

My ML studies

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January 28, 2024

Contents

1	Introduction	4
1.1	General	4
2	Supervised learning	5
2.1	Terms	5
2.2	SL: Decision tree	6
2.2.1	Introduction	6
2.2.2	Representation of the decision tree:	7
2.2.3	Algorithm to build a decision tree	7
2.2.4	Expressiveness	7
2.2.5	ID3 algorithm to create a decision tree	8
2.2.6	Inductive bias	11
2.2.7	Extending ID3 algorithm-other consideration	12
2.2.8	Regression with Decision tree	13
2.2.9	Changing the information gain formula is another option	14
2.2.10	Advantages and Disadvantages of Decision Trees (copied from a text)	14
2.2.11	When to use a decision tree	16
2.2.12	Random forest (Tree ensembles)	16
2.2.13	Boosted tree (XGBoost)	17
2.3	SL: Regression and classification	17
2.3.1	Linear regression	18
2.3.2	Non-linear/polynomial regression	18
2.3.3	Error	19
2.3.4	Multiple Linear regression (multiple features)	19
2.3.5	Other cases	19
2.3.6	Classification	19
2.4	SL: Neural network	20

2.4.1	Perceptron	20
2.5	SL: Instance based learning	21
2.6	SL: Ensemble B&B	21
2.7	SL: Kernel methods and SVMs	22
2.8	SL: Comp Learning Theory	22
2.9	SL: VC dimensions	22
2.10	SL: Bayesian Learning	22
2.11	SL: Bayesian inference	22
3	Unsupervised learning	23
3.1	Clustering	23
3.1.1	K-means clustering	24
3.1.2	Principal Component Analysis (PCA)	24
4	Reinforced Learning	26
4.1	Markov Decision Process	26
5	Miscellaneous topics	27
5.1	One hot encoding for categorical features	27
5.2	Cross validation	28
5.3	F1 score, precision, and recall	30
5.4	Overfitting vs underfitting	30
5.5	Gradient descent (steepest descent)	31
5.5.1	Cost function	31
5.5.2	Gradient descent method	33
5.5.3	Learning rate selection	35
5.6	Model validation	36
5.7	Data processing/cleaning: Missing Values	36
5.8	Data processing & Feature engineering	37
5.8.1	Feature engineering	37
5.8.2	How to create new features	38
5.8.3	scaling vs normalization	41
5.8.4	Scaling a feature	42
5.8.5	Mean normalization	43
5.8.6	z-score normalization	43
5.8.7	Combining features	43
5.9	Ensemble methods	43
5.9.1	Gradient Boosting	44

5.9.2	Data leakage	44
5.10	Python	46
5.11	ML Checklist	46
5.11.1	Time series	46
5.12	Time series	46
5.12.1	Trend	47
5.12.2	Seasonality	47
5.12.3	Cycles: serial dependence (time series as features) . . .	51
5.12.4	Forecasting with hybrid models: Components and residuals	53
5.12.5	Forecasting	54
Bibliography		57

Chapter 1

Introduction to ML

1.1 General

- Supervised learning (SL): functional approximation from labeled data.
- Unsupervised learning (UL): functional description. Learning from unlabeled data.
- Reinforcement learning (RL): Learning from delayed reward.

Chapter 2

Supervised learning (SL)

There are two types of supervised learning:

- classification: taking some inputs and mapping it to some discrete labels. (true or false; male or female; SUV or sedan or truck; class1, class2, class3.)
- regression: returns continuous valued function. Mapping from input to some **real number**. Something like age is more like discrete number, so, it is also classification.

2.1 Terms

- Instances: Inputs, such as pictures, pixels, etc.
- Concept: A set of *functions* that maps inputs to outputs.
- Target concept: The actual function that can map inputs to outputs. This is the actual answer.
- Hypothesis class: Set of all the functions that we are going to think about.
- Sample (Training set): A set of instances with correct labels.
- Candidate: The best approximation of the target concept.

- Testing set: A set of instances with correct labels that was not visible to the learning algorithm during the training phase. It's used to determine the algorithm performance on novel data. we can argue that we learned something by memorization, but indeed, we just memorized the concepts. What we want is generalization.

Remark:

There are generally two ways a regression algorithm can make predictions: either by transforming the features or by transforming the target. Feature-transforming algorithms learn some mathematical function that takes features as an input and then combines and transforms them to produce an output that matches the target values in the training set. Linear regression and neural nets are of this kind.

Target-transforming algorithms use the features to group the target values in the training set and make predictions by averaging values in a group; a set of feature just indicates which group to average. Decision trees and nearest neighbors are of this kind.

The important thing is this: feature transformers generally can extrapolate target values beyond the training set given appropriate features as inputs, but the predictions of target transformers will always be bound within the range of the training set. If the time dummy continues counting time steps, linear regression continues drawing the trend line. Given the same time dummy, a decision tree will predict the trend indicated by the last step of the training data into the future forever. Decision trees cannot extrapolate trends. Random forests and gradient boosted decision trees (like XGBoost) are ensembles of decision trees, so they also cannot extrapolate trends.

2.2 SL: Decision tree

2.2.1 Introduction

Decision tree is a classification learning in the form of a sequence of decisions based on the attributes/features/questions (which forms the nodes) applied to every instance to assign it to a specific class. Answers to the questions would be the edges of the trees. For example, deciding to eat at a restaurant or not, or classification of vehicles into sedans, SUVs, trucks, etc.

2.2.2 Representation of the decision tree:

A decision tree is a structure of nodes, edges and leaves that can be used to *represent* the data. We always start at the root of the tree, otherwise we don't look at any other attribute in the tree.

- Nodes represent attributes where you ask a question about it. (vehicle length, vehicle height, number of doors, etc.).
- Edges represent values/answers, a specific value for each attribute/question.
- Leaves represent the output (or final answer). For example, vehicle's type.

2.2.3 Algorithm to build a decision tree

Algorithm means how to create the decision tree. A decision tree *algorithm* is a sequence of steps that will lead you to the desired output. To form a decision tree, we need to come up with the attributes that can split the space, roughly in half.

- Pick the best attribute (the one that can split the data roughly in half). If this attribute added no valuable information (not a good split), it might cause overfitting.
- Ask a question about this attribute.
- Follow the correct answer path.
- Loop back to (1) till you narrow down the possibilities to one answer (the output).

Note that the usefulness of a question depends upon the answers we got to previous questions.

Purity: means all the samples are of the same kind. This is the ideal case for the leaf nodes. We have impurity if it is still a mix of various categories.

2.2.4 Expressiveness

- Decision trees can basically express any function using the input attributes.

- For Boolean functions (AND, OR, XOR, etc.), the truth table row will be translated into a path to a leaf.
- How many decision trees we can generate for a specific function/problem? For n boolean attributes with boolean output, the decision tree hypothesis space is very huge ($2^{(2^n)}$). (Babak note: this number of decision tree is not really distinct, see my notebook). This is why we need to design algorithms to efficiently search the hypothesis space for the best decision tree.

Decision trees with AND and OR are linear (they need linear number of nodes-ANY type problems). But XOR is a hard problem (requires 2^n nodes-PARITY type of problems).

2.2.5 ID3 algorithm to create a decision tree

We need to find the best attributes for each node, to narrow down the space with each question. ID3 (Inducing Decision Tree (3)) builds decision trees using a top-down, greedy approach. The greedy part of the approach comes from the fact that it will decide which attribute should be at the root of the tree by looking just one move ahead. It compares all available attributes to find which one classifies the data the best, but it doesn't look ahead (or behind) at other attributes to see which combinations of them classify the data the best. ID3 algorithm returns an optimal decision tree, but as the size of the training data and the number of attributes increase, it becomes more likely that running ID3 on it will return a suboptimal decision tree.

To train a decision tree, answer these questions:

- How to find the best attribute/feature for the decision tree at each level?
- When do you stop splitting?

Pseudo code:

1. Pick the best attribute A (the definitions of best attribute comes later). To select this attribute, a statistical test is used to determine for each attribute how well it alone classifies the training examples.

2. Split the data into subsets that correspond to the possible values of the best attribute.
3. Assign A as a decision attribute for a node.
4. For each value of A, create a descendant node.
5. Sort training examples to leaves.
6. Stopping criteria (see down there): f examples perfectly classified (means all data point are of the same class) or there is no more attributes – Stop splitting – else –Iterate over leaves

How to find the best attribute/feature for the decision tree at each level:

There are a couple of options. The most common method is called information gain: a measure that expresses how well an attribute splits the data into groups based on classification (maximize purity or minimize impurity). For example, an attribution returns *low information gain*, if it divides samples to two classes with an even yes and no, but the information gain is high, if each class has more of yeses or nos.

It quantifies the reduction in randomness (Entropy) over the labels we have with a set of data, based upon knowing the value of a particular attribute. A mathematical way to measure the gain, is entropy. It measures the homogeneity of a data set S's classifications. *Entropy ranges from 0, which means that all of the classifications in the data set are the same (either yes or no), to \log_2 of the number of different classifications, which means that the classifications are equally distributed within the data set.* For a binary classification the entropy is only $\log_2 1 = 1$ (if yes and no samples are equally divided). entropy is calculated as follows:

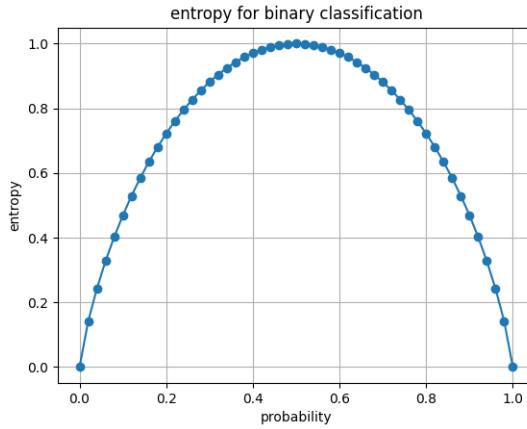
$$Entropy(S) = \sum_{i=1}^c -p_i \log_2(p_i) \quad (2.1)$$

where:

- c corresponds to the number of different classifications (either for the attribute or the final output)
- p_i corresponds to the proportion of the data with the classification i

Here is the plot of entropy for a binary classifier, as the proportional of yes and no samples change:

Figure 2.1: Entropy



Information gain measures the reduction in entropy that results from partitioning the data on an attribute A, which is another way of saying that it represents how effective an attribute is at classifying the data. Given a set of training data S and an attribute A, the formula for information gain is:

$$Gain(S, A) = Entropy(S) - \sum_v \frac{|S_v|}{|S|} Entropy(S_v) \quad (2.2)$$

where v is all the possible values of attribute the attribute (for example, sunny, cloudy, rainy), and S_v is the total number of samples corresponding to this value of attribute (for example sunny).

For if *I play tennis game* (yes and no is the final output) with attributes weather (sunny, cloudy, rainy), temperature (hot, cold, mild), humidity (normal, high), first, we calculate the entropy of the entire set ($Entropy(S)$) (wrt the the final output classification, yes and no). For each attribute, we calculate the the entropy corresponding to each value of entropy, then we calculate the final entropy.

We want to maximize information gain, so we want the entropies of the partitioned data to be as low as possible, which explains why attributes that exhibit high information gain split training data into relatively heterogeneous groups.

As the size of the training data and the number of attributes increase, it becomes likelier that running ID3 on it will return a sub-optimal decision tree.

The other option we can use instead of Entropy is the **Gini function**.

When do you stop splitting?

- when a node is 100% pure
- when splitting a node will result in the tree exceeding a maximum depth (to avoid over-fitting)
- when improvement in purity score (information gain) are below a threshold
- when the number of examples in a node is below a threshold

2.2.6 Inductive bias

Two types of bias for classifiers:

- Restriction Bias: Describes the hypothesis set space (H) that we will consider for learning the tree. Complete hypothesis space (low Restriction Bias). Instead of looking at infinitely many functions, we only consider those that can be represented by the decision tree.
- Preference Bias: Describes the subset of hypothesis n ($n \in H$), from the hypothesis set space H , that we prefer.

Inductive bias of ID3 algorithm:

- it prefers the decision tree with good splits at top (even if a bad split generates the same outcome). This is because ID3 is greedy using info gain.
- it prefers correct outcome over incorrect because ID3 repeats until the labels are correctly classified.
- it prefers shorter trees (comes from the fact that we use good splits from the top).

2.2.7 Extending ID3 algorithm-other consideration

For continuous values attributes/features, we can classify the attributes based on thresholds (that exists in the data set). Without threshold, the continuous data attribute provides the most information gain, while giving a decision tree that is not generalize well. To find the threshold, we can plot the values and decide based on a threshold the returns the best outcome, by calculating the information gain values for each threshold. One way to select the threshold is to take all the values that are mid points between the sorted list of training. For example, for 10 training samples, we need to test the info gain for 9 values, for this specific feature. We can even have multiple threshold for one feature (by creating multiple features).

Does it make sense to repeat an attribute along a path in a decision tree? No, it does not make sense for discrete values, but for continuous values, it makes sense, because indeed we are asking a different question (for a different range).

If the data for some attributes is missing, see 5.7.

Over-fitting + When do we stop? When everything classified correctly or if there is no more attribute. What if we have noise in data (different answer for the same instance)? Causes an infinite loop. What would be the stopping criterion, then? We want generalization, and we should avoid **over-fitting**. If the tree is too big/complicated, there is a chance that it over-fits. There are two popular approaches to avoid over-fitting in decision trees: stop growing the tree before it becomes too large or prune the tree after it becomes too large. Typically, a limit to a decision tree's growth will be specified in terms of the maximum number of layers, or depth, it's allowed to have.

One option to avoid over-fitting is that we can grow the trees, and use cross-validation to prevent over-fitting. The data available to train the decision tree will be split into a training set and validation/test set and we keep growing the tree with various maximum depths will be created based on the training set and then test it against the test set. The best will be selected (when the error grows, we stop growing the tree).

Pruning the tree, on the other hand, involves testing the original tree against pruned versions of it. Leaf nodes are taken away from the tree as long as the pruned tree performs better against test data than the larger tree.

One-hot encoding: If there are multiple categories for a feature, we can use one-hot encoding to convert each category to a binary feature. Thus, if a

feature can take k values, one-hot encoding creates k binary features. There are libraries in the sklearn library for this task. See the details in the 5.1.

Regression: how to adapt decision trees for regression type of problems (continuous outputs)? Decision trees as we've defined them here don't transfer directly to regression problems. We no longer have a useful notion of information gain, so our approach at attribute sorting falls through. Instead, we can rely on purely statistical methods (like variance and correlation) to determine how important an attribute is. For leaves, too, we can do averages, local linear fit, or a host of other approaches that mathematically generalize with no regard for the meaning of the data.

2.2.8 Regression with Decision tree

We can use decision trees for classification (DecisionTreeClassifier) or for regression (DecisionTreeRegressor). Training a regressor is not any different from the classifier, but for the leaf node, we use the average of the continuous values of all the samples in that node.

The major difference here is that how you choose to split the data at the node. Instead of maximizing the entropy, we try to minimize the variance of the values for the continuous feature. Thus, we calculate the variance for the values at each leaf separated by the feature, then we use a weighted method to combine it.

minimize the variance (means choose the feature with largest value) =
variance of all samples at the root –

$$\left[\frac{\text{num of samples in the left leaf}}{\text{num of total samples}} \times \text{variance of left leaf} + \frac{\text{num of samples in the right leaf}}{\text{num of total samples}} \times \text{variance of right leaf} \right] \quad (2.3)$$

For example, if a feature divides 10 samples into two leaf nodes with 4 and 6 samples in each leaf node, then, the weighted average of variance is $\frac{4}{10} \times \text{variance of left leaf} + \frac{6}{10} \times \text{variance of right leaf}$.

2.2.9 Changing the information gain formula is another option

The information gain formula used by the ID3 algorithm treats all of the variables the same, regardless of their distribution and their importance. This is a problem when it comes to continuous variables or discrete variables with many possible values because training examples may be few and far between for each possible value, which leads to low entropy and high information gain by virtue of splitting the data into small subsets, but results in a decision tree that might not generalize well.

One successful approach to deal with this is using a formula called GainRatio in the place of information gain. GainRatio tries to correct for information gain's natural bias toward attributes with many possible values by adding a denominator to information gain called SplitInformation. SplitInformation attempts to measure how broadly partitioned an attribute is and how evenly distributed those partitions are. In general, the SplitInformation of an attribute with n equally distributed values is $\log_2 n$. These relatively large denominators significantly affect an attribute's chances of being the best attribute after an iteration of the ID3 algorithm and help to avoid choices that perform particularly well on the training data but not so well outside of it.

$$\begin{aligned}GainRatio(S, A) &= \frac{Gain(S, A)}{SplitInformation(S, A)} \\SplitInformation(S, A) &= - \sum_{i=1}^c \frac{|S_i|}{S} \log_2 \frac{|S_i|}{|S|}\end{aligned}$$

2.2.10 Advantages and Disadvantages of Decision Trees (copied from a text)

Advantages:

- Simple to understand and to interpret.
- Requires little data preparation. Other techniques often require data normalization, dummy variables need to be created and blank values to be removed.

- The cost of using the tree (i.e., predicting data) is logarithmic in the number of data points used to train the tree.
- Able to handle both numerical and categorical data. Other techniques are usually specialized in analyzing datasets that have only one type of variable.
- Able to handle multi-output problems.
- Uses a white box model. If a given situation is observable in a model, the explanation for the condition is easily explained by Boolean logic. By contrast, in a black box model (e.g., in an artificial neural network), results may be more difficult to interpret.
- Possible to validate a model using statistical tests. That makes it possible to account for the reliability of the model.
- Performs well even if its assumptions are somewhat violated by the true model from which the data were generated.

Disadvantages:

- Can create over-complex trees that do not generalize the data well. This is called overfitting. Mechanisms such as pruning (setting the minimum number of samples required at a leaf node or setting the maximum depth of the tree) are necessary to avoid this problem.
- Decision trees can be unstable because small variations in the data might result in a completely different tree being generated. This problem is mitigated by using decision trees within an ensemble (random forest/XGBoost).
- The problem of learning an optimal decision tree is known to be NP-complete under several aspects of optimality and even for simple concepts. Consequently, practical decision-tree learning algorithms are based on heuristic algorithms such as the greedy algorithm where locally optimal decisions are made at each node. Such algorithms cannot guarantee to return the globally optimal decision tree. This can be mitigated by training multiple trees in an ensemble learner, where the features and samples are randomly sampled with replacement.

- There are concepts that are hard to learn because decision trees do not express them easily, such as XOR, parity or multiplexer problems.
- Decision tree learners create biased trees if some classes dominate. It is therefore recommended to balance the dataset prior to fitting with the decision tree.

2.2.11 When to use a decision tree

Decision trees and tree ensembles:

- Works well on tabular/structured data
- Not recommended for unstructured data such as text, image, audio. Use NN here.
- Decision tree is fast in training.
- Small decision trees may be human interpretable.

Neural Networks

- Works well on all types of data, including tabular/structured and unstructured data.
- May be slower than the decision tree for training.
- Works with transfer learning.
- When building a system of multiple models working together, it might be easier to string together multiple neural networks.

2.2.12 Random forest (Tree ensembles)

A single decision tree can be highly sensitive to small changes in the data. The random forest uses many trees, and it makes a prediction by averaging the predictions of each component tree. It generally has much better predictive accuracy than a single decision tree and it works well with default parameters. If you keep modeling, you can learn more models with even better performance, but many of those are sensitive to getting the right parameters.

To build a tree ensemble (random forest), we use a technique called *Sampling With Replacement*. We are going to construct random sets of the same size of the original set, that are slightly different from the original set, by randomly selecting instances from the set (so, some of the training instances might be repeated in each set). Then, we train a decision tree using this data set. We continue this process to build B decision trees (Bagged decision tree). To randomize the feature choice further, at each node, when choosing a feature to use to split, if n features are available, pick a random subset of $k < n$ features and allow the algorithm to only choose from that subset of features. If n is large \sqrt{n} is valid.

Pseudo code:

Given training set of size m

For $b=1$ to B :

- use sampling with replacement to create a new training set of size m
- train a decision tree on the new dataset

2.2.13 Boosted tree (XGBoost)

This is the most commonly used method of decision tree on samples. It requires a modification to the Bagged decision tree from the previous section 2.2.12. Basically, it is focusing on the part the data that the tree is not doing well.

Pseudo code:

Given training set of size m

For $b=1$ to B :

- use sampling with replacement to create a new training set of size m
- Instead of picking from all examples with equal $1/m$ probability, make it more likely to pick misclassified examples from previously trained trees.
- train a decision tree on the new dataset

2.3 SL: Regression and classification

Regression is the mapping of continuous inputs to continuous outputs, as opposed to the classification where we had mapping from discrete input to

discrete output. Regression is similar to function approximation. Back then, regression meant falling back to the average/mean, but now, we mean, using functional form to approximate a bunch of points.

We use regression because the data itself is not accurate and has noise. If the data is exact, we need to use interpolation and spline methods, to exactly fit the line with the data.

2.3.1 Linear regression

Finding a linear function/relationship between the input data and the output. It might not be a good fit though. We want to find a line (linear function) such that it minimizes the deviation, or to be more precise, the squared error between the data points and the line. This is least square regression. Basically, this is fitting data with a curve, so that we can predict the results based on the model. Here we do not try to intersect every point, rather the curve is designed to follow the pattern of points. (The other approach is interpolation that we try to pass the line/curve through each data point.)

