality

Adding more features increase the probability of having sparse datasets (similar to stratified sampling -> stratum size). even when the data is randomly generated an n-space on average has a higher distance between two generated points than a n-1 space.

you can reduce, in general, a higher dimensional space into a lower dimensional space using projection (a hyperplane with lower dimension will act as a new plane). If this plane is flat on the n-lower dimension is called projection, but if the plane is generated curving that plane on the higher dimensional space is called "manifold"

projection (PCA, random projection)

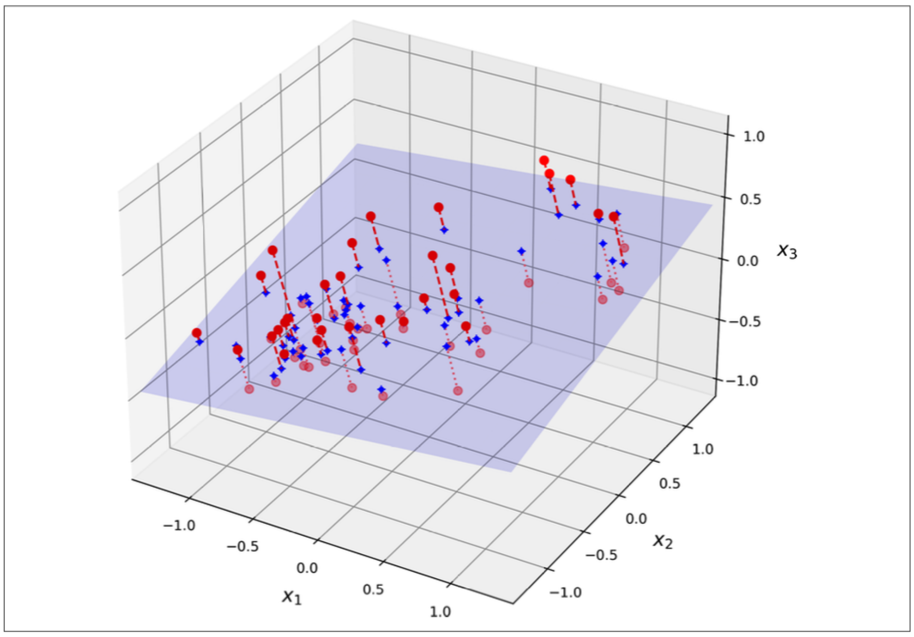


Figure 8-2. A 3D dataset lying close to a 2D subspace

manifold

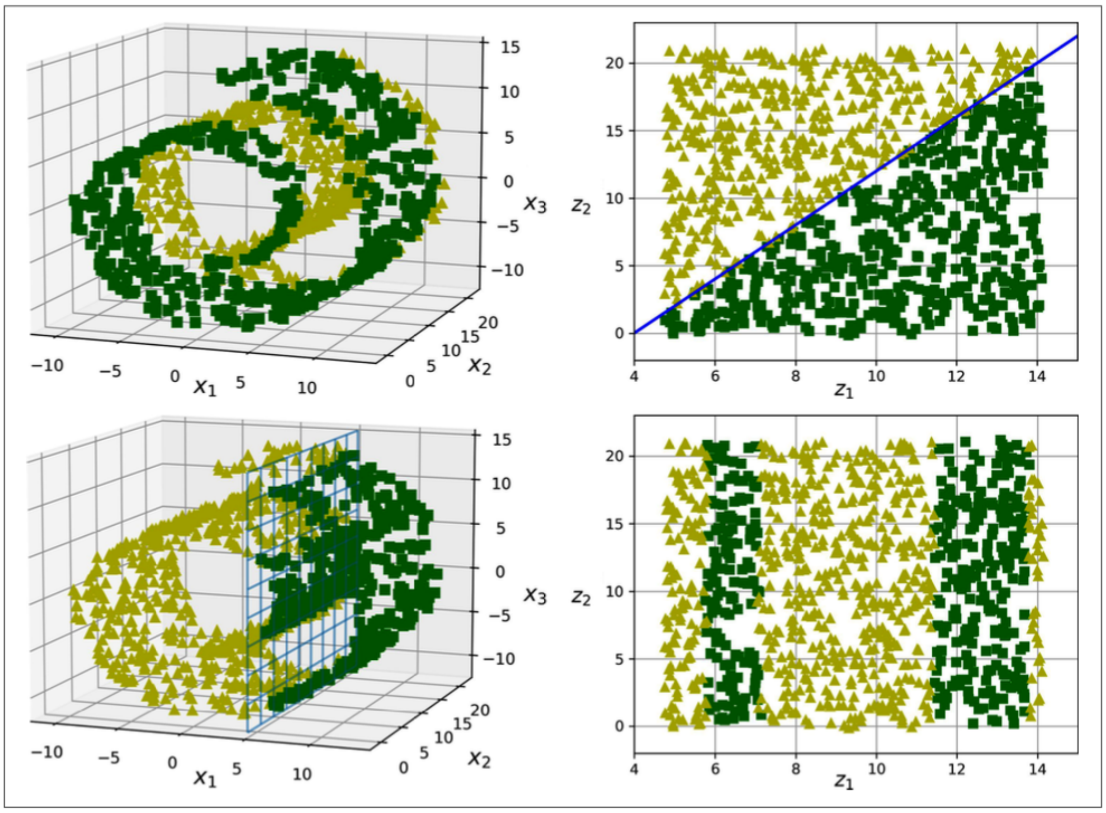


Figure 8-6. The decision boundary may not always be simpler with lower dimensions

PCA

This is a projection algorithm that finds the principal components and then makes a plane with n-k dimensions using the components with higher variance explained. you can optimize the amount of dimensions using a thershold on explained variance percentage, choosing the `n_components` parameter. -or alternative the actual n dimensions of your desired new space-

```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

LLE (local linear embeding)

Locally linear embedding (LLE) is a nonlinear dimensionality reduction (NLDR) technique. It is a manifold learning technique that does not rely on projections, unlike PCA and random projection. In a nutshell, LLE works by first measuring how each training instance linearly relates to its nearest neighbors, and then looking for a low-dimensional representation of the training set where these local relationships are best preserved

Chapter 9

K Means algorithm

Start by placing the centroids randomly (e.g., by picking k instances at random from the dataset and using their locations as centroids). Then label the instances, update the centroids, label the instances, update the centroids, and so on until the centroids stop moving. The algorithm is guaranteed to converge in a finite number of steps (usually quite small). That's because the mean squared distance between the instances and their closest centroids can only go down at each step, and since it cannot be negative, it's guaranteed to converge.

k-means algorithm does not behave very well when the blobs have very different diameters because all it cares about when assigning an instance to a cluster is the distance to the centroid.

by default kmeans will have `n_init` different initiation centroids, and it will keep the solution with the lower cost, the cost is equal to the sum of distance of all samples to their centroid (also called inertia):

$$ \text{intertia: } C=\sum_{i,j-centroid}{min_j{||x_i-C_j||^2}} $$

An important improvement to the k-means algorithm, k-means++, was proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii. They introduced a smarter initialization step that tends to select centroids that are distant from one another, and this improvement makes the k-means algorithm much less likely to converge to a suboptimal solution. **The `KMeans` class uses this initialization method by default**.