Machine Learning Foundations
Unit 3: Train Common ML Models

Table of Contents

- Assignment: Optimizing KNN
- Module Wrap-up: Implement K-Nearest Neighbors

Module Introduction: Implement Decision Trees

- Watch: Information Theory Overview
- Read: Information Theory Formalized
- Watch: Building a Decision Tree
- Quiz: Check Your Knowledge: Entropy Scenarios
- Watch: Making Predictions Using the Decision Tree
- Quiz: Check Your Knowledge: Decision Trees Part 1
- Tool: Decision Trees Cheat Sheet
- Ask the Expert: Mehrnoosh Sameki on Decision Trees
- Quiz: Check Your Knowledge: Decision Trees Part 2
- Watch: Optimizing a Tree
- Ask the Expert: Mehrnoosh Sameki on Overfitting and Underfitting
- Read: Model Complexity Revisited
- Ask the Expert: Annie Wong on Bias and Variance Errors
- Assignment: Optimizing Decision Trees
- Assignment: Unit 3 Assignment - Train Decision Trees After Data Preparation
- Assignment: Unit 3 Assignment - Written Submission
- Module Wrap-up: Implement Decision Trees
- Ask the Expert: Mehrnoosh Sameki on Comparing DTs and KNNs
- Ask the Expert: Kathy Xu on Using DTs vs. KNNs
- Assignment: Lab 3 Assignment

Homepage

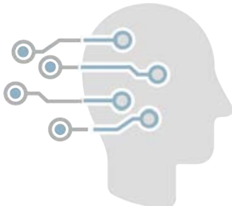
Video Transcript

If you're here watching this video, you're probably already aware that artificial intelligence and machine learning are important technologies. I'd go as far as saying they are critical in today's digital society. Nearly every action in today's economy involves data, and AI helps organizations more objectively and efficiently perform the core tasks, such as delivering content or assessing risk. AI can and will impact us all as consumers in this modern economy. All of the AI is built by a small set of people with highly specialized and sought-after skills. Given the breadth of AI's reach, it is important that the people building it are able to understand the diverse perspectives and lived experiences of the people it affects. As the use of AI matures, we're hearing more and more about how AI might be used as a tool for oppression, silently capturing and reinforcing society's biases. But AI-driven problems can be contained and constrained with responsible and inclusive design and testing guardrails that look for potential problems. This is an important part you will play and why diversity in the people who build AI systems is critical. Diversity in tech is how AI gets built for the people by the people.

What you'll do

- **Understand the machine learning life cycle and explore common machine learning packages**
- **Perform exploratory analysis to understand your data and prepare your data for machine learning applications**
- **Train and optimize two popular supervised learning algorithms: k-nearest neighbors and decision trees**
- **Understand the mechanics of linear models and implement a common linear model from scratch**
- **Define the model evaluation metrics for specific applications by selecting the appropriate model candidates and hyperparameters for testing**
- **Understand the principle of ensemble models and how to use them to improve model performance**

- **Explore the fields of computer vision and natural language processing then implement deep learning models to solve problems in these areas**
- **Identify performance issues and societal failures then find solutions to address these issues**



Course Description

Machine learning (ML) is increasingly a part of people's daily lives. Think about some of the technologies you use every day, such as the suggestions that appear on YouTube and emails being diverted to the spam folder. All are practical applications of ML, a branch of artificial intelligence (AI) that allows computer programs to automatically improve through experience. Looking ahead, some of the world's most complex problems — such as future pandemics — could depend on ML as a solution.

With a curriculum taught by Cornell Tech's Visiting Lecturer Brian D'Alessandro, with content from Cornell University and Boston University faculty, and developed in concert with industry leaders, this "Machine Learning Foundations" summer course offers you the skills that will enable you to build ML solutions in real-world conditions through an ethical and inclusive lens. In this skills-based program, you will work with industry-relevant tools to analyze real-world data sets to identify patterns and relationships in data. By the end of this nine-week course, you will have hands-on experience solving real-world problems by working through the ML life cycle to build machine learning models.

Weekly synchronous lab sessions will give you the opportunity to explore these skills in a collaborative environment and gain hands-on experience in machine learning and data science. Ultimately, the foundational skills you acquire in this "Machine Learning Foundations" curriculum will prepare you to take on real-world industry challenges in Studio this fall.

During this part of the **Break Through Tech** machine learning program, you can expect to spend about eight to ten hours per week on asynchronous online content and about three hours per week on synchronous lab sessions with other students. For a detailed list of what is required to successfully complete this course, visit the "Syllabus" link under **Course Resources** in the left navigation menu.

Brian D'Alessandro
Head of Data Science, Social Impact
Instagram

Brian D'Alessandro is a practicing data science executive with 20 years of experience building machine learning and statistical models for industrial decision making. Mr. D'Alessandro currently leads data science for Instagram's Well Being and Integrity teams. Prior to Instagram, he held leadership roles at Capital One, Zocdoc, and Dstillery. Within these roles, Mr. D'Alessandro led the development and execution of AI and ML systems enhancing digital experiences serving healthcare and financial service needs. Mr. D'Alessandro has also served as an adjunct professor for NYU's Center for Data Science Master's of Data Science program. He developed and taught core ML classes for incoming Master's students and has helped over 1,000 students start their careers as data scientists and machine learning engineers.

Dr. Kilian Weinberger
Associate Professor
Computing and Information Science, Cornell University

Dr. Kilian Weinberger is an Associate Professor in the Department of Computer Science at Cornell University. He received his Ph.D. from the University of Pennsylvania in Machine Learning under the supervision of Lawrence Saul and his undergraduate degree in Mathematics and Computer Science from the University of Oxford. During his career, Dr. Weinberger has won several best paper awards at ICML (2004), CVPR (2004, 2017), AISTATS (2005), and KDD (2014, runner-up award). In 2011, he was awarded the Outstanding AAAI Senior Program Chair Award, and in 2012 he received an NSF CAREER award. Dr. Weinberger was elected co-program chair for ICML 2016 and for AAAI 2018. In 2016, he was the recipient of the Daniel M. Lazar '29 Excellence in Teaching Award. Dr. Weinberger's research focuses on machine learning and its applications; in particular, he focuses on learning under resource constraints, metric learning, machine-learned web-search ranking, computer vision, and deep learning. Before joining Cornell University, Dr. Weinberger was an Associate

Professor at Washington University in St. Louis and had previously worked as a research scientist at Yahoo! Research.

Dr. Linda K. Nozick
Professor and Director of Civil and Environmental Engineering
College of Engineering, Cornell University

Dr. Linda K. Nozick is Professor and Director of Civil and Environmental Engineering at Cornell University. She is a past Director of the College Program in Systems Engineering, a program she co-founded. Dr. Nozick has been the recipient of several awards, including a CAREER award from the National Science Foundation and a Presidential Early Career Award for Scientists and Engineers from President Clinton for "the development of innovative solutions to problems associated with the transportation of hazardous waste." She has authored over 60 peer-reviewed publications, many focused on transportation, the movement of hazardous materials, and the modeling of critical infrastructure systems. Dr. Nozick has been an associate editor for Naval Research Logistics and a member of the editorial board of Transportation Research Part A. She has served on two National Academy Committees to advise the U.S. Department of Energy on renewal of their infrastructure. During the 1998-1999 academic year, she was a Visiting Associate Professor in the Operations Research Department at the Naval Postgraduate School in Monterey, California. Dr. Nozick holds a B.S. in Systems Analysis and Engineering from George Washington University and an M.S.E and Ph.D. in Systems Engineering from the University of Pennsylvania.

Dr. Chris Myers
Senior Research Associate and Adjunct Professor
Center for Advanced Computing, Cornell University

Dr. Chris Myers has been with the Center for Advanced Computing at Cornell University since 2017, having previously been a member of the research staff of the Bioinformatics Facility of the Institute of Biotechnology (2007-2017) and the Cornell Theory Center (1993-1997, 1998-2007). In addition, he is an Adjunct Professor in the Department of Physics at Cornell and a member of the graduate faculty in the fields of Physics, Computational Biology, Applied Mathematics, and Computational Science and Engineering. Dr. Myers works primarily in the field of computational biology, addressing problems in the systems biology of cellular regulation, signaling, metabolism, development, virulence and immunity, and in host-pathogen interactions and the spread of infectious diseases on populations, networks, and landscapes.

Dr. Mehrnoosh Sameki

Adjunct Professor, Boston University

Senior Technical Program Manager, Microsoft

Dr. Mehrnoosh Sameki is a senior technical program manager at Microsoft, responsible for leading the product efforts on machine learning interpretability and fairness within the Open Source and Azure Machine Learning platform. She co-founded Fairlearn and Responsible-AI-widgets and has been a contributor to the InterpretML offering. Dr. Sameki earned her Ph.D. degree in Computer Science at Boston University, where she currently serves as an Adjunct Assistant Professor offering courses in responsible AI. Previously, she was a data scientist in the retail space, incorporating data science and machine learning to enhance customers' personalized shopping experiences.

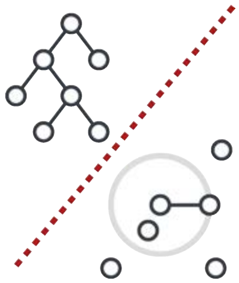
Unit 3: Train Common ML Models Overview

Video Transcript

We are now ready to dive into the core of machine learning, which is the process of creating predictive models from data. Referring back to the ML development lifecycle, this is where we start model training. We can assume now that you have specified the problem statement and have prepared data to have a label and features. So far we've discussed supervised learning, which is where we build a model using labeled data. In this section, we will cover two core methods used in supervised learning. These methods are K-nearest neighbors and decision trees. Our goals will be to understand the core mechanics of these methods, but also gain practical knowledge on how to build and optimize them. These two algorithms have a unique way in which they are trained. I'll show you how to set these up and train using scikit-learn. In addition to the mechanics of these core algorithms, we'll discuss a few other fundamental concepts that apply to supervised learning. One such concept is loss functions, which are functions that quantify how well a model is performing. Additionally, we'll cover model complexity and how it leads to overfitting. Overfitting is a model failure mode that causes model generalization performance to be poor. We will learn to control overfitting by adjusting model hyperparameters, and hyperparameters are algorithms specific inputs that control how the model is built. Each of our core algorithms has different hyperparameters and choosing them carefully is key to getting good generalization performance.