In summary, this is an approximate function that fits the shape or general trend of the data w/o necessarily matching the individual points. To find the line:

$$\begin{aligned} & \text{data points: } \{(x_i, y_i) : i = 1 \dots n\} \\ & \text{find a and b for the linear fit: } y_i = ax_i + b \\ & \text{such that minimizes error: } e = \sum_{i=1}^n (y_i - (ax_i + b))^2 \end{aligned} \tag{2.4}$$

To find the two unknowns of the linear fit, a and b, take the derivative of the error with respect to a and b and set it zero. That would be a system of equations with two unknowns. After solving the equation you have the fit. To have a nonlinear fit, we can use a polynomial model, as discussed in the next section.

To do linear regression, we can use `sklearn.linear_model.LinearRegression`.

2.3.2 Non-linear/polynomial regression

$$f(x_i) = a_0 + a_1 x_i + a_2 x_i^2 + \dots \tag{2.5}$$

The unknowns are a_0, a_1, \dots . See my class notes for more details. To better fit the regression model, we can use higher order polynomial, but it leads to over-fitting.

2.3.3 Error

Training data has errors due to various reasons such as reading errors, sensor errors, transcription error, maliciously given data, etc. This is the reason we are using the regression not the interpolation.

To calculate the parameters of the model, we need to form the cost function (see 5.5.1) and minimize the error using an optimization technique, such as gradient descent 5.5.2.

2.3.4 Multiple Linear regression (multiple features)

For the regression, we can have multiple independent variables/features for the regression (x_1, \dots, x_n) .

2.3.5 Other cases

Using discrete numbers is also possible for regression, however this is no trivial. We need to encode the attributes. For example, by enumerating the categories (giving a number to each possible value of this feature). It is a bit misleading because a correlation between the ordering of the enumeration and its value can be interpolated. The other option is represent the value of the feature as a Boolean.

2.3.6 Classification

The output variable y would be a small handful of cases (as opposed to the linear regression with infinite range of numbers). Examples of (binary) classifications, include email spam detection, tumor detection, etc. One method is to use linear regression and map all predictions greater than 0.5 as a 1 and all less than 0.5 as a 0. This method doesn't work well because classification is not actually a linear function. Instead we need logistic regression. Logistic/Sigmoid function is (output values between 0 and 1, which is the probability of each category/class):

$$g(z) = \frac{1}{1 + e^{-z}} \text{ where } 0 < g(z) < 1 \quad (2.6)$$

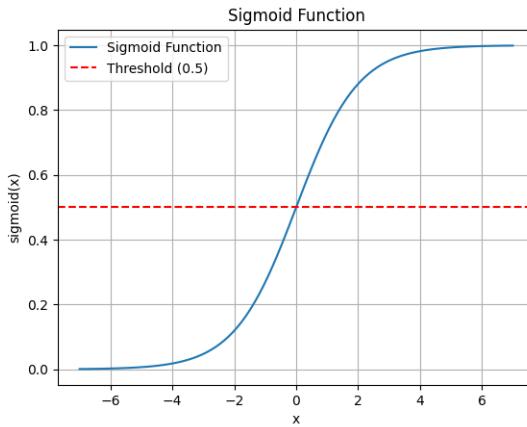


Figure 2.2: Sigmoid

In the language of linear regression, it means we feed the sigmoid func with the output of linear regression:

$$f_{\vec{w}, b}(\vec{x}) = g(\vec{w} \cdot \vec{x} + b) \quad (2.7)$$

In order to get our discrete 0 or 1 classification, we can define a *decision boundary*, such as 0.5, so, if $g(z) > 0.5 \rightarrow y = 1$, this means $z = \vec{w} \cdot \vec{x} + b > 0$. By setting $\vec{w} \cdot \vec{x} + b = 0$, we can find/plot the decision boundary.

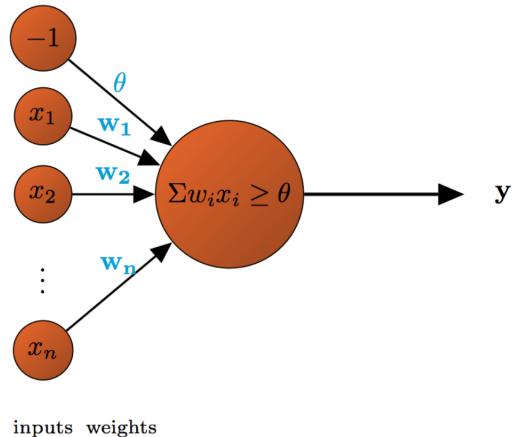
2.4 SL: Neural network

2.4.1 Perceptron

simplest model of a brain cell. The Perceptron calculates the sum of products of the inputs X and their corresponding weights W, and then compare the result with an activation threshold. If the sum is greater than or equal the firing threshold θ , the perceptron returns one, otherwise, it is zero.

$$\sum_{i=1}^k X_i W_i \geq \theta \Rightarrow y = 1 \text{ otherwise } y = 0 \quad (2.8)$$

Figure 2.3: Perceptron



2.5 SL: Instance based learning

2.6 SL: Ensemble B&B

Ensemble Learning is in general the process of combining some simple rules into a more complex rule that can generalize well.

It works by dividing the data into smaller subsets, learn over each individual subset to come up with a rule, then combine all these rules in a single more complex rule. If we looked at the whole data, it would be hard to come up with simple rules.

2.7 SL: Kernel methods and SVMs

2.8 SL: Comp Learning Theory

2.9 SL: VC dimensions

2.10 SL: Bayesian Learning

2.11 SL: Bayesian inference

Chapter 3

Unsupervised learning (UL)

Unsupervised algorithms don't make use of a target; instead, their purpose is to learn some property of the data, to represent the structure of the features in a certain way. In the context of feature engineering for prediction, you could think of an unsupervised algorithm as a "feature discovery" technique.

3.1 Clustering

Clustering simply means the assigning of data points to groups based upon how similar the points are to each other. When used for feature engineering, we could attempt to discover groups of customers representing a market segment, for instance, or geographic areas that share similar weather patterns. The motivating idea for adding cluster labels is that the clusters will break up complicated relationships across features into simpler chunks. Our model can then just learn the simpler chunks one-by-one instead having to learn the complicated whole all at once. It's a "divide and conquer" strategy.

There are multiple methods for clustering. They differ primarily in how they measure *similarity* or *proximity* and in what kinds of features they work with. Clustering algorithms include: Distribution-based methods (expectation-maximization algorithm), Centroid-based methods (K-means), Connectivity-based methods (hierarchical algorithms), Density model (DBSCAN), and subspace clustering.

3.1.1 K-means clustering

It measures similarity using ordinary straight-line distance (Euclidean distance). It creates clusters by placing a number of points, called centroids, inside the feature-space. Each point in the dataset is assigned to the cluster of whichever centroid it's closest to. The "k" in "k-means" is how many centroids it creates.

The k-means algorithm is sensitive to scale. This means we need to be thoughtful about how and whether we rescale our features since we might get very different results depending on our choices. As a rule of thumb, if the features are already directly comparable (like a test result at different times), then you would **not** want to rescale. On the other hand, features that aren't on comparable scales (like height and weight) will usually benefit from rescaling. Sometimes, the choice won't be clear though. In that case, you should try to use common sense, remembering that features with larger values will be weighted more heavily.

What you should take away from this is that the decision of whether and how to rescale features is rarely automatic – it will usually depend on some domain knowledge about your data and what you're trying to predict. Comparing different rescaling schemes through cross-validation can also be helpful.

To find out the best K for a data set, we can test various K numbers and plot K vs variance, this is called an elbow plot. The best K is the one that the slope of variance reduces. If K is equal to the number of items in the dataset, then, the variance would be zero.

3.1.2 Principal Component Analysis (PCA)

Just like clustering is a partitioning of the dataset based on proximity, you could think of PCA as a partitioning of the variation in the data. PCA is a great tool to help you discover important relationships in the data and can also be used to create more informative features. PCA is typically applied to standardized data. With standardized data "variation" means "correlation". With unstandardized data "variation" means "covariance". All data in this course will be standardized before applying PCA. The main idea of PCA: instead of describing the data with the original features, we describe it with its axes of variation. The axes of variation become the new features. The new features PCA constructs are actually just linear combinations (weighted

sums) of the original features. These new features are called the principal components of the data. The weights themselves are called loadings.

PCA also tells us the amount of variation in each component. We can see from the figures that there is more variation in the data along the Size component than along the Shape component. PCA makes this precise through each component's percent of explained variance. It's important to remember, however, that the amount of variance in a component doesn't necessarily correspond to how good it is as a predictor: it depends on what you're trying to predict.

Chapter 4

Reinforced Learning (RL)

4.1 Markov Decision Process

Chapter 5

Miscellaneous topics

5.1 One hot encoding for categorical features

source1 and source2

A categorical feature takes only a few limited number of values. There are three options to deal with the categorical features:

- Drop the feature: this option works only if the feature does not provide any useful information.
- Ordinal encoding: assigning a value to each category (**ordinal variables**). This method works for tree-based (decision tree) models.
- One-hot encoding: creating one feature for each category, and assigning binary values. This method works particularly well if there is no clear ordering in the categorical data. We refer to categorical variables without an intrinsic ranking as **nominal variables**. One-hot encoding generally does not perform well if the categorical variable takes on a large number of values (15 and more). We refer to the number of unique entries of a categorical variable as the cardinality of that categorical variable. High cardinality columns can either be dropped from the dataset, or we can use ordinal encoding.

A one hot encoding is a representation of categorical features as binary vectors. This first requires that the categorical values be mapped to integer values. Then, each integer value is represented as a binary vector that is all zero values except the index of the integer, which is marked with a 1.

Example: assume we have a sequence of labels with the values *red* and *green*. We can assign *red* an integer value of 0 and *green* the integer value of 1. As long as we always assign these numbers to these labels, this is called an integer encoding. Consistency is important so that we can invert the encoding later and get labels back from integer values, such as in the case of making a prediction. Next, we can create a binary vector to represent each integer value. The vector will have a length of 2 for the 2 possible integer values. The *red* label encoded as a 0 will be represented with a binary vector [1, 0] where the zeroth index is marked with a value of 1. In turn, the *green* label encoded as a 1 will be represented with a binary vector [0, 1] where the first index is marked with a value of 1. If we had the sequence: *red*, *red*, *green*, we could represent it with the integer encoding: 0, 0, 1. And the one hot encoding of: [1, 0], [1, 0], and [0, 1].

Why Use a One Hot Encoding? A one hot encoding allows the representation of categorical data to be more expressive. Many machine learning algorithms cannot work with categorical data directly. The categories must be converted into numbers. This is required for both input and output variables that are categorical. We could use an integer encoding directly, rescaled where needed. This may work for problems where there is a natural ordinal relationship between the categories, and in turn the integer values, such as labels for temperature *cold*, *warm*, and *hot*.

There may be problems when there is no ordinal relationship and allowing the representation to lean on any such relationship might be damaging to learning to solve the problem. An example might be the labels dog and cat.

In these cases, we would like to give the network more expressive power to learn a probability-like number for each possible label value. This can help in both making the problem easier for the network to model. When a one hot encoding is used for the output variable, it may offer a more nuanced set of predictions than a single label.

We can use libraries such as scikit-learn and keras to encode a categorical feature for ML.

5.2 Cross validation

The goal is always to generalize the model to fit the real world data. The test set is just a representation of the data that we may see in future. The model should be complex enough to model the training set without over-fitting.

The data points that we are using for training are assumed to be Independent and Identically Distributed (IID), which means that there's no inherent difference between training, testing and real-world data and all the data is coming from the same source. This is the *Fundamental Assumption of Supervised Learning*.

A fixed validation set leaves some random chance in determining model scores. That is, a model might do well on the fixed validation set, even if it would be inaccurate on a different set. The larger the validation set, the less randomness (aka *noise*) there is in our measure of model quality, and the more reliable it will be. Unfortunately, we can only get a large validation set by removing rows from our training data, and smaller training datasets mean worse models! The idea is that we select part of the training set as the test set, not touching the actual test during the training set. This is indeed the cross validation set.

Cross Validation steps:

- Randomly partition the training data into k folds of equal size.
- Train the model on all the folds except for one ($k-1$).
- Validate the model's performance using the fold that was not used in training.
- Repeat steps 2 and 3 using different combinations of these folds.
- Average the error in predicting the polynomial trained on the training folds.

Cross-validation gives a more accurate measure of model quality, which is especially important if you are making a lot of modeling decisions. However, it can take longer to run, because it estimates multiple models (one for each fold). For small datasets, where extra computational burden isn't a big deal, you should run cross-validation. For larger datasets, a single validation set is sufficient. Your code will run faster, and you may have enough data that there's little need to re-use some of it for holdout. There's no simple threshold for what constitutes a large vs. small dataset. But if your model takes a couple minutes or less to run, it's probably worth switching to cross-validation. Alternatively, you can run cross-validation and see if the scores for each experiment seem close. If each experiment yields the same results,

a single validation set is probably sufficient. Note that we no longer need to keep track of separate training and validation sets.

To use cross validation, it is more convenient to implement a pipeline.

Observation for using cross validation with linear regression:

- Average cross validation error is higher than training error for lower orders .
- Average cross validation error decreases as the polynomial order increases (same for training error).
- After the golden degree, increasing the degree of polynomial will result in overfitting, and the Cross Validation error will start to increase.

5.3 F1 score, precision, and recall

Refer to this source.

Precision (P) is defined as the number of true positives (T_p) over the number of true positives plus the number of false positives (F_p): $P = \frac{T_p}{T_p + F_p}$.

Recall (R) is defined as the number of true positives (T_p) over the number of true positives plus the number of false negatives (F_n): $R = \frac{T_p}{T_p + F_n}$.

These quantities are also related to the (F1) score, which is defined as the harmonic mean of precision and recall: $F1 = 2 \frac{R * P}{P + R}$.

The F1 score can be interpreted as a harmonic mean of the precision and recall, where an F1 score reaches its best value at 1 and worst score at 0.

5.4 Overfitting vs underfitting

This is a phenomenon called overfitting, where a model matches the training data almost perfectly, but does poorly in validation and other new data. On the flip side, if we make our tree very shallow, it doesn't divide up the houses into very distinct groups.

At an extreme, if a tree divides houses into only 2 or 4, each group still has a wide variety of houses. Resulting predictions may be far off for most houses, even in the training data (and it will be bad in validation too for the same reason). When a model fails to capture important distinctions and

patterns in the data, so it performs poorly even in training data, that is called underfitting.

Since we care about accuracy on new data, which we estimate from our validation data, we want to find the sweet spot between underfitting and overfitting. Visually, we want the low point of the (red) validation curve in the figure below.

5.5 Gradient descent (steepest descent)

5.5.1 Cost function

The cost function gives you a way to measure how well a specific set of parameters fits the training data. Thereby gives you a way to try to choose better parameters.

Let's use the concept of multiple linear regression to discuss the cost function.

Parameters/coefficients/weights of the model (In ML, parameters of a model are the variables that you can do training in order to improve the model):

$$w_1, \dots, w_n, b \equiv \vec{w}, b \quad (5.1)$$

Here is the model:

$$f_{\vec{w}, b}(\vec{x}) = w_1 x_1 + \dots + w_n x_n + b \quad (5.2)$$

data points $\{(x_i, y_i) : i = 1 \dots m\}$

$$\hat{y}^{(i)} = f_{\vec{w}, b}(\vec{x}^{(i)}) = \vec{w} \cdot \vec{x}^{(i)} + b \quad (5.3)$$

Problem statement: find \vec{w}, b such that $\hat{y}^{(i)}$ is close to $y^{(i)}$ for all $(x^{(i)}, y^{(i)})$.
 $(\hat{y}^{(i)} - y^{(i)})^2$, the error for one single sample is called the loss function.

To find \vec{w}, b , we form the the cost function using squared error cost:

find \vec{w}, b :

$$\text{minimize: } J(\vec{w}, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}^{(i)} - y^{(i)})^2 = \frac{1}{2m} \sum_{i=1}^m (wx^{(i)} + b - y^{(i)})^2$$

(5.4)

m is the total number of data points. The extra 2 in the denominator is just for convenience. This is the squared error cost function, which is widely used. However, there are other options for the cost functions as well.

Loss function: Used when we refer to the error for a single training example. Cost function: Used to refer to an average of the loss functions over an entire training dataset.

The squared error cost function is not an ideal cost function for logistic regression. The reason is that the logistic regression model, which is defined by:

$$f_{\vec{w}, b}(\vec{x}) = \frac{1}{1 + e^{-(\vec{w} \cdot \vec{x}^{(i)} + b)}} \quad (5.5)$$

is non-convex, as opposed to linear regression model which is convex. To have a convergent gradient descent method, the cost function should be convex.

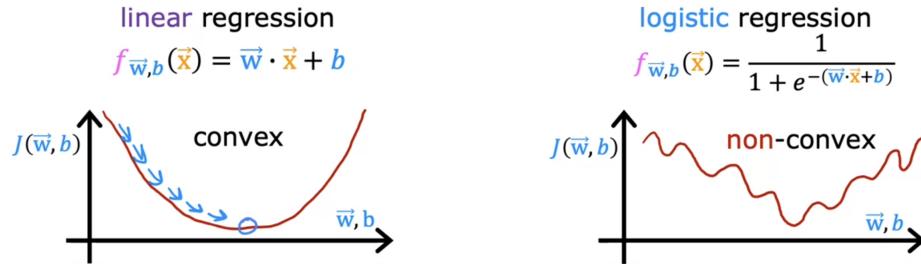


Figure 5.1: cost function for logistic function

To convert the logistic function to a convex function, we need to use the following loss definition (see ML C1W3):

$$J(\vec{w}, b) = \frac{1}{m} \sum_{i=1}^m \frac{1}{2} L(\hat{y}^{(i)} - y^{(i)}) = \frac{1}{m} \sum_{i=1}^m \frac{1}{2} L(f_{\vec{w}, b}(\vec{x}^{(i)}) - y^{(i)})$$

$$L(f_{\vec{w}, b}(\vec{x}^{(i)}) - y^{(i)}) = \begin{cases} -\log(f_{\vec{w}, b}(\vec{x}^{(i)})) & \text{if } y^{(i)} = 1 \\ -\log(1 - f_{\vec{w}, b}(\vec{x}^{(i)})) & \text{if } y^{(i)} = 0 \end{cases} \quad (5.6)$$

If $y^{(i)} = 1$ then, if the predicted value $f_{\vec{w}, b}(\vec{x}^{(i)})$ is close to one, the loss function is close to zero (reduces the loss), but if the predicted value is close to zero, then the function penalize the loss function with a large number. The other way around for $y^{(i)} = 0$.

Logistic loss function

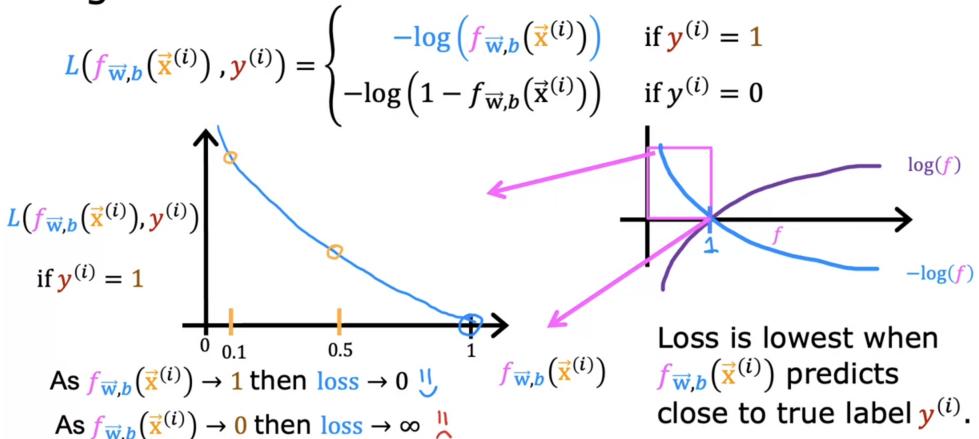


Figure 5.2: cost function for logistic function

5.5.2 Gradient descent method

An optimization method to minimize any function. Depending on the initial starting point, the method may end up at a different local minimum.

Method:

For a cost function $J(\vec{w}, b)$, we want to find w_1, w_2, \dots to minimize J .

Algorithm:

- start with some initial \vec{w}, b .
- update w_j simultaneously until the algorithm converges, meaning you reach a local minimum, where additional iteration does not change the point. It is incorrect to use new values of w_j to update other parameters in the same iteration.

$$\begin{aligned}
 w_j &= w_j - \alpha \frac{\partial}{\partial w_j} J(\vec{w}, b) = w_j - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y}^{(i)} - y^{(i)}) x_j^{(i)} \\
 &= w_j - \alpha \frac{1}{m} \sum_{i=1}^m (f_{\vec{w}, b}(\vec{x}^{(i)}) - y^{(i)}) x_j^{(i)} \quad \text{for each } j \\
 b &= b - \alpha \frac{\partial}{\partial b} J(\vec{w}, b) = b - \alpha \frac{1}{m} \sum_{i=1}^m (f_{\vec{w}, b}(\vec{x}^{(i)}) - y^{(i)}) \quad \text{for each } i
 \end{aligned} \tag{5.7}$$

The negative is because we want to move in the opposite direction.