What you'll do:

- **Define the core foundational elements of model training and evaluation**
- **Develop intuition for different classes of algorithms**
- **Analyze the mechanics of two popular supervised learning algorithms: decision trees and k-nearest neighbors**
- **Develop intuition on tradeoffs between different algorithmic choices**



Unit Description

Over the next two weeks, you will be introduced to the fourth step in the machine learning life cycle: modeling. You will focus on the model training process for supervised learning models and explore a few supervised learning algorithms that are commonly used. You will also begin to explore model evaluation.

Recall that supervised learning attempts to discover the relationship between features and some associated labels for the purpose of prediction. This week, Mr. D'Alessandro introduces the model training for two popular supervised learning algorithms: k-nearest neighbors (KNN) and decision trees (DT). Both models are fairly simple and intuitive to understand. Both are non-parametric models, meaning that neither hold prior assumptions about the structure or distribution of the data and the relationships between features and the label. In the following unit, you'll learn about a class of parametric models called linear models, which assume a linear relationship between features and a label.

Although both KNN and DT models can be used for regression and classification problems, the focus of this week will mostly be on their applicability to classification problems. You will practice creating your own ML models using a popular Python package for machine learning called scikit-learn.

Note: This course uses version 0.22.2 of the scikit-learn library. Some of the features of scikit-learn that are covered in this course may be deprecated in newer versions of scikit-learn.

Also note: Throughout this program, you may often see classification models referred to as "classifiers." Recall that in classification, the labels are discrete or categorical values. You may often see "labels" referred to as "classes" or "class labels."

Back to Table of Contents

Tool: Unit 3 Glossary

Though most of the new terms you will learn about throughout the unit are defined and described in context, there are a few vital terms that are likely new to you but undefined in the course videos.
While you won't need to know these terms until later in the unit, it can be helpful to glance at them briefly now. Click on the link to the right to view and download the new terms for this unit.

Download the Tool

Use this **Unit 3 Glossary** as a reference as you work through the unit and encounter unfamiliar terms.

Back to Table of Contents

Discussion: Unit 3: Train Common ML Models

Welcome to the discussion thread for Unit 3! This is a space where you can ask any questions you have about training common ML models.

To get the most helpful responses from your peers and instructional teams, be specific about the concepts you're struggling with and share what you've understood so far.

Guidelines for Posting in Discussion Threads:

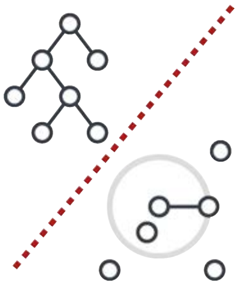
1. **Stay On Topic:** Make sure your questions and contributions are relevant to the unit's content. This helps keep discussions focused and beneficial for everyone.
2. **Be Specific:** When you post a question, include specific details and context. Mention particular concepts, lectures, assignments, you're referring to. This makes it easier for others to provide accurate and helpful responses.
3. **Quote or Cite Materials:** If your question is about a specific part of the course materials, quote or cite the section to help others understand and reference the context of your query. You can even use a link to the specific course page!
4. **Constructive Language:** Use respectful and constructive language in all your interactions. Encourage and appreciate responses, and offer positive feedback when others help you.
5. **Use Clear and Concise Language:** Keep your questions and comments clear and to the point. Avoid overly complex language that might confuse your peers or instructional teams.
6. **Collaborative Learning:** Encourage discussion by not only asking questions but also responding to others. Sharing your insights and understanding can contribute significantly to collective learning.
7. **Confidentiality and Respect:** Do not share personal information or content that hasn't been publicly discussed in the course materials. Always respect the privacy

and intellectual rights of your peers and instructors.

8. **Search Before Posting:** Before posting a question, check if someone else has asked something similar and whether it has already been answered. This helps reduce duplicate questions and leverages existing discussions.
9. **Use Proper Formatting:** If you're sharing code, equations, or specific formatting-dependent content, use the appropriate formatting tools provided by the discussion platform to enhance readability.
10. **Review and Edit Before Posting:** Before you submit your post, review it for clarity and errors. A well-written post is more likely to receive useful responses.
11. **Maintain Academic Integrity:** Do not post exact answers to assignment questions. Instead, focus on discussing concepts and problem-solving approaches. This helps preserve the integrity of the learning process and ensures everyone benefits fairly from the course materials.

Back to Table of Contents

Module Introduction: Introduction to Model Training



In this module, Mr. D'Alessandro will introduce the training and evaluation process for supervised learning models. Recall that the goal is to train a model that can generalize well to new data. You will familiarize yourself with new terms, key concepts, and the methods used in the training process with the goal of generalization in mind. You will also be introduced to the scikit-learn package, a key package for doing machine learning in Python. This package supports techniques for supervised learning and will make programming your model much easier.

Back to Table of Contents

Watch: Training With the Goal of Generalization

The goal of the training process is to create an accurate model that generalizes well to new data. There are a few things to consider in order to reach that goal.

First, you want to minimize loss, or the measure of how many mistakes your model made. Loss is a way of measuring the difference between a training example's label and the label that the model predicts. The goal is to produce a model in which there are little to no prediction errors, therefore little to no loss. This measure is often referred to as training loss or training error.

Second, you want to avoid one common problem that may occur when training your model with the goal of having low to zero loss. While a model may successfully have a low training loss, it may adapt so well to training data that it cannot generalize to new data. This is called overfitting. The goal is to create the best model possible without overfitting.

In this video, you will be introduced to these core concepts. Please note that logistic regression will be further discussed next week.

Video Transcript

We are now ready to start formally learning the algorithms behind supervised learning. There are several algorithms we'll learn. Each varies in how they learn a prediction model, but they all have the same goal in the end, which is to be able to generalize to new data. I'll explain this concept more in this video. In this course, we won't cover all of the possible algorithms. I chose a core set with two goals in mind. The first goal is to learn the fundamental conceptual building blocks that will ultimately help you better understand any learning algorithm. These building blocks are represented by the three algorithms in the less complex group here. The second goal is to pick up practical experience on the algorithms that are most generally used in practice. These are represented in the more complex group here. Before we discuss any one algorithm, I want to introduce a few concepts that are important for all of them. I have mentioned several times that the goal of machine learning is generalization, which is the model's ability to adapt to new previously unseen data.

For supervised learning, I can make this more explicit. Instead of saying, adapt to new data, I can say we want to be able to accurately predict the label in previously unseen data. This idea of generalization can be expressed mathematically. The core tool we use to do this is called the loss function. The loss function is a specific mathematical expression that measures how good your predictions are. The most common loss function is the simple idea of error, i.e. on average, how often is your prediction exactly equal to the label? We will use loss functions in the model-building process, which is called training, as well as in evaluation. There are several loss functions to choose from, and the one to use will be driven by the problem. Our general goal with supervised learning is to minimize the loss function.

But there is a very important distinction to make. We don't technically want to minimize the loss function on the data we have. Instead, we want to optimize or minimize the loss on new previously unseen data. This is called minimizing the expected loss as opposed to the training loss. This is a bit abstract, so let's illustrate this a bit. The plot on the left represents a theoretical data distribution. This is the data that could be generated from a data generating process. This is where you would sample your training data from. On the right we have our observed data sample. These data points come from the same distribution as the left, but we should assume it is a finite sample. When we build a model, we use only the sample training data. There is a phenomenon where our model becomes finely tuned to the finite training sample and fully minimizes the loss function on that data, and at the same time, the model doesn't perform well on new data. This is what we call overfitting. Overfitting is one of the most important concepts in machine learning, and a lot of your work will be focused on avoiding it. Here is another illustration of it. In this case, we have a scatter plot where a classification label is represented by the color. The line represents our supervised learning model and the goal has been to optimally separate the two labels. If this data represents our training data, then the green line makes perfect predictions. At face value, this might seem great. But when new data comes in and we might observe that the green line fit too much the nuances or noise of the specific training dataset. The black line is a lot smoother and we might observe in practice that this is more accurate on new data. When we overfit, our model adapts to the training data so well that the model does not generalize well, just as we can see in this illustration. Again, pretty much everything we'll learn from this point on has the core goal of creating the best model possible without overfitting the data. This is essentially how we will approach the goal of generalization.

Back to Table of Contents

Read: Overfitting and Underfitting

The goal of supervised learning is to build a model from known labeled examples to predict outcomes, or labels, from unlabeled data. As you have seen, generalization is a machine learning model's ability to accurately predict new, unseen data. A good ML model generalizes well to new data.

There are two failures that can occur when training your model: Your model can "overfit" the training data or "underfit" the training data. Overfitting occurs when the model is too complex, while underfitting occurs when the model is too simple.

☆ **Key Points**

Having a low training loss does not always mean that your model will generalize well to new data.

Overfitting occurs when a model is too complex; an overfit model has low training error and poor generalization.

Underfitting occurs when the model is too simple; an underfit model has high training error and poor generalization.

What is overfitting?

Just because a model performs well and has low training loss (training error) on training data does not mean it will also perform well with new, unseen data. If the model learns the idiosyncrasies that are particular to **only** the training data set, it will fail to generalize to new data. This is known as overfitting.

The model has learned relationships among features and labels that are too specific to the training data only and therefore cannot be used to accurately infer anything about unseen data. This happens when a model is too **complex**, which allows it to fit extremely well against all detailed information that is thrown at it. While this may sound like a good thing, it is not. Although training loss may be low, the model becomes so fixated on the training data that it may not be able to make accurate predictions on unseen data, as the model makes decisions based on patterns which exist only in the training data and not in the broader data distribution.

Consider this example: You are training your model to recognize trees. You would start off by giving it a bunch of images of various trees during training. In this case, you were able to obtain various images of palm, oak, and spruce. Your goal is to have your model recognize green leaves and a brown trunk so that next time a different kind of tree with these characteristics shows up, your model will be able to confidently predict it as a tree.