α is the learning rate (step size). The choice of learning rate affects the efficiency of gradient descent. If it is too small, it converges very slowly. If it is too large (overshoot), may cause divergence and never reaches the minimum. If we are exactly at the minimum, since slope is zero, the value of the learning does not affect the results. Thus, even a fixed learning can reach the minimum.

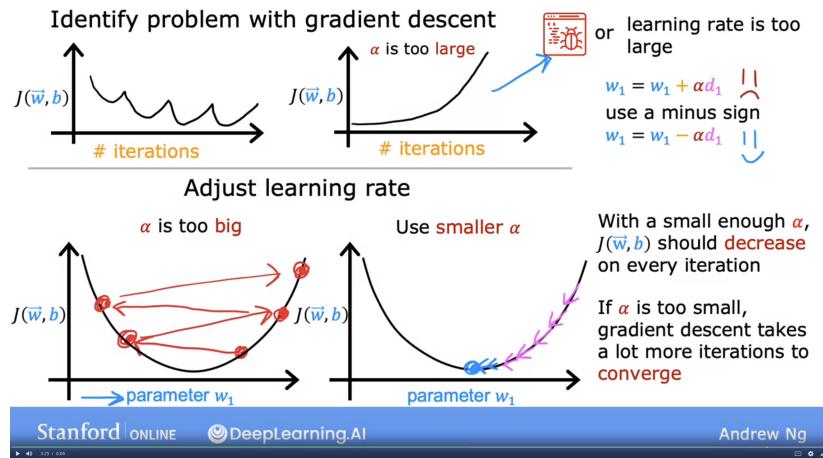
Various types of gradient descent:

Batch gradient descent: each step of gradient descent uses all the training examples. While this batching provides computation efficiency, it can still have a long processing time for large training datasets as it still needs to store all of the data into memory. Batch gradient descent also usually produces a stable error gradient and convergence, but sometimes that convergence point isn't the most ideal, finding the local minimum versus the global one.

Mini-batch gradient descent updates the parameters using a subset of training samples.

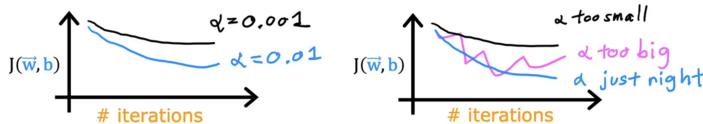
5.5.3 Learning rate selection

If the learning rate is too small, it would be very slow, and if it too large, it may diverge. To start, we can set the learning rate to a very small number, and check if the cost function decreases with every single iteration. If not, there is bug in the code. We can plot the cost function (learning curve) with each iteration of the gradient descent. The learning rate α should be selected such that the cost function decreases as iterations increases. If this is not the case, then the learning rate is high. Generally, we need to test many learning rates and select the most optimized one.



Values of α to try:

$$\dots \xrightarrow{3X} 0.001 \xrightarrow{\approx 3X} 0.003 \xrightarrow{3X} 0.01 \xrightarrow{\approx 3X} 0.03 \xrightarrow{3X} 0.1 \xrightarrow{\approx 3X} 0.3 \xrightarrow{\approx 3X} 1 \dots$$



5.6 Model validation

Always start with the dataset documentation.

In most (though not all) applications, the relevant measure of model quality is predictive accuracy. In other words, will the model's predictions be close to what actually happens.

There are many metrics for summarizing model quality, but we'll start with one called Mean Absolute Error (also called MAE). With the MAE metric, we take the absolute value of each error. This converts each error to a positive number. We then take the average of those absolute errors. This is our measure of model quality. `sklearn` has a function, `mean_absolute_error`, to calculate MAE.

Many people make a mistake when measuring predictive accuracy. They make predictions with their training data and compare those predictions to the target values in the training data. This is not valid. The most straightforward way to validate the model is to exclude some data from the model-building process, and then use those to test the model's accuracy on data it hasn't seen before. This data is called validation data.

5.7 Data processing/cleaning: Missing Values

Before we treat missing data, we need to know **Is this value missing because it wasn't recorded or because it doesn't exist?** If a value is missing because it doesn't exist (like the height of the oldest child of someone who doesn't have any children) then it doesn't make sense to try and guess what it might be. These values you probably do want to keep as NaN. On the other hand, if a value is missing because it wasn't recorded, then you can try to guess what it might have been based on the other values in that column and row. There are many ways the data misses: wrong measurement, data is private, data is not available, etc.

Generally, there are three approaches deal with the missing data. These are quick and dirty approaches that probably remove some useful info or adding some noise to your dataset.

- The simplest option: drop columns or features with missing values. Unless most values in the dropped columns are missing, the model loses

access to a lot of (potentially useful!) information with this approach.

- Imputation: fills in the missing values with some number. For instance, we can fill in the mean value along each column, or we can choose the most popular data for the missing item. We can also assign the probability of each value of the attribute to the missing entries. The imputed value won't be exactly right in most cases, but it usually leads to more accurate models than you would get from dropping the column entirely.
- Extending imputation: we impute the missing values, as before. And, additionally, for each column with missing entries in the original dataset, we add a new column that shows the location of the imputed entries. For example, if the size of bedroom is missing for some instances, we add a new column, missing_bedroom_size, and set it to FALSE for all valid instances and TRUE for all missing instances. This will meaningfully improve results. In other cases, it doesn't help at all.

In pandas, we can use `.isnull()` to detect columns with missing data. We can use `.drop` to drop columns. We can also use `dropna` to either drop columns or instances.

5.8 Data processing & Feature engineering

5.8.1 Feature engineering

The goal of feature engineering is simply to make your data better suited to the problem at hand. You might perform feature engineering to:

- improve a model's predictive performance
- reduce computational or data needs
- improve interpretability of the results

Feature engineering is possible through:

- determine which features are the most important with mutual information

- invent new features in several real-world problem domains (e.g. square the length of land, to get area, which is a more reasonable feature. It can predicate parabola now.)
- encode high-cardinality categoricals with a target encoding
- create segmentation features with k-means clustering
- decompose a dataset's variation into features with principal component analysis

A great first step is to construct a ranking with a feature utility metric, a function measuring associations between a feature and the target. Then you can choose a smaller set of the most useful features to develop initially and have more confidence that your time will be well spent. The metric we'll use is called "mutual information". It can **detect any kind of relationship, while correlation only detects linear relationships**. The mutual information (MI) between two quantities is a measure of the extent to which knowledge of one quantity reduces uncertainty about the other. Mutual Info varies between 0 (independent quantities) to $+\infty$. It is a logarithmic func, and barely reaches to 2. It's possible for a feature to be very informative when interacting with other features, but not so informative all alone. MI can't detect interactions between features. It is a univariate metric. The actual usefulness of a feature depends on the model you use it with. A feature is only useful to the extent that its relationship with the target is one your model can learn.

Scikit-learn has two mutual information metrics in its feature_selection module: one for real-valued targets (mutual_info_regression) and one for categorical targets (mutual_info_classification).

5.8.2 How to create new features

mathematical transform

Use arithmetic operations to create new features based on other features. For example, find the area of land by multiplying width by length.

count

Features describing the presence or absence of something often come in sets, the set of risk factors for a disease, say. You can aggregate such features by

creating a count. These features will be binary (1 for Present, 0 for Absent) or boolean (True or False). In Python, booleans can be added up just as if they were integers.

Example:

```
accidents[“RoadwayFeatures”] = accidents[roadwayFeatures].sum(axis=1)
```

building up and breaking down features

Add or breakdown strings to create new features. For example, break down phone numbers to area codes.

clustering

Use, for example, K-means to cluster data points and add it as a feature. It requires a knowledge about the domain.

Principal Component Analysis (PCA)

There are two ways you could use PCA for feature engineering.

- The first way is to use it as a descriptive technique. Since the components tell you about the variation, you could compute the MI scores for the components and see what kind of variation is most predictive of your target. That could give you ideas for kinds of features to create.
- The second way is to use the components themselves as features. Because the components expose the variational structure of the data directly, they can often be more informative than the original features. Here are some use-cases:
 - Dimensionality reduction: When your features are highly redundant (multicollinear, specifically), PCA will partition out the redundancy into one or more near-zero variance components, which you can then drop since they will contain little or no information.
 - Anomaly detection: Unusual variation, not apparent from the original features, will often show up in the low-variance components. These components could be highly informative in an anomaly or outlier detection task.

- Noise reduction: A collection of sensor readings will often share some common background noise. PCA can sometimes collect the (informative) signal into a smaller number of features while leaving the noise alone, thus boosting the signal-to-noise ratio.
- Decorrelation: Some ML algorithms struggle with highly-correlated features. PCA transforms correlated features into uncorrelated components, which could be easier for your algorithm to work with.

PCA basically gives you direct access to the correlational structure of your data. You'll no doubt come up with applications of your own!

PCA Best Practices- there are a few things to keep in mind when applying PCA:

- PCA only works with numeric features, like continuous quantities or counts.
- PCA is sensitive to scale. It's good practice to standardize your data before applying PCA, unless you know you have good reason not to.
- Consider removing or constraining outliers, since they can have an undue influence on the results.

Target Encoding

This method, as opposed to all other methods, targets categorical features. It is similar to one-hot or label encoding, with the difference that it also uses the target to create the encoding. This makes it what we call a supervised feature engineering technique.

A target encoding is any kind of encoding that replaces a feature's categories with some number derived from the target. For example, *mean encoding*, takes the average of the numerical target based on a categorical feature (ex. average/mean price of a car brand (make)). **Bin counting** is the equivalent encoded feature applied to a binary target.

Target encoding is great for:

- High-cardinality features: A feature with a large number of categories can be troublesome to encode: a one-hot encoding would generate too many features and alternatives, like a label encoding, might not be

appropriate for that feature. A target encoding derives numbers for the categories using the feature's most important property: its relationship with the target.

- Domain-motivated features: From prior experience, you might suspect that a categorical feature should be important even if it scored poorly with a feature metric. A target encoding can help reveal a feature's true informativeness.

There are at least two concerns with the target encoding:

- unknown categories: Target encodings create a special risk of overfitting, which means they need to be trained on an independent "encoding" split. When you join the encoding to future splits, Pandas will fill in missing values for any categories not present in the encoding split. These missing values you would have to impute somehow.
- rare categories: When a category only occurs a few times in the dataset, any statistics calculated on its group are unlikely to be very accurate.

A solution to these problems are **smoothing**. The idea is to blend the in-category average with the overall average. Rare categories get less weight on their category average, while missing categories just get the overall average.

In pseudocode: $\text{encoding} = \text{weight} * \text{in_category}$ (ex. mean of the category for that feature) + $(1 - \text{weight}) * \text{overall}$ (ex. mean of all categories for that feature). Where weight is a value between 0 and 1 calculated from the category frequency. An easy way to determine the value for weight is to compute an m-estimate: $\text{weight} = n / (n + m)$, where n is the total number of times that category occurs in the data. The parameter m determines the "smoothing factor". Larger values of m put more weight on the overall estimate. When choosing a value for m, consider how noisy you expect the categories to be. Does the price of a vehicle vary a great deal within each make? Would you need a lot of data to get good estimates? If so, it could be better to choose a larger value for m; if the average price for each make were relatively stable, a smaller value could be okay.

5.8.3 scaling vs normalization

In both cases, you're transforming the values of numeric variables so that the transformed data points have specific helpful properties. The point is to

help with the gradient descent to converge faster. The difference is that: in **scaling**, you're changing the range of your data, while in **normalization**, you're changing the shape of the distribution of your data.

scaling

This means that you're transforming your data so that it fits within a specific scale, like 0-100 or 0-1. You want to scale data when you're using methods based on measures of how far apart data points are, like support vector machines (SVM) or k-nearest neighbors (KNN). With these algorithms, a change of "1" in any numeric feature is given the same importance. By scaling your variables, you can help compare different variables on equal footing.

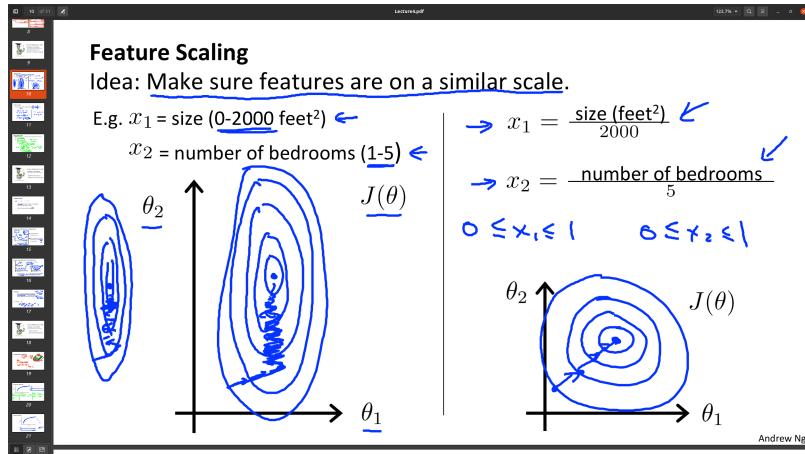
normalization

Scaling just changes the range of your data. Normalization is a more radical transformation. The point of normalization is to change your observations so that they can be described as a normal distribution.

In general, you'll normalize your data if you're going to be using a machine learning or statistics technique that assumes your data is normally distributed. Some examples of these include linear discriminant analysis (LDA) and Gaussian naive Bayes. (Pro tip: any method with "Gaussian" in the name probably assumes normality.)

5.8.4 Scaling a feature

Having two features with large and small values may have adverse impact on our training. For example, for regression, it may cause large round off error, or affects the shape of gradient descent contours and as a result may cause slow convergence or even divergence. To avoid that, it is recommended to scale features so that they have the same range. After scaling, the data range would be 0 to 1.



5.8.5 Mean normalization

In this method, we first find the average of the feature (μ). Each item of the feature is normalized as:

$$x_i = \frac{x_i - \mu}{max - min} \quad (5.8)$$

Then, we have the range for each feature between -1 and 1.

5.8.6 z-score normalization

In this method, we first find the standard deviation (σ) and the average (μ) of the feature. Each item of the feature is normalized as:

$$x_i = \frac{x_i - \mu}{\sigma} \quad (5.9)$$

Then, we have the range for each feature between -1 and 1.

5.8.7 Combining features

Using intuition to design new features by transforming or combining original features.

5.9 Ensemble methods

Ensemble methods combine the predictions of several models (e.g., several trees, in the case of random forests).

5.9.1 Gradient Boosting

Gradient boosting is a method that goes through cycles to iteratively add models into an ensemble.

It begins by initializing the ensemble with a single model, whose predictions can be pretty naive. (Even if its predictions are wildly inaccurate, subsequent additions to the ensemble will address those errors.)

Then, we start the cycle:

- First, we use the current ensemble to generate predictions for each observation in the dataset. To make a prediction, we add the predictions from all models in the ensemble.
- These predictions are used to calculate a loss function (like mean squared error, for instance).
- Then, we use the loss function to fit a new model that will be added to the ensemble. Specifically, we determine model parameters so that adding this new model to the ensemble will reduce the loss. (Side note: The "gradient" in "gradient boosting" refers to the fact that we'll use gradient descent on the loss function to determine the parameters in this new model.)
- Finally, we add the new model to ensemble,
- repeat!

XGBoost stands for extreme gradient boosting, which is an implementation of gradient boosting with several additional features focused on performance and speed. (Scikit-learn has another version of gradient boosting, but XGBoost has some technical advantages.) scikit-learn API for XGBoost (`xgboost.XGBRegressor`) allows us to build and fit a model just as we would in scikit-learn. The `XGBRegressor` class has many tunable parameters. See the code.

5.9.2 Data leakage

Data leakage (or leakage) happens when your training data contains information about the target, but similar data will not be available when the model is used for prediction. This leads to high performance on the training set

(and possibly even the validation data), but the model will perform poorly in production.

In other words, leakage causes a model to look accurate until you start making decisions with the model, and then the model becomes very inaccurate.

There are two main types of leakage: target leakage and train-test contamination.

Target leakage occurs when your predictors include data that will not be available at the time you make predictions. It is important to think about target leakage in terms of the timing or chronological order that data becomes available, not merely whether a feature helps make good predictions.

Example: People take antibiotic medicines after getting pneumonia in order to recover. The raw data shows a strong relationship between those columns, but *took antibiotic medicine* is frequently changed after the value for *got pneumonia* is determined. This is target leakage. Since validation data comes from the same source as training data, the pattern will repeat itself in validation, and the model will have great validation (or cross-validation) scores. But the model will be very inaccurate when subsequently deployed in the real world, because even patients who will get pneumonia won't have received antibiotics yet when we need to make predictions about their future health.

To prevent this type of data leakage, any variable updated (or created) after the target value is realized should be excluded.

Train-Test Contamination A different type of leak occurs when you aren't careful to distinguish training data from validation data.

Recall that validation is meant to be a measure of how the model does on data that it hasn't considered before. You can corrupt this process in subtle ways if the validation data affects the preprocessing behavior. This is sometimes called train-test contamination.

For example, imagine you run preprocessing (like fitting an imputer for missing values) before calling `train_test_split()`. The end result? Your model may get good validation scores, giving you great confidence in it, but perform poorly when you deploy it to make decisions.

After all, you incorporated data from the validation or test data into how you make predictions, so the model may do well on that particular data even if it can't generalize to new data. This problem becomes even more subtle (and more dangerous) when you do more complex feature engineering.

As we discussed in the tutorial, to avoid overfitting, we need to fit the

encoder on data heldout from the training set.

If your validation is based on a simple train-test split, exclude the validation data from any type of fitting, including the fitting of preprocessing steps. This is easier if you use scikit-learn pipelines. When using cross-validation, it's even more critical that you do your preprocessing inside the pipeline!

5.10 Python

Use vectorization in python to improve the performance (for example: `np.dot(W,x)`).

5.11 ML Checklist

- Inspect all features, look for duplicate features.
- Manage missing data (drop items with missing target, and impute missing items).
- Manage categorical/object features (categorical, one-hot, etc.)

5.11.1 Time series

- Plot lags to find seasonality/cycles and calculate correlation, and add new lag features if there is a high correlation.
- Plot partial autocorrelation, and add new lag features if there is a high correlation.

5.12 Time series

The basic object of forecasting is the time series, which is a set of observations recorded over time. In forecasting applications, the observations are typically recorded with a regular frequency, like daily or monthly.

One of the main forecasting approaches is the Linear regression method for forecasting ($\text{target} = \text{weight_1} * \text{feature_1} + \text{weight_2} * \text{feature_2} + \text{bias}$). But, first we need to generate the features corresponding to the time series. There are three kinds of features unique to time series: time-step features and lag features.

Time-step features are features we can derive directly from the time index. The most basic time-step feature is the time dummy, which counts off time steps in the series from beginning to end. Time-step features let you model time dependence. A series is time dependent if its values can be predicted from the time they occurred.

Lag (and lead) features are the second types of features that we can generate from the time series. To make a lag feature, we shift the observations of the target series so that they appear to have occurred later in time. Lag features let you model *serial dependence*. A time series has serial dependence when an observation can be predicted from previous observations. **Adapting machine learning algorithms to time series problems is largely about feature engineering with the time index and lags.**

Seasonal features such as seasonal *indicators* or Fourier transform features (will be discussed later).

There are three patterns/components of dependence in a time series:

Series = **trend** (moving average or linear regression (with different polynomial order) with time-step feature) + **seasonality** (weekly, monthly, etc. using indicator features (for short seasons) or Fourier method (if season is longer)) + **cycles** (serial dependence using lag feature) + **error**. Each of these items is called a component.

The residuals of a model are the difference between the target the model was trained on and the predictions the model makes – the difference between the actual curve and the fitted curve, in other words.

Trend, seasonality, and cycles will be discussed next.

5.12.1 Trend

This portion of the time series can be captured by moving average rolling windows, or using linear regressions with the time-step feature. The trend models we learned about in this lesson turn out to be useful for a number of reasons. Besides acting as a baseline or starting point for more sophisticated models, we can also use them as a component in a "hybrid model" with algorithms unable to learn trends (like XGBoost and random forests).

5.12.2 Seasonality

We say that a time series exhibits seasonality whenever there is a regular, periodic change in the mean of the series. Seasonal changes generally follow

the clock and calendar – repetitions over a day, a week, or a year are common.

There are two kinds of features that model seasonality. The first kind, *indicators*, is best for a season with few observations, like a weekly season of daily observations (7 observation in the season). The second kind, *Fourier features*, is best for a season with many observations, like an annual season of daily observations (365 observations per season).

we can use a seasonal plot to discover seasonal patterns. A seasonal plot shows segments of the time series plotted against some common period, the period being the "season" you want to observe.

Seasonal indicators

A seasonal plot shows segments of the time series plotted against some common period, the period being the "season" you want to observe. Seasonal indicators are binary features that represent seasonal differences in the level of a time series. Seasonal indicators are what you get if you treat a seasonal period as a categorical feature and apply one-hot encoding. For example, by one-hot encoding days of the week, we get weekly seasonal indicators. Creating weekly indicators for the Trigonometry series will then give us six new "dummy" features. (Linear regression works best if you drop one of the indicators; we chose Monday in the frame below. This means the in the one-hot model, if all Tue Sun is 0, it is Monday.)