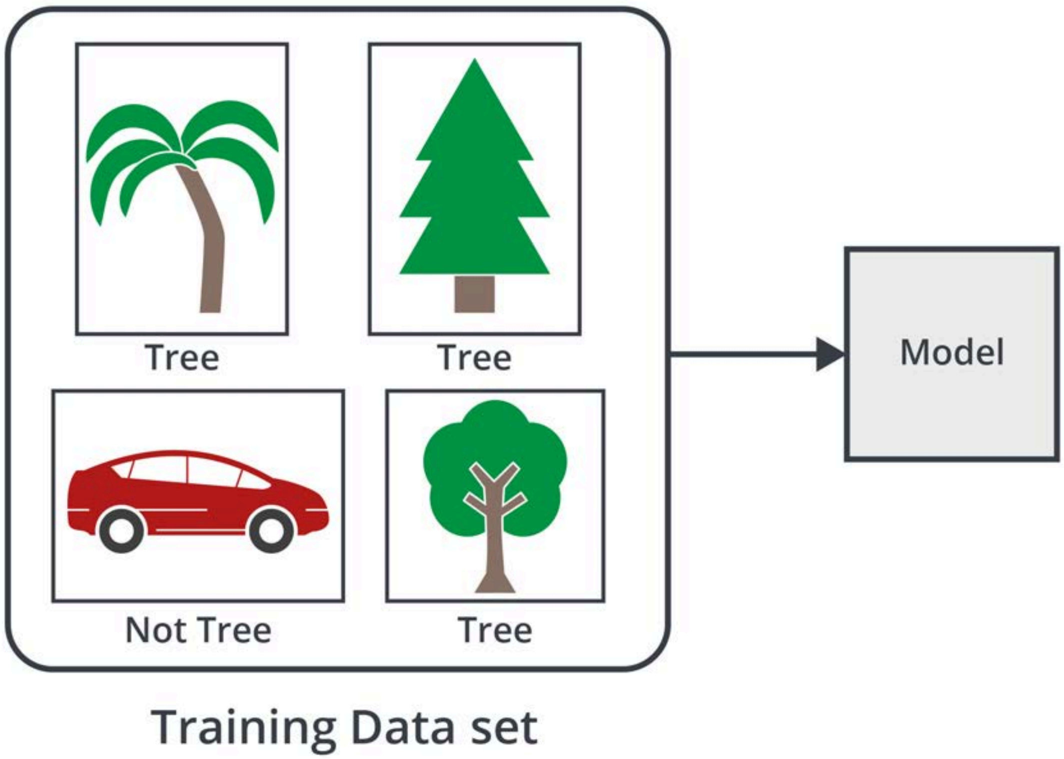


Figure 1. Training phase of a tree recognizer.

If your model is overly complex, it will start to learn characteristics such as leaf shape, trunk shape, and the height-to-width ratio of these trees from the training data set. As such, your tree recognizer, in this case, becomes very good at recognizing just palm, spruce, and oak. If the model sees a willow tree, it will predict it as a non-tree even though it also has green leaves and a brown trunk.

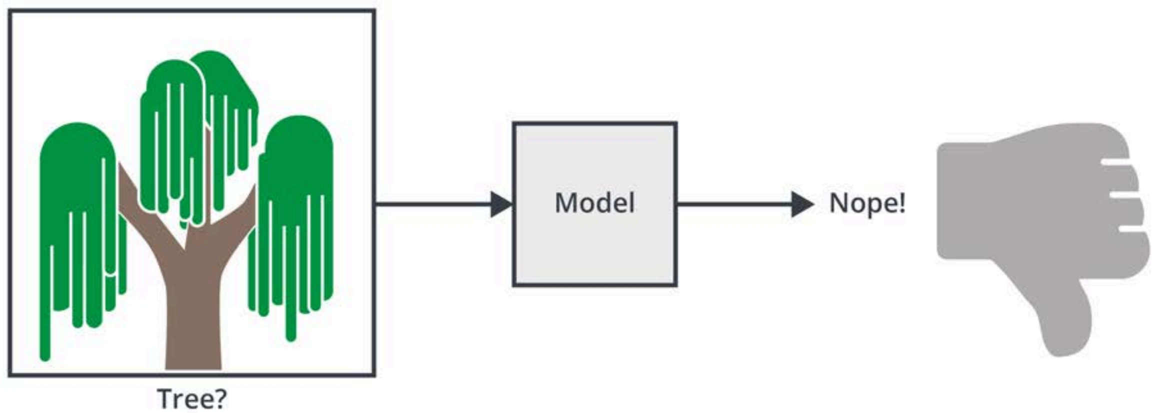


Figure 2. Overly complex model.

What is underfitting?

While an overfit model performs well on training data but generalizes poorly to new data, an underfit model never performs well on training data from the beginning. An underfit model has high training error and therefore can't generalize well to new data either. In the case of an underfit model, it is too simple and has not captured relevant details and relationships among features and labels necessary to make proper predictions; therefore, it will be unable to make predictions on new data and will perform poorly.

In the tree recognizer example, an underfit model may have only learned to recognize a tree as anything that is green.

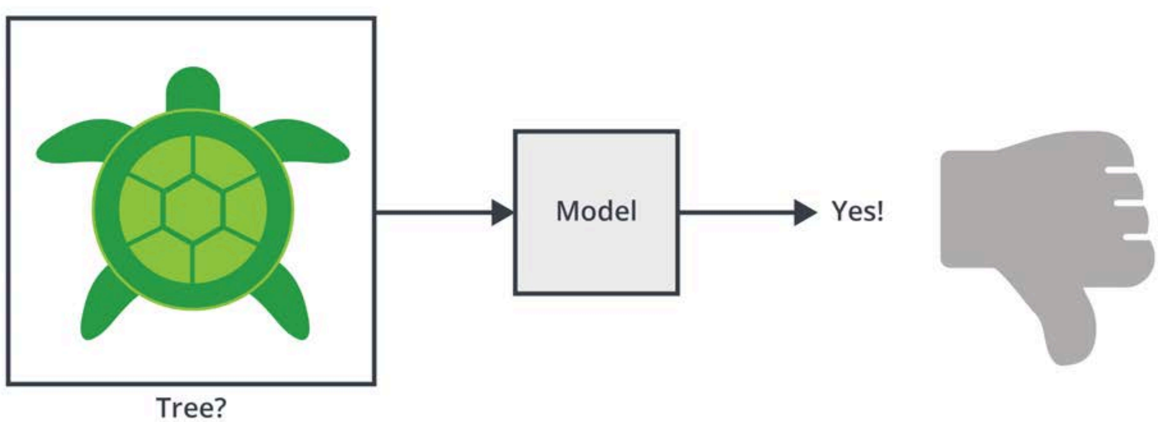


Figure 3. Overly simple model.

Back to Table of Contents

Read: Training and Test Data Sets

How to avoid overfitting?

You have seen that due to overfitting, a low training error does not necessarily mean that your model will perform well on new, unlabeled data. So how can you properly evaluate your model's performance and prevent overfitting? To evaluate your model's ability to generalize well to new data, you have to test your model on data that your model has not seen before. But how can you test your model on new data if you only have the data set on which your model was trained? A common technique in machine learning is to split your original data set into two partitions: training data and test data.

☆ Key Points

Splitting your data set into training, validation, and test sets allows you to properly evaluate your model's performance and prevent overfitting.

- **Training set** — a partition to train a model
- **Test set** — a partition to test the model

You will train your model on the training data set and evaluate the model on your test data set. The beauty of this technique is that since you will be making your test set from your initial labeled data set, you will have both the features and the labels. This means you will have all of the actual values in advance. You will test your model on the features and compare your model's predictions with the labels. For example, in a classification problem, you will be able to see what fraction of the email examples were accurately classified as "spam" emails. In a regression problem, you will be able to see the difference between the predicted and actual values of housing prices.

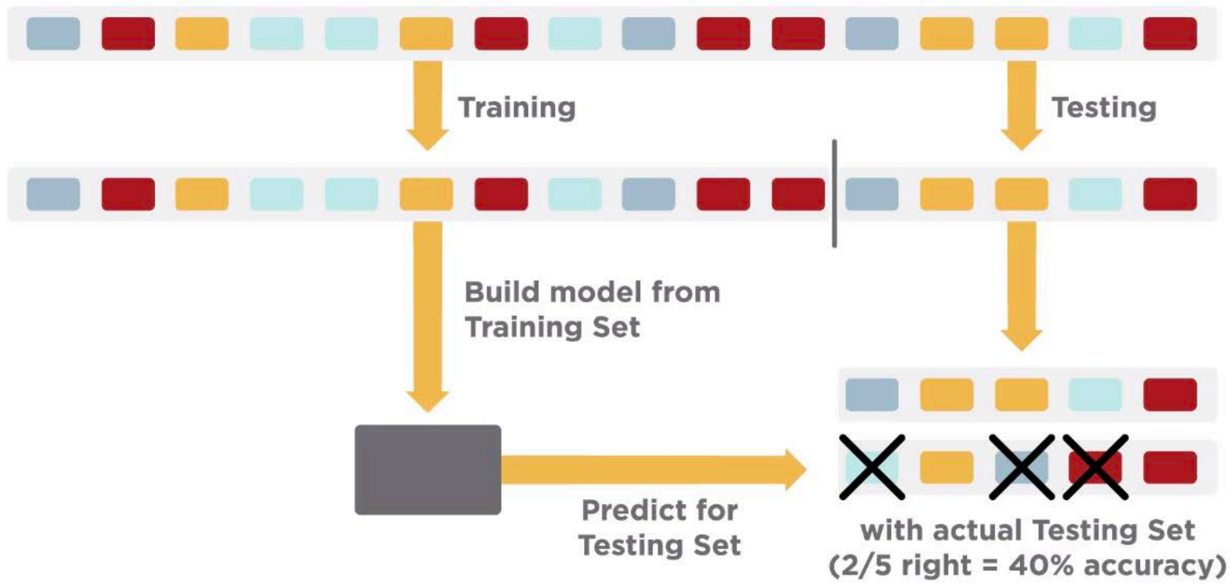


Figure 1. Split full data set into a training set and a test set.