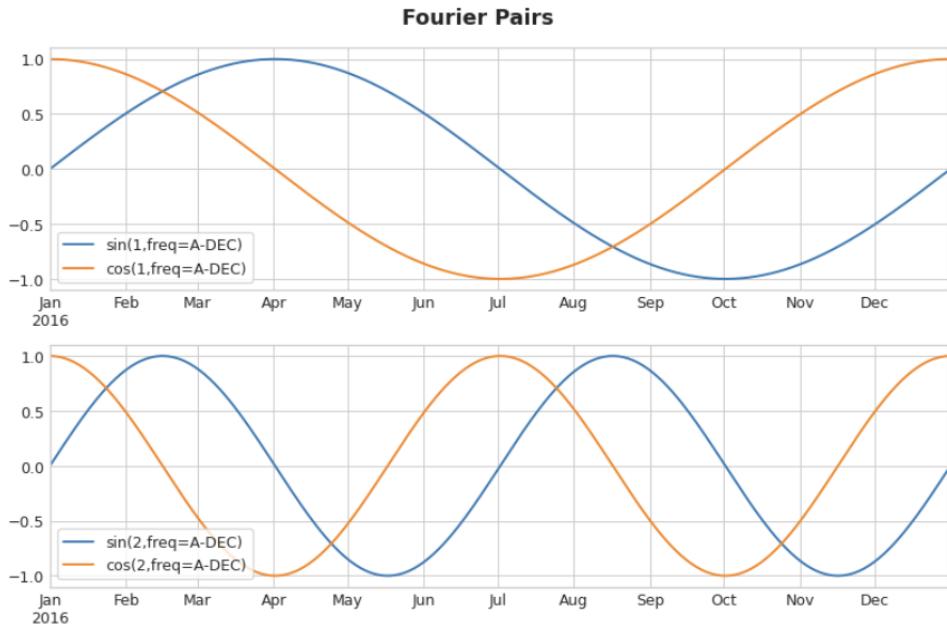
THE TRIGONOMETRY SERIES WILL THEN GIVE US SIX NEW "DUMMY" FEATURES. (LINEAR REGRESSION WORKS BEST IF YOU DROP ONE OF THE INDICATORS; WE CHOSE MONDAY IN THE FRAME BELOW.)

Date	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday
2016-01-04	0.0	0.0	0.0	0.0	0.0	0.0
2016-01-05	1.0	0.0	0.0	0.0	0.0	0.0
2016-01-06	0.0	1.0	0.0	0.0	0.0	0.0
2016-01-07	0.0	0.0	1.0	0.0	0.0	0.0
2016-01-08	0.0	0.0	0.0	1.0	0.0	0.0
2016-01-09	0.0	0.0	0.0	0.0	1.0	0.0
2016-01-10	0.0	0.0	0.0	0.0	0.0	1.0
2016-01-11	0.0	0.0	0.0	0.0	0.0	0.0
...

Figure 5.3: seasonal indicators

Fourier features and periodogram

The kind of feature we discuss now are better suited for long seasons over many observations where indicators would be impractical. Instead of creating a feature for each date, Fourier features try to capture the overall shape of the seasonal curve with just a few features. It is these frequencies within a season that we attempt to capture with Fourier features. The idea is to include in our training data periodic curves having the same frequencies as the season we are trying to model. Fourier features are pairs of sine and cosine curves, one pair for each potential frequency in the season starting with the longest. Fourier pairs modeling annual seasonality would have frequencies: once per year, twice per year, three times per year, and so on.

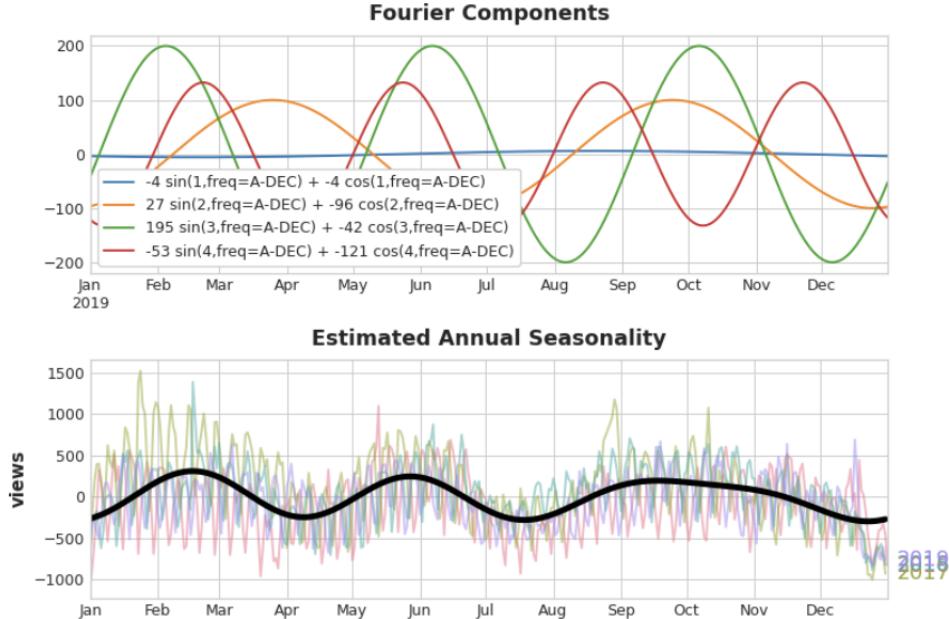


*The first two Fourier pairs for annual seasonality. **Top:** Frequency of once per year. **Bottom:** Frequency of twice per year.*

Figure 5.4: Fourier features

If we add a set of these sine / cosine curves to our training data, the linear regression algorithm will figure out the weights that will fit the seasonal com-

ponent in the target series. The figure illustrates how linear regression used four Fourier pairs to model the annual seasonality in the Wiki Trigonometry series.



Top: Curves for four Fourier pairs, a sum of sine and cosine with regression coefficients. Each curve models a different frequency. **Bottom:** The sum of these curves approximates the seasonal pattern.

Notice that we only needed eight features (four sine / cosine pairs) to get a good estimate of the annual seasonality. Compare this to the seasonal indicator method which would have required hundreds of

Figure 5.5: Fourier features

Notice that we only needed eight features (four sine / cosine pairs) to get a good estimate of the annual seasonality. Compare this to the seasonal indicator method which would have required hundreds of features (one for each day of the year). By modeling only the "main effect" of the seasonality with Fourier features, you'll usually need to add far fewer features to your training data, which means reduced computation time and less risk of overfitting.

Choosing Fourier features with the Periodogram:

How many Fourier pairs should we actually include in our feature set? We can answer this question with the periodogram. The periodogram tells you the strength of the frequencies in a time series. Specifically, the value on the y-axis of the graph is $(a^{**} 2 + b^{**} 2) / 2$, where a and b are the coefficients of the sine and cosine at that frequency (as in the Fourier Components plot above).

Removing from a series its trend or seasons is called **detrending** or **de-seasonalizing** the series.

Once Fourier or seasonal indicator features created, we can use the linear (nonlinear/polynomial) regression for forecasting.

5.12.3 Cycles: serial dependence (time series as features)

Some time series, have *time dependent properties*, that is, we could derive the feature directly from the time index (for example, weekly dependence). However, some other time series properties can only be modeled as serially dependent properties, that is, using as features past values of the target series. Plotted against past values (with lag) reveals the structure.

Cycles

One especially common way for serial dependence to manifest is in cycles. Cycles are patterns of growth and decay in a time series associated with how the value in a series at one time depends on values at previous times, but not necessarily on the time step itself. Cyclic behavior is characteristic of systems that can affect themselves or whose reactions persist over time. Economies, epidemics, animal populations, volcano eruptions, and similar natural phenomena often display cyclic behavior. What distinguishes cyclic behavior from seasonality is that cycles are not necessarily time dependent, as seasons are. What happens in a cycle is less about the particular date of occurrence, and more about what has happened in the recent past. The (at least relative) independence from time means that cyclic behavior can be much more irregular than seasonality.

To investigate possible serial dependence (like cycles) in a time series, we need to create "lagged" copies of the series. Lagging a time series means to

shift its values forward one or more time steps, or equivalently, to shift the times in its index backward one or more steps. In either case, the effect is that the observations in the lagged series will appear to have happened later in time. The lagged data can be used as a feature to predict the target.

Lag plot

A **lag plot** of a time series shows its values plotted against its lags. Serial dependence in a time series will often become apparent by looking at a lag plot. The most commonly used measure of serial dependence is known as **autocorrelation**, which is simply the correlation a time series has with one of its lags. Autocorrelation varies between -1 to +1.

Choosing lags

When choosing lags to use as features, it generally won't be useful to include every lag with a large autocorrelation. The partial autocorrelation tells you the correlation of a lag accounting for all of the previous lags – the amount of "new" correlation the lag contributes, so to speak. Plotting the partial autocorrelation can help you choose which lag features to use.

A plot like that above is known as a correlogram. The correlogram is for lag features essentially what the periodogram is for Fourier features.

Finally, we need to be mindful that autocorrelation and partial autocorrelation are measures of linear dependence. Because real-world time series often have substantial non-linear dependencies, it's best to look at a lag plot (or use some more general measure of dependence, like mutual information) when choosing lag features. The Sunspots series has lags with non-linear dependence which we might overlook with autocorrelation.

Lag features require that the lagged target value is known at the time being forecast. A lag 1 feature shifts the time series forward 1 step, which means you could forecast 1 step into the future but not 2 steps. We just assumed that we could always generate lags up to the period we wanted to forecast (every prediction was for just one step forward, in other words). But, in reality, we need to forecast a few steps ahead. Machine learning can help with this.

5.12.4 Forecasting with hybrid models: Components and residuals

We could imagine learning the components of a time series as an iterative process: first learn the trend and subtract it out from the series, then learn the seasonality from the detrended residuals and subtract the seasons out, then learn the cycles and subtract the cycles out, and finally only the unpredictable error remains. Add together all the components we learned and we get the complete model. This is essentially what linear regression would do if you trained it on a complete set of features modeling trend, seasons, and cycles.

We can use a single algorithm (linear regression) to learn all the components at once. But it's also possible to use one algorithm for some of the components and another algorithms for the rest. This way we can always choose the best algorithm for each component. To do this, we use one algorithm to fit the original series and then the second algorithm to fit the residual series. We'll usually want to use different feature sets (X_{train_1} and X_{train_2} above) depending on what we want each model to learn. If we use the first model to learn the trend, we generally wouldn't need a trend feature for the second model, for example.

```
# 1. Train and predict with first model model_1.fit(X_train_1, y_train)
y_pred_1 = model_1.predict(X_train)

# 2. Train and predict with second model on residuals model_2.fit(X_train_2,
y_train - y_pred_1)
y_pred_2 = model_2.predict(X_train_2)

# 3. Add to get overall predictions y_pred = y_pred_1 + y_pred_2
```

While it's possible to use more than two models, in practice it doesn't seem to be especially helpful. In fact, the most common strategy for constructing hybrids is the one we've just described: a simple (usually linear) learning algorithm followed by a complex, non-linear learner like GBDTs or a deep neural net, the simple model typically designed as a "helper" for the powerful algorithm that follows.

There are many ways you could combine machine learning models besides the way we've outlined in this lesson. Successfully combining models, though, requires that we dig a bit deeper into how these algorithms operate.

Important remark: there are generally two ways a regression algorithm can make predictions: either by *transforming the features* or by transforming the target. Feature-transforming algorithms learn some mathematical function that takes features as an input and then combines and transforms

them to produce an output that matches the target values in the training set. Linear regression and neural nets are of this kind. *Target-transforming* algorithms use the features to group the target values in the training set and make predictions by averaging values in a group; a set of feature just indicates which group to average. Decision trees and nearest neighbors are of this kind.

Feature transformers generally can extrapolate target values beyond the training set given appropriate features as inputs, but the predictions of target transformers will always be bound within the range of the training set. If the time dummy continues counting time steps, linear regression continues drawing the trend line. Given the same time dummy, a decision tree will predict the trend indicated by the last step of the training data into the future forever. Decision trees cannot extrapolate trends. Random forests and gradient boosted decision trees (like XGBoost) are ensembles of decision trees, so they also cannot extrapolate trends.

This difference is what motivates the hybrid design in this lesson: use linear regression to extrapolate the trend, transform the target to remove the trend, and apply XGBoost to the detrended residuals. To hybridize a neural net (a feature transformer), you could instead include the predictions of another model as a feature, which the neural net would then include as part of its own predictions. The method of fitting to residuals is actually the same method the gradient boosting algorithm uses, so we will call these boosted hybrids; the method of using predictions as features is known as "stacking", so we will call these stacked hybrids.

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5.12.5 Forecasting

There are two things to establish before designing a forecasting model:

- what information is available at the time a forecast is made (features),

and,

- the time period during which you require forecasted values (target).

The **forecast origin** is time at which you are making a forecast. Practically, you might consider the forecast origin to be the last time for which you have training data for the time being predicted. Everything up to the origin can be used to create features.

The **forecast horizon** is the time for which you are making a forecast. We often describe a forecast by the number of time steps in its horizon: a "1-step" forecast or "5-step" forecast, say. The forecast horizon describes the target.

The time between the origin and the horizon is the **lead time** (or sometimes latency) of the forecast. A forecast's lead time is described by the number of steps from origin to horizon: a "1-step ahead" or "3-step ahead" forecast, say. In practice, it may be necessary for a forecast to begin multiple steps ahead of the origin because of delays in data acquisition or processing.

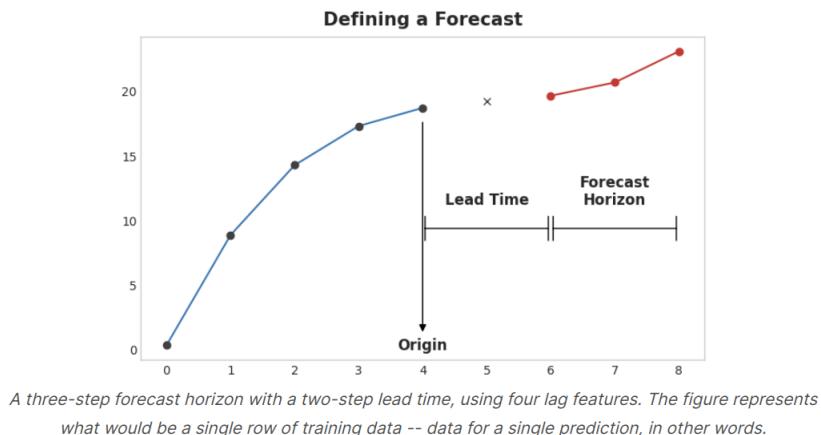


Figure 5.6: Defining a forecast

Prepare data for forecasting

We can create lag/lead features or time steps for linear regression. Additionally, we can create features based on the target for decision tree. How we

do this depends on the forecasting task. For example, table 5.7, shows the dataframe for 5.6 (I don't know why we need lags 5 and 6!). Note also that the lagged data is used as feature and the lead data is used as the target.

	Targets			Features				
	y_step_3	y_step_2	y_step_1	y_lag_2	y_lag_3	y_lag_4	y_lag_5	y_lag_6
Year								
2010	2	1	0	nan	nan	nan	nan	nan
2011	3	2	1	nan	nan	nan	nan	nan
2012	4	3	2	0	nan	nan	nan	nan
2013	5	4	3	1	0	nan	nan	nan
2014	6	5	4	2	1	0	nan	nan
2015	7	6	5	3	2	1	0	nan
2016	8	7	6	4	3	2	1	0
2017	9	8	7	5	4	3	2	1
2018	10	9	8	6	5	4	3	2
2019	11	10	9	7	6	5	4	3

Figure 5.7: features for a forecast

Multistep forecasting strategies

Here are strategies for producing the multiple target steps required for a forecast.

Multioutput model: Use a model that produces multiple outputs naturally. Linear regression and neural networks can both produce multiple outputs (extrapolation). This strategy is simple and efficient, but not possible for every algorithm you might want to use. XGBoost can't do this, for instance (XGBoost is only for interpolation).

Direct strategy Train a separate model for each step in the horizon: one model forecasts 1-step ahead, another 2-steps ahead, and so on. Forecasting 1-step ahead is a different problem than 2-steps ahead (and so on), so it can help to have a different model make forecasts for each step. The downside is that training lots of models can be computationally expensive.

Recursive strategy Train a single one-step model and use its forecasts to update the lag features for the next step. With the recursive method, we feed a model's 1-step forecast back in to that same model to use as a lag feature for the next forecasting step. We only need to train one model, but *since errors will propagate from step to step, forecasts can be inaccurate for long horizons.*

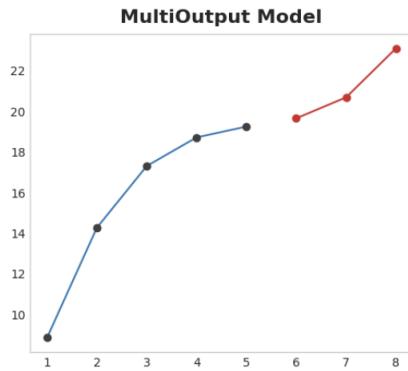


Figure 5.8: MultiOutput Model

DirRec strategy A combination of the direct and recursive strategies: train a model for each step and use forecasts from previous steps as new lag features. Step by step, each model gets an additional lag input. Since each model always has an up-to-date set of lag features, *the DirRec strategy can capture serial dependence better than Direct, but it can also suffer from error propagation like Recursive.*

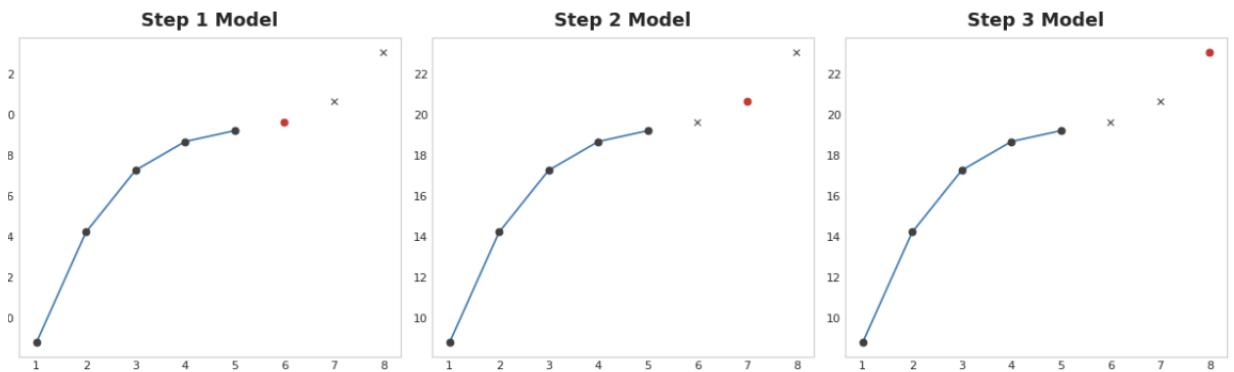


Figure 5.9: Direct strategy

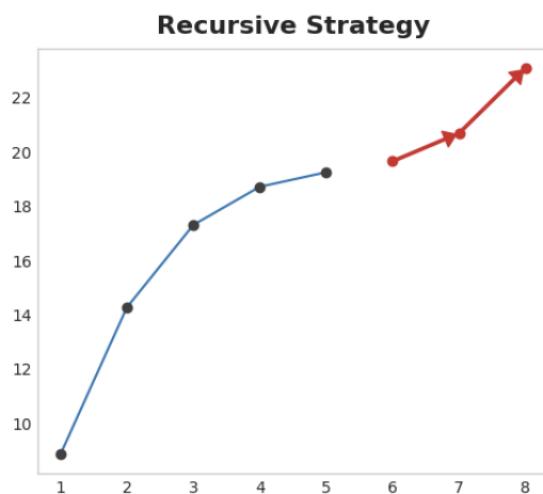


Figure 5.10: Recursive strategy

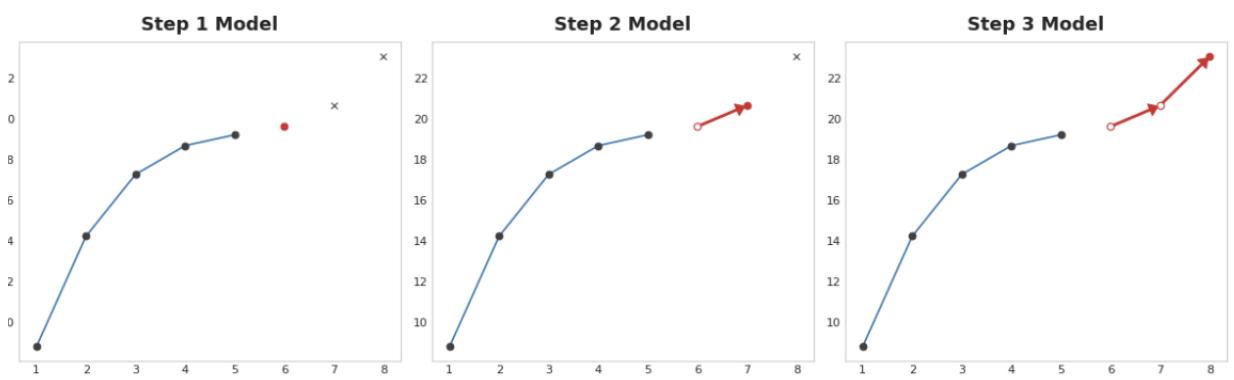


Figure 5.11: DirRec strategy