There are pitfalls in using the test set over and over. After evaluating your model's performance, you may find that you must improve your model, but you cannot tweak your model then train and test again using the same test data set. Continuing this process will inadvertently change the model to do well on the test data set and lead you to overfit your model on the test set. Testing more than once on a test set may incorrectly lead you to believe that your model will perform well on unseen data. Since you should only use the test data set once, you can also use a validation data set to improve your model before testing.

Therefore, your data set should be initially split into three partitions:

- **Training set** — a partition to train a model
- **Validation set** — a partition to validate the model's performance
- **Test set** — a partition to test the model

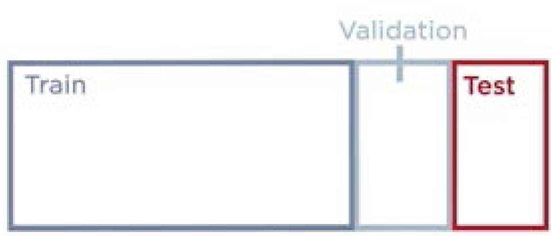


Figure 2. Split full data set into a training set, a validation set, and a test set.

You train your model on the training set, evaluate the model on the validation set, adjust the model accordingly, and continue this process as many times as needed until you improve your model and the validation error (validation loss) improves to an acceptable level. Once you feel that you are ready to test your model to obtain an accurate assessment of the model's performance, you can then complete an evaluation of your model on the test set. This will allow for an unbiased evaluation of the model's performance.

Note: Training and validation sets are often referred to as just a training set.

Evaluation techniques

There are different ways to partition your data set to create training, validation, and test sets. There are also different ways to analyze your model to determine loss and accuracy during both the training and validation phases. These techniques can vary per model. These techniques include:

- Loss functions
- Evaluation metrics

You will cover these techniques in a later course. In this course, you will begin by using just two sets: a training data set and a test data set. You will train the model on the training set and evaluate the model on the test set using a very simple evaluation metric built into scikit-learn for classification models: accuracy. While the measure of loss and accuracy are not the same, the accuracy metric you will use is essentially equivalent to the zero-one loss function used to evaluate binary and multiclass classification models. Both count the number of predictions that are correct and incorrect.

Back to Table of Contents

Read: Hyperparameters

One way to avoid the problems of overfitting and underfitting is to incorporate a validation phase after model training. In the validation phase, you can evaluate your model's performance, make necessary changes, and then retrain the model. One key mechanism of a supervised learning model that can be adjusted during the validation phase is a model's hyperparameters.

Hyperparameters are the knobs that programmers tweak in machine learning algorithms. The best way to think about hyperparameters is to view them as the settings of an algorithm that can be adjusted to optimize performance, just as you might turn the knobs of a radio to get a clearer signal. You choose hyperparameter values prior to commencing training. In order to improve a machine learning model's performance after training, a model's hyperparameters may be adjusted during the validation phase. The model will subsequently go through the training process again with these adjustments. You will read in further detail about what hyperparameters are and why they are so important.

☆ **Key Points**

Hyperparameters are the settings of an algorithm that can be adjusted to optimize performance; it's the same idea as turning the knobs of a radio to get a clearer signal.

To ensure your model is not susceptible to overfitting or underfitting, you want to tune the model’s hyperparameters to some optimal values.

A machine learning engineer’s job is to experiment with various values of hyperparameters and evaluate the models to ensure that the models developed are not overfitted or underfitted.

What is a hyperparameter in a machine learning model?

A model hyperparameter is a configuration that is external to the model itself. Hyperparameters declare the mechanics of the model, such as its complexity, and determine how the model is trained, such as how fast it learns.

Hyperparameters are often:

- Used to adapt a model to a particular setting
- Specified by the practitioner
- Set using heuristics
- Tuned for a given predictive modeling problem

Hyperparameter optimization

When creating a machine learning model, you'll be presented with design choices as to how to define your model architecture, including a model's hyperparameters. Often, you won't immediately know what the optimal model hyperparameters should be for a given model. You cannot know the best value of a model hyperparameter for a given problem and cannot estimate these values from data. To find the optimal hyperparameters for your model, you may use common approaches, copy values used on other models, or search for the best value by trial and error. You can explore a range of possibilites. When a machine learning algorithm is tuned for a specific problem, essentially you are tuning the hyperparameters of the model to discover the model that results in the most accurate predictions. This is known as hyperparameter optimization.

Examples of model hyperparameters

Below are some hyperparameters you will encounter throughout the course:

- **Size of neighborhood** in KNN
- **Depth of tree** in decision trees
- **Learning rate**, or step size, in gradient descent

[Back to Table of Contents]

Watch: The Core Sklearn API

One of the reasons Python is the number one language for machine learning is the wealth of available open-source packages out there. One of the packages commonly used in the machine learning community is scikit-learn (sklearn for short). Not only does sklearn contain a comprehensive collection of classes and methods for performing common machine learning tasks, but it is also well-documented. In this video, Mr. D'Alessandro will go over the core API in sklearn, including model instantiation, model fitting/training, and model prediction and evaluation.

Video Transcript

I think it is fair to say that great software is one of the reasons machine learning has become so popular. The discipline has been around for several decades in academic circles. The emergence of the tech industry has also brought the data and use cases that were perfect for machine learning. In the early 2000s, it still took deep and specialized knowledge to be a machine learning engineer. This is because the software we have today did not exist. If you wanted to build a model, you often had to build the model training code from scratch, and this significantly slowed down our limited execution progress. There are now many great software options available today, but arguably the most influential has been scikit-learn and Python. In this video will introduce the core APIs that make this software so powerful and popular. Scikit-learn has a very wide range of algorithmic options covering regression, classification, and unsupervised learning. It also provides rich libraries for data preparation, model selection, and evaluation. One of the most powerful design features of the package is the consistency and ease of use of actually training a model. Independent of the algorithm, scikit-learn has reduced modeling to three core steps. These are model specification where you instantiate the model class and tell scikit-learn how you want to configure the specific algorithm, then is model fitting, which is another way to say training the model. At that point, you have your model. When you want to use the model for evaluation or prediction purposes, the third step kicks in.

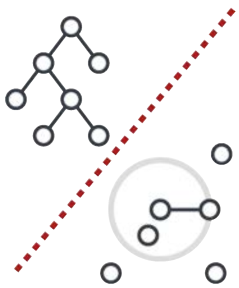
Here are the same steps represented as actual code. There are four lines here because you have to import the specific algorithm first, of course. In the first line I am creating a model object from the model class. Across the different algorithms, this is where the code will be different because each of the core algorithms will have its own class as well as different input parameters. Next, we call the fit method. We pass in the data which consists of the features represented by X here and the label represented by Y. DF here is just a variable that holds a data frame. This is where scikit-learn runs the actual optimization routines. This method doesn't return anything, but under the hood, the model object is now filled with data that represents the actual model. At this stage, the training is complete. When we want to use the model to either evaluate or make actual predictions, we call the predict method. We'll cover this more later, but this particular method returns the predicted class. If you want to predict a probability score, for instance, you'll want to use a different one. When we build models, we commonly want to try out different algorithms. Scikit-learn makes this particularly easy with its common API. In this code example, we can call the training and a loop. First, we import the different algorithms. Notice that each one comes from a separate submodule of scikit-learn. I then created a dictionary here where each element is a different algorithm. After that, I call the fit method within the loop. The common API gives us the ability to automate the process of testing and choosing different algorithms. This is a process called model selection that we'll discuss in more detail later. Despite some common APIs, scikit-learn still has a lot to remember. I personally don't remember it all after many years of using it. Even if I know the name of the class like I need, I still might forget the exact names of the input parameters, or what the defaults are. The scikit-learn documentation is quite robust and accessible though. A common sequence in your workflow will be to Google scikit-learn plus the name of the action you want to do. The documentation usually comes up first, and I think scikit-learn has some of the best documentation of any Python package out there. As you get more advanced, the source code is linked to the documentation itself. So if you want to really understand how an algorithm works, there's no better thing to do than study the actual source code.

Back to Table of Contents

Module Wrap-up: Introduction to Model Training

In this module, Mr. D'Alessandro explained the basics for training and properly evaluating a supervised learning model. You explored how to create a model with low training loss and ways to overcome the perils of overfitting your model to training data. Mr. D'Alessandro also introduced a popular Python package scikit-learn, that is commonly used in machine learning. You will use this package to implement and evaluate future supervised learning models. **Back to Table of Contents**

Module Introduction: Implement K-Nearest Neighbors



The first supervised learning algorithm Mr. D'Alessandro introduces is the k-nearest neighbors (KNN) algorithm. KNN is a simple algorithm in that can make predictions about an example based on the labels of other examples "near" it.

KNN can be used in regression or classification problems. For regression problems, it can make predictions for a *continuous* label; in this case, the predicted value is the average of the labels for the k-nearest neighbors. For classification problems, KNN can be used to classify a *categorical* label; in this case, we look at the distinct categories for the k-nearest neighbors, and the category that occurs most often is our predicted label (class).

In this module, Mr. D'Alessandro focuses on how k-nearest neighbors is used in classification. You will explore the k-nearest neighbors classifier and see how it is used to classify examples as you explore its applications and limitations.

Back to Table of Contents

Watch: Introduction to KNN

In this video, Mr. D'Alessandro introduces you to your first machine learning algorithm: k-nearest neighbors (KNN). KNN is straightforward to implement and is therefore often used to introduce the key components of a machine learning algorithm. Watch as Mr. D'Alessandro explains how this model works and what it means for KNN to be an instance-based learning algorithm.

Video Transcript

Here, we'll cover the learning algorithm called k-nearest neighbors or KNN for short. KNN is unique amongst the algorithms you'll commonly use. It's an example of what we call instance-based learning. Nearly all other algorithms can be represented by a parameterized data object. These objects typically typically take the form of equations or logical tree-based structures. KNN, on the other hand, is represented by the training data. As a matter of fact, one doesn't technically train a KNN model. Predictions are made at prediction time and involve just a query on the original training examples. To illustrate how KNN works, let's start with a common picture. Here we have a scatter of two features called X1 and X2. Each point represents a different example with those two features. Each example has a class label which we represent with the color. You can see here that most of the green points tend to cluster to the upper right, but we also see some overlap between the two classes. Recall that all of our learning algorithms work by attempting to find a reasonable separating line between the two colors. With KNN, we start with the point we are predicting.

In this case, it's the large red dot. When we look for the K closest points using some distance formula that we choose, this is where the k-nearest neighbor name comes from. Once we have found the K closest points are separating boundary is essentially a circle around our point, and the radius would be the distance to the farthest point in that set of k-neighbors. Once we have our neighborhood and a set of points within it, we make a prediction by looking at the class labels of the neighbors. Just as it is illustrated in this chart, to make a prediction for a single example, we can ignore all points outside of the circle. Our predictions can be the most common class if this is a classification problem; we can also take the averages of the label. This means we can use the exact same algorithm for regression problems, or classification problems when we're trying to predict a class label probability instead of a class label alone. This process will be repeated for every new example we are predicting. Each example will get its own custom neighborhood and the prediction will be based only on the points in that specific neighborhood. In this example, we can see how label values tend to be concentrated in different regions of the feature space. Pretty much all classification algorithms operate under this basic assumption. The more that labels cluster, the better performing our algorithms likely will be. KNN is the most explicit algorithm capturing a fundamental concept in supervised learning. This concept is that examples that are near each other in the feature space are likely to have the same label.

Back to Table of Contents

Read: An Overview of KNN

Most supervised learning models are represented by some underlying data structure derived from training examples, such as the tree structure that is produced by the decision tree supervised learning algorithm. This is known as model-based learning. Another type of supervised learning is known as instance-based learning. Instance-based learning models simply store training examples in memory and utilize those examples on-demand to make predictions for a new, previously unseen example.

K-nearest neighbors — KNN for short — is one such algorithm that belongs in instance-based learning. One way to think of it is that there really is no such thing as training in instance-based learning; all that you are doing is making the data available at prediction time so you can consult the data on the fly as you make predictions.

☆ **Key Points**

KNN is an instance-based type of supervised learning model that stores training examples in memory and uses them to predict the labels of new examples.

Distance functions are used to measure similarity (nearness) between two points. The distance function is one of KNN's hyperparameters.

K is a hyperparameter chosen by the machine learning engineer; it can be determined based on domain knowledge, heuristics, or experimentation.

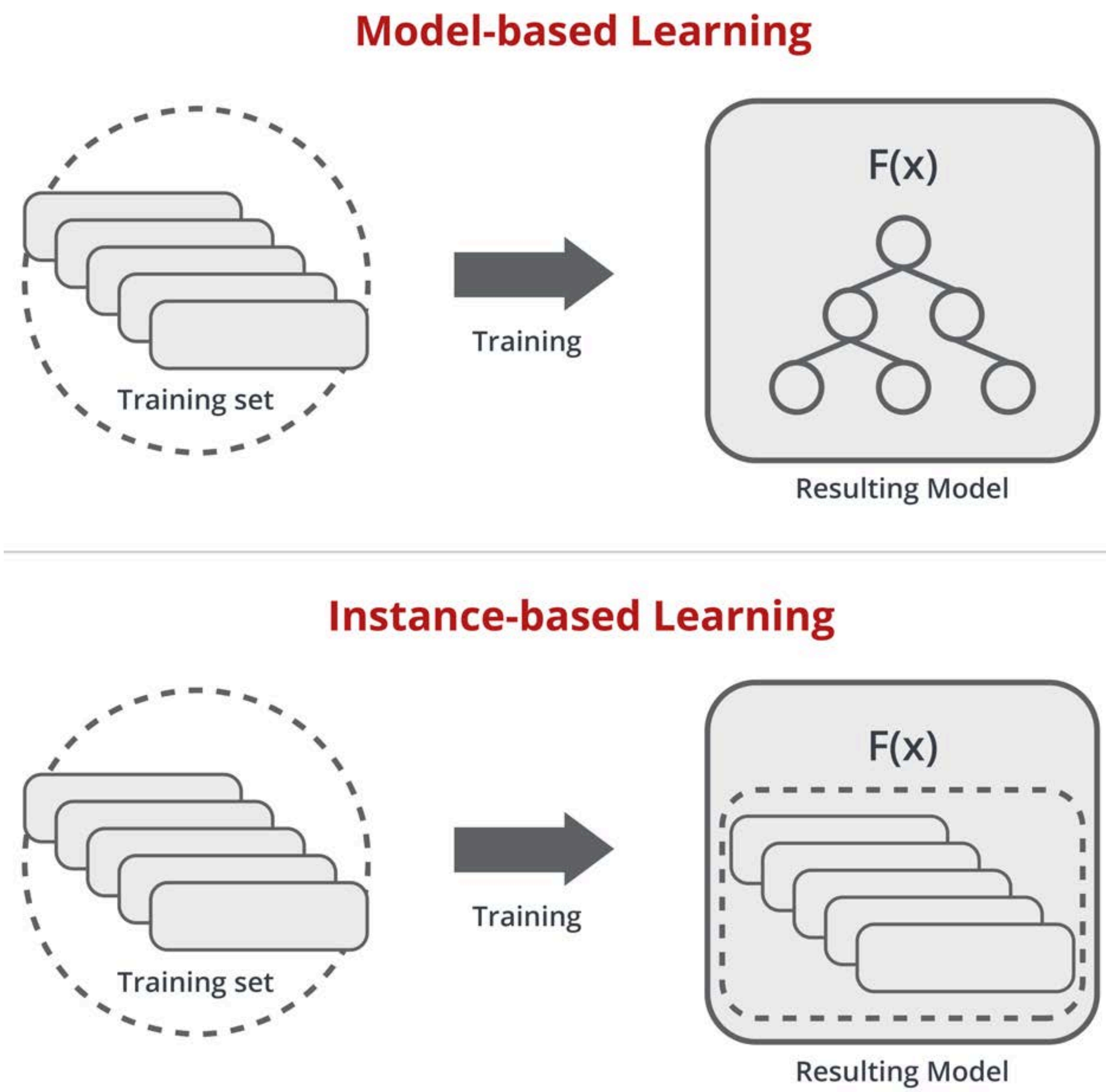


Figure 1. Model-based learning vs. instance-based learning.

Take a look at an example of a KNN classifier in action. In Figure 2 below, blue and red markers represent training examples containing two features, x1 and x2. When a new, unlabeled example comes in, as indicated by the green marker, how should we classify it? We first choose a size for K (K=number of nearest neighbors); in this case. three. We then find the K closest examples to our green marker and look for the most common class label in this group. Since there are two blue markers and one red marker, we determine that our green example should be classified as blue, given that it is the most common marker in this group.

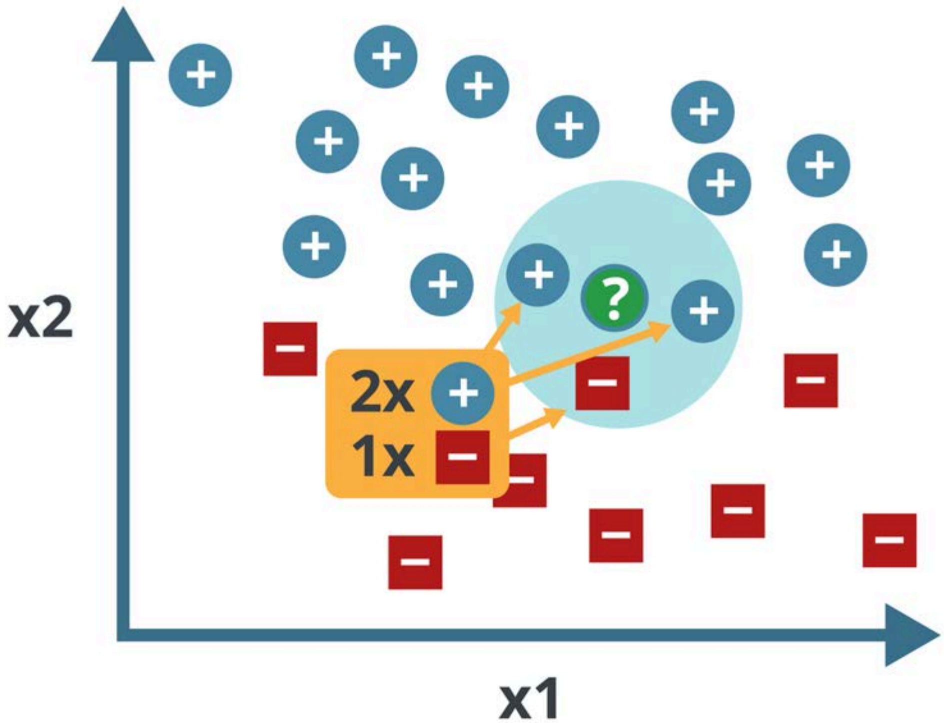


Figure 2. KNN example

In KNN, the K is also known as a **hyperparameter**; it represents the number of neighboring examples that will be used to make a prediction. This number is usually determined based on domain knowledge, heuristics, or experimentation, though experimentation is recommended. Too low of a K or too high of a K can both lead to poor performance. You will get into more details on hyperparameter tuning in the later lessons.

Another concept is the notion of closeness or similarity. In our example above, we use Euclidean distance as our similarity measure, but there are other methods for measuring similarities, such as Manhattan distance and Mahalanobis distance. These similarity measures are known as **distance functions**, which you will go over in greater detail in subsequent sections.

To summarize, KNN is an instance-based learning that stores training examples in its memory. When a new, previously unseen example comes in, KNN first looks for the K most similar examples based on some distance function and makes the prediction based on the labels of those examples.

Back to Table of Contents

Tool: KNN Cheat Sheet

The tool linked to this page provides an overview of the k-nearest neighbors algorithm for your reference. You'll find information about the applicability, underlying mathematical principles, assumptions, and other details of KNN.

Download the Tool

Use this **KNN Cheat Sheet** when referring to algorithm parameters.

Back to Table of Contents

Code: KNN Demo

In this activity, you will see how to implement a KNN model using scikit-learn. You will practice how to create training and test data sets from a raw data set, use the training data train a KNN model, and use the test data set to evaluate your model's performance. You will work with a popular data set, the **Iris Data Set**, which is used to classify the species of an iris flower.

Note: This week you will use just two sets: a training data set and a test data set. You will train the model on the training set, and evaluate the model on the test set. You will not use a validation data set.

This activity will not be graded.

Please complete this activity in the course.

Back to Table of Contents

Watch: Distance Functions

The core of KNN lies in the concept of distance function. Distance function allows KNN to evaluate the similarity between two different data points (examples). In this video, Mr. D'Alessandro goes over how distance functions work in detail and its role in KNN. He further explains how to compute common distance with a demonstration of Euclidean distance.

Video Transcript

K-nearest neighbors is probably the simplest supervised learning algorithm from a mathematical perspective: The most important mathematical elements are what we use to evaluate the idea of nearness. We do this using a special type of function called a distance function. Distance functions are typically defined between two points — let's start there. The concept is easiest to illustrate in two dimensions, but everything we discuss here applies to any number of dimensions. When I use the word dimension here, I simply am referring to the number of features in your data. The simplest way to think of distance is the length of a straight line connecting two points. The most commonly used distance function is called Euclidean distance. The distance function represents the concept I just mentioned, which was the straightest distance between two points. If you look at the formula, it should be actually pretty familiar. This is none other than the Pythagorean theorem. This formula is easily generalized to multiple dimensions. Again, there are a few other distance functions that are relevant for k-nearest neighbors, but Euclidean distance is the most common starting point. Once you learn the different options and circumstances in which you may use each one, you can specify the distance functioned when building the KNN model in scikit-learn. As shown here in the scikit-learn documentation, the parameter for distance function in the code is called metric. The choice of distance metric can be another type of hyperparameter you can test to ultimately find your best model.

Back to Table of Contents

Read: Common Distance Functions

There are many common distance functions that are used to compute the similarity of two data points (i.e., examples). The optimal distance function for a problem can be selected based on domain knowledge, heuristics, and experimentation. You will begin with three distance functions commonly used in KNN: Euclidean, Mahalanobis, and Manhattan.

☆ Key Points

Euclidean distance is the most straightforward distance metric, but it does not account for the correlation and scale among features.

Mahalanobis distance can be thought of as an improved version of Euclidean distance that accounts for both correlation and scale among features.

Manhattan distance is another common distance metric that is calculated by taking the sum of the absolute difference between data points.

Euclidean distance

Most people are familiar with Euclidean distance as it is what is used to calculate the hypotenuse of a triangle. The equation below is the generalized form of the Euclidean distance function for a n-dimensional feature space where x_i^a is the i-th feature of a given example A and x_i^b is the i-th feature of another example B that you are comparing against.

$$d(A,B) = \sqrt{\sum_{i=1}^{n} (x_i^b - x_i^a)^2}$$

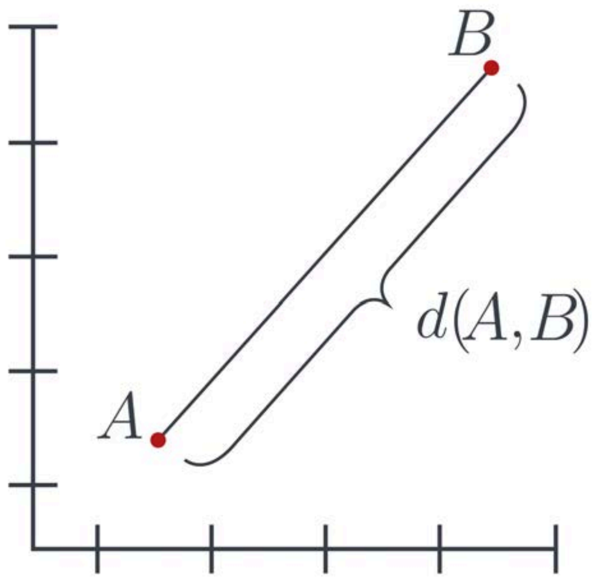


Figure 1. Euclidean distance.

Euclidean distance is straightforward to work with and familiar to most people., but it does not account for covariance and scale among features. If you want to account for these among features, you will need to use something more elaborate, such as Mahalanobis distance.

Mahalanobis distance

Mahalanobis can be thought of as an improved version of Euclidean distance in order to account for correlation among features and scale. Here, S is the covariance matrix. If S is the identity matrix, meaning that there is no correlation among any of the features, then Mahalanobis distance simply reduces to Euclidean distance.

$$d(A,B) = \sqrt{(\mathbf{x^b} - \mathbf{x^a})^T S^{-1} (\mathbf{x^b} - \mathbf{x^a})}$$

In the example below, even though the Euclidean distance between red/blue and between green/blue is the same, green would be considered a lot closer to blue in Mahalanobis distance, since it lies along the first principal component of the data set. The first principal component is basically the direction of the highest variance. Intuitively speaking, it is the direction where data is most stretched out. Principal component analysis is a useful technique under feature engineering, but it is outside the scope of this course. You are encouraged to read up on it when it is convenient for you.

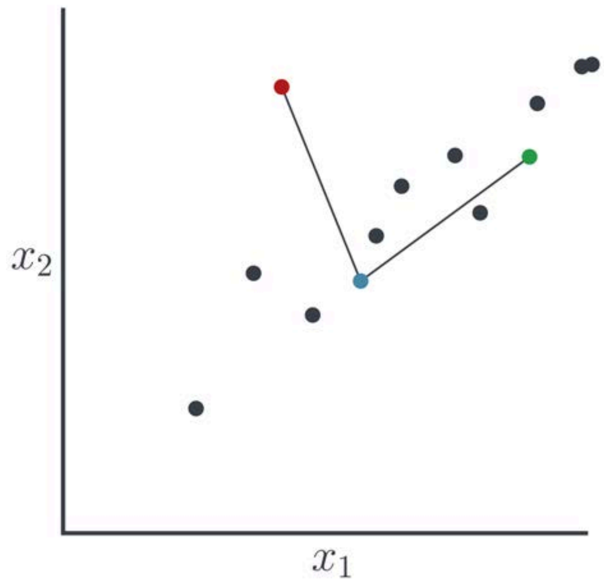


Figure 2. Mahalanobis distance.

Manhattan distance

Manhattan distance takes the sum of the absolute difference between each feature:

$$d(A, B) = \sum_{i=1}^{n} \left|x_i^b - x_i^a\right|$$

It is also known as the taxicab metric due to its likeness to the distance traveled in the city with grid layout, as depicted in Figure 3 below.

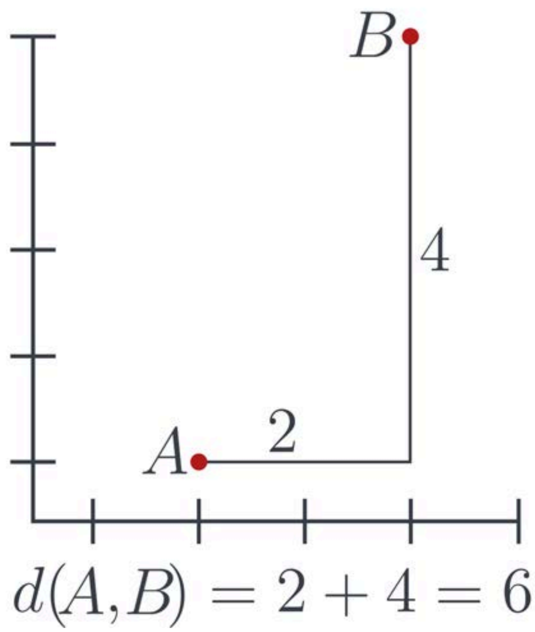


Figure 3. Manhattan distance.

Summary

The type of distance to use for a given problem can be determined based on domain knowledge, heuristics, or experimentation. Oftentimes, it is worthwhile to experiment with various distance functions to find the one that yields the best performance.

Back to Table of Contents

Assignment: Computing the Euclidean Distance

In this exercise, you will see how the Euclidean distance is used to find the k-nearest neighbors of an unlabeled example. You will write a function to find the Euclidean distance. In this assignment and for the remaining activities and assignments in this unit, you will work with a new data set called **Cell2Cell**, which is used to predict whether a customer will remain with its current telecom service.

This exercise will be graded.

When you finish your work:

1. Save your notebook by selecting the "Save and Checkpoint" entry from the "File" menu at the top of the notebook. If you do not save your notebook, some of your work may be lost.
2. Submit your work by clicking **Education —> Mark as Completed** in the upper left of the Activity window. 

3. This assignment will be auto-graded and can be resubmitted. After submission, the Jupyter Notebook will remain accessible in the first tabbed window of the exercise. To reattempt the work, you will first need to click **Education —> Mark as Uncompleted,** then proceed to make edits to the notebook. Once you are ready to resubmit, follow steps one and two.

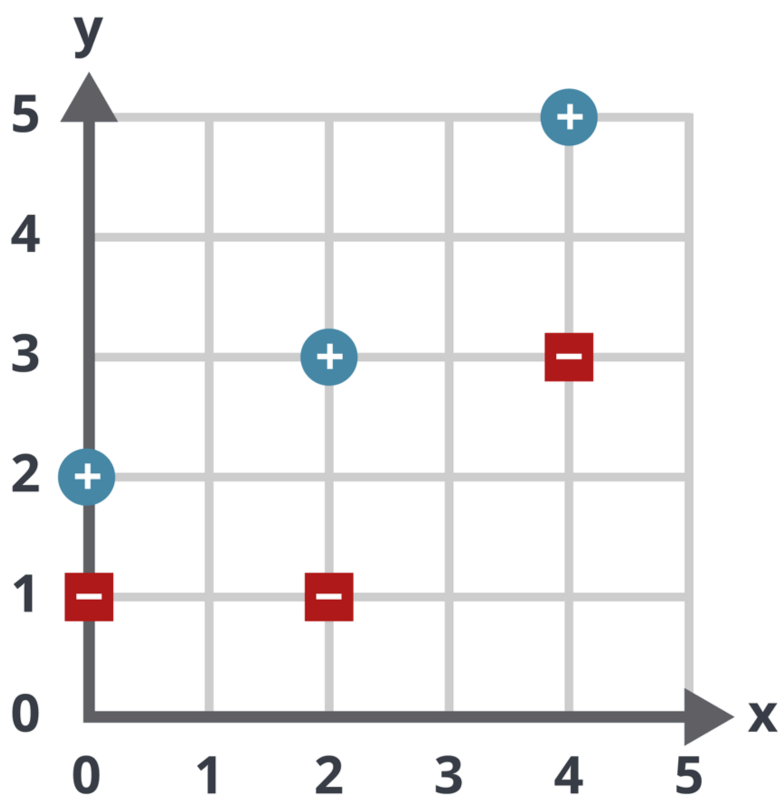
This exercise will be auto-graded.

Please complete this activity in the course.

Back to Table of Contents

Activity: Find a Decision Boundary

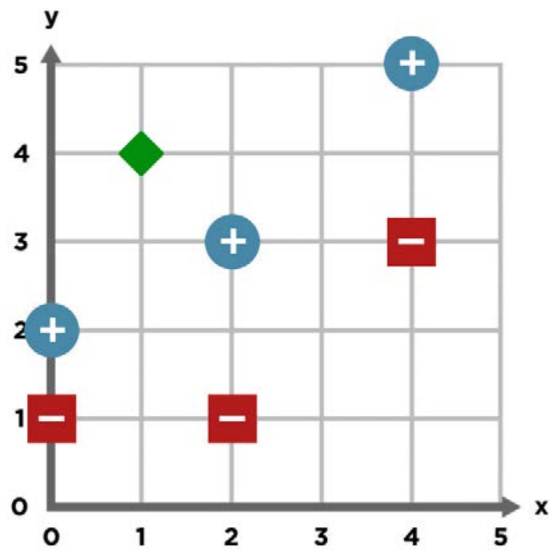
The KNN decision boundary is influenced by the number of nearest neighbors and the position of points from each class. In the case of binary classification using 1-NN (1-nearest neighbor), the decision boundary for a set of data might look like this:



Distance metric

Note that your choice of distance metric also influences the determination of the decision boundary: If you choose Euclidean distance as in the example above, the shortest distance between two points is along the line that connects them.

Alternatively, if you choose a different distance metric, such as taxicab (Manhattan) distance, you can only travel along vertical and horizontal axes, much like a taxicab driving through a city grid. For example, you need to determine the taxicab distance between the green diamond at (1,4) and the positive labeled data point at at (0,2) on the graph below. To get to the point (0,2) from (1,4), you have to take 2 steps down and one step left. Thus, the taxicab distance between these points is 3.



Determining the boundary by hand

One trick to finding the boundary for 1-NN (1-nearest neighbor) by hand is to find two points of opposite class that you suspect are near the boundary (e.g., the + at (2,3) and the - at (2,1)). Their midpoint (2,2) is likely to be on the boundary. You can continue to look for opposite-class pairs of points that are close together; this midpoint will also be on the boundary.

Activity instructions

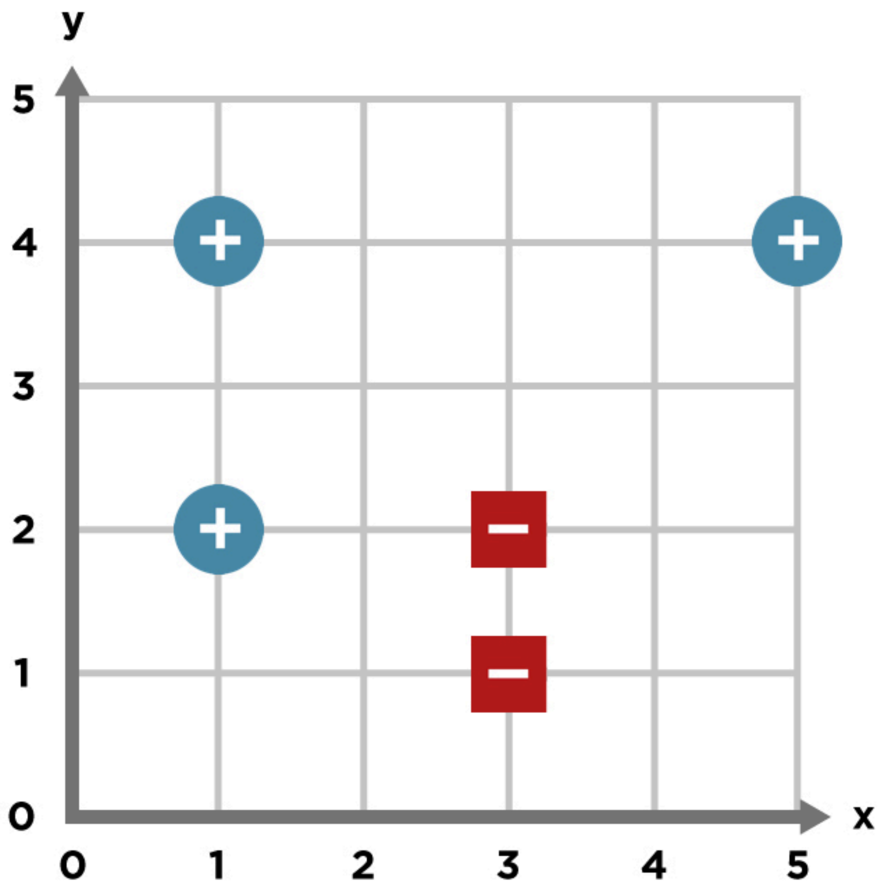
Suppose you have a data set and you want to draw a decision boundary. You have chosen to use 1-NN (1-nearest neighbor) and you will use the Euclidean distance metric. You have the following data points, strictly confined within a [0, 5] x [0, 5] grid:

- Class +: (1, 2), (1, 4), (5,4)
- Class -: (3, 1), (3, 2)

Answer the following prompts. When you are ready, click the **Show Solution** button below to reveal the answers.

1. Find the decision boundary for the data displayed in the graph below (using 1-nearest neighbor). You may find it helpful to plot these points out and draw the

boundary by hand.
2. How would a new test data point (5,1) be classified, given your decision boundary?



Hide SolutionShow Solution

Back to Table of Contents

Ask the Expert: Mehrnoosh Sameki on KNNs

So far we have been focusing on implementing KNNs for classification problems, but KNN can also be used to solve regression problems. In this video, Dr. Mehrnoosh Sameki compares regression KNN and classification KNN.

Note: The job title listed below was held by our expert at the time of this interview.

Mehrnoosh Sameki

Product Manager, Microsoft

Dr. Mehrnoosh Sameki is a Senior Technical Program Manager at Microsoft, responsible for leading the product efforts on machine learning interpretability and fairness within the Open Source and Azure Machine Learning platforms. Dr. Sameki also co-founded Fairlearn and Responsible-AI-widgets and has been a contributor to the InterpretML offering.

Can you compare KNN for regression vs. KNN for classification?

Video Transcript

The key differences are KNN regression tries to predict the value of the output variable by using a local average of the neighbors, and so it predicts a value by using the mean of the k-nearest neighbors. Versus in classification, the attempt is to predict the class to which the output variable belongs by computing the local probability. And so in that case, KNN classifier predicts a class by using the highest majority category among its k-nearest neighbors.

[Back to Table of Contents](#)

Watch: KNN Optimization

In most cases, machine learning algorithms need to be optimized based on the data you are working with. KNN is no exception. In this video, Mr. D'Alessandro will introduce the idea of hyperparameters. Hyperparameters are tunable parameters that are used to improve model performance. Mr. D'Alessandro also explains the idea of model complexity and how it relates to a model's ability to generalize, as well as the functionality of normalization and the effect it has on KNN's performance. You will discover what it means for a model to overfit and underfit in the context of model complexity.

Video Transcript

Every supervised learning algorithm has input parameters that control what we call the complexity of the model. These input parameters defined how flexible the model is in terms of its ability to fit small variations in the data. We'll generally refer to these input parameters as model hyperparameters, and the process of finding the best ones is called hyperparameter optimization. A model's complexity is its ability to adapt to small variations in the data. We run a hyperparameter optimization to choose a complexity that enables us to generalize the best. This idea of complexity is an incredibly important concept, and we'll discuss every algorithm through this lens. The main complexity parameter for k-nearest neighbors is usually just called K or the number of neighbors to be used for prediction. It is advisable to always spend some time to test different options for K and to find a value that is best for your data. There are other design parameters that are important to consider as well. We have choices for distance function, and even within a given function, we have the option to weigh each instance using some function of the distance. Another important design choice is normalization, which is a process to scale each feature so that they have similar magnitudes. We'll discuss why this is so important. As with all hyperparameters that control a model's complexity, we need to empirically test a range of options to see which performs the best. We'll cover exactly how to do this in a different lecture. This picture illustrates three different levels of K. On the left, we have a high value of K. Given a fixed set of data points, increasing K means using points that are farther away. We can see in the left-hand plot that the circle is so wide that we're mixing in too much of the different classes. At the most extreme case, the circle covers all points and we're just averaging over the whole data set. Using far away or unrepresentative points leads to what we call underfitting. Underfitting is when the model doesn't learn real nuances of the data, and we will also learn later that underfitting is associated with a type of error we call model estimation bias. On the right-hand side, we have a small value of K. This solves the problem we introduced with high K. We can see that within any small circle, the points are more likely to have similar labels, but at the same time, the predictions depend heavily on only a few points. When the data is noisy, which in this case translates to the different colored points being in the same circle, there was a high, random chance that the very closest neighbors to a point are there from the opposite class. This heightened sensitivity to just a few nearby points leads to what we call overfitting, and again, we'll show later that overfitting is associated with a type of model error called estimation variance.

The best option is likely to be somewhere in the middle, a smaller circle means the nearby points are likely to be representative of the example being predicted, but we want it to be large enough to not be too sensitive to just a few points. This idea of finding the middle ground will be common in a lot of algorithms we use. Next, let's discuss the idea of normalization and why it's important. Normalization would be a preprocessing step, so you wouldn't specify this when calling the scikit-learn KNN class. Normalization generally improves performance with this algorithm, so I highly recommend doing it. Let's use a simple Euclidean distance example to illustrate the point. In this case, we have age and income as features, and we're computing the distance between two points. Imagine the average age is 40 and the average income is 50,000. The two red arrows start from the same point and jump the same relative distance. The size of the arrows are misleading because each of these features are on different scales. But, in this case, moving 50 percent along the x-axis results in a distance value of 20, but on the y-axis, it is 25,000. So without normalizing, similar relative movements on features that have a larger scale will dominate the distance function. Let's also see this another way. Going from age 40 to 60 is pretty significant, but raising one's annual income by $20 likely isn't, at least for prediction purposes. With Euclidean distance, these changes are considered equivalent, so the bottom line is that features with higher scale will receive a higher implicit weight in KNN. The distance functions will be more sensitive to these features, sometimes to the point where other features don't even matter. This is generally undesirable, so we normalize to equalize each features contribution to the model. This process of normalization maintains the predictive properties of an individual feature, but changes its distribution. Again, we do this to ensure each feature has a similar scale of distribution, which results in them having equal importance in the distance function. Here is an illustration on how normalization affects the shape of the distribution. We can see that the new distribution is shifted, so its mean is zero, and it also has a lower variance, which is depicted by the width of the bell curves. When we normalize, we perform this shift and rescaling on each features so that the distributions look more like the orange plot here. After normalization, each feature would have a distribution similar to the orange one here, no matter its starting point. This process doesn't hurt the predictive performance because the normalized values still have the same correlation with the label.

[Back to Table of Contents](#)

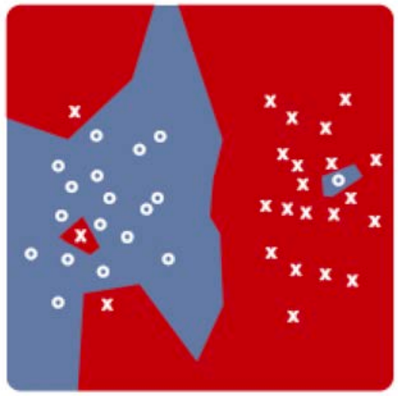
Techniques for Improving KNN

How can you improve the performance of a KNN model? To optimize KNN, you can experiment with different values of its hyperparameter K (the size of the neighborhood) to find the best model complexity and avoid underfitting or overfitting. You can also optimize KNN by choosing the appropriate distance function. You can even perform pre-processing steps to normalize each feature's contribution to the model, thus avoiding the pitfalls of a distance function weighing some features more heavily than others and resulting in certain features being "ignored." Below, you will see how choosing different values for hyperparameter K affects performance as well as some normalization techniques.

- **Hyperparameter optimization**
- **Normalization techniques**

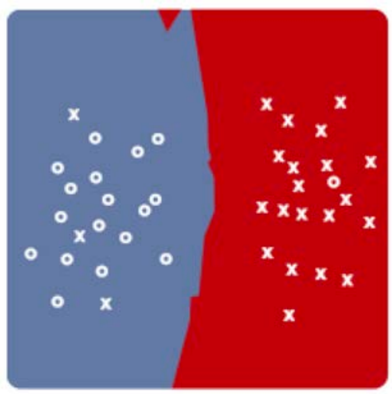
Hyperparameter optimization

As you will recall, a model's complexity defines how flexible a model is in terms of its ability to fit small variations in data. Hyperparameters are the configurable aspects of your model that can be adjusted to control model complexity and improve a model's performance. The KNN model has exactly one hyperparameter, and that is k, the size of the neighborhood that you pick to infer the label. The best choice of k depends on the specific data set. You typically choose odd numbers to avoid ties, especially with binary classification problems, though you can set k equal to any number. So what happens when you change k?



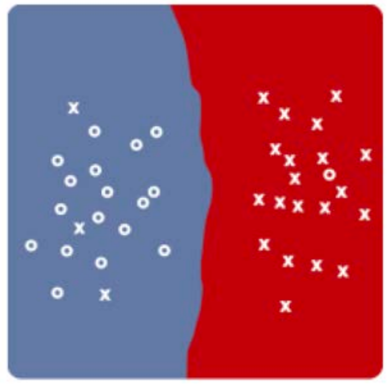
eucdist k = 1

The KNN decision boundary here for 1-nearest neighbor is actually quite rough and picks up on little movements in the data set. You might also see “islands” of misclassified and mislabeled examples, as KNN carves out regions around these mislabeled examples. If you suspect your data set is noisy, meaning some points are mislabeled in your data, 1-NN might be too sensitive to accurately generalize to future data.



eucdist k = 3

If you increase k to 3, you're now averaging local neighborhoods and the little “islands” get washed out as they are outvoted by the other examples. The complexity of the boundary decreases and becomes smoother with 3-NN.



eucdist k = 9

The decision boundary becomes smoother and less susceptible to noise as you increase k further. In this example, the decision boundary of 9-NN is well defined and even smoother than 3-NN. You may find, however, that 9-NN begins misidentifying significant groups of data points, which becomes more likely as you increase the number of neighbors used.

Normalization techniques

Some machine learning models are sensitive to the range of feature values; KNN is one such algorithm. For example, say you want to predict whether a loan will default based on a person's age and income level. A typical range for age will be between 18 and 100, while income level can be upward of thousands to hundreds of thousands. In this case, income level will have a much higher influence in our distance calculation than age does. In Figure 1, you would typically expect red and green dots to be considered closer to each other than blue and green. Yet based on un-normalized values, our distance function determines that blue and green are actually closer than red and green.

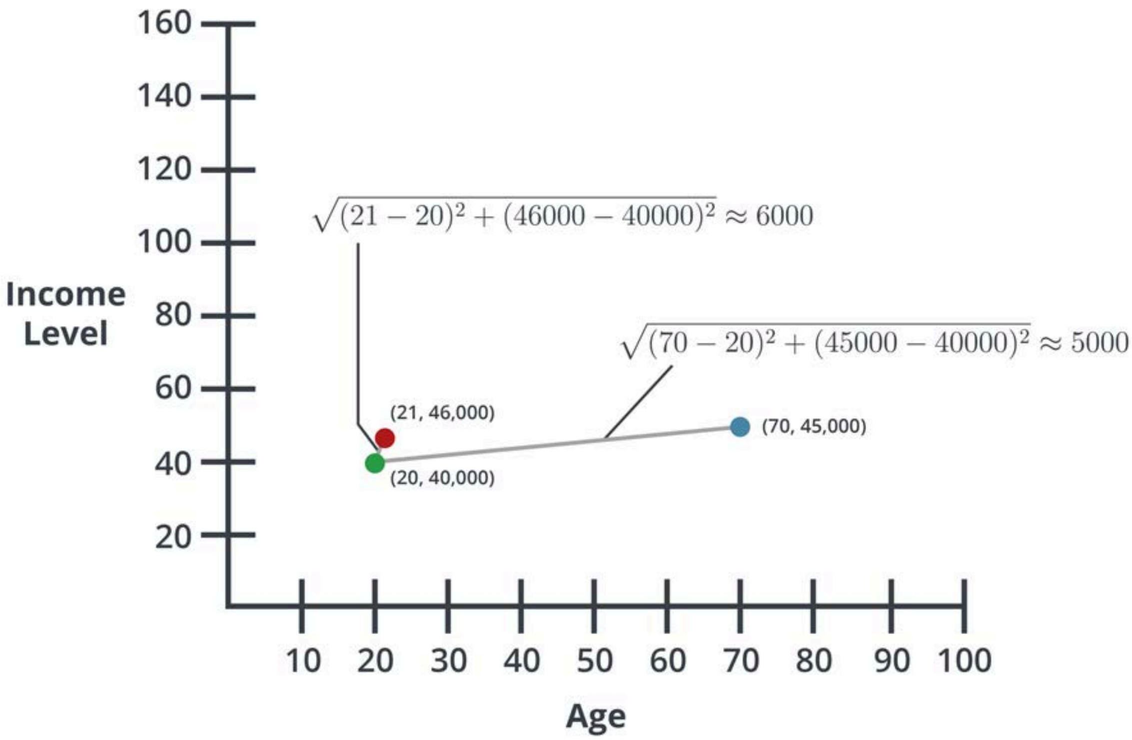


Figure 1. Loans with two features: age and income level.

To combat the behavior illustrated above, introduce the technique of normalization. Normalization essentially transforms the values of features into the same scale. This allows distance function to give equal weight to each feature. The two most common normalization techniques are standardization and min-max normalization. (Note that some literature uses normalization interchangeably with min-max normalization.)

Standardization

In standardization, you transform the values within a feature to have a mean of zero and a standard deviation of one. You do this by subtracting the mean for each feature then dividing this by the feature's standard deviation. Another name for standardization is standard scaler. Standard scaler typically works well with features that follow normal distribution and are less sensitive to outliers.

$$x_{i,\text{normalized}} = \frac{x_i - \overline{x}}{\sigma}$$

where $\overline{x}$ is the mean and σ is the standard deviation.

Min-max normalization

In min-max normalization, you transform the values within a feature to be between certain min/max range. Here, subtract the min value of the feature from the example then divide this by the range of the feature. Another name for min-max normalization is min-max scaler. Min-max normalization typically works well with features that don't follow normal distribution and are more sensitive to outliers.

$$x_{i,\text{normalized}} = \frac{x_i - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$

Summary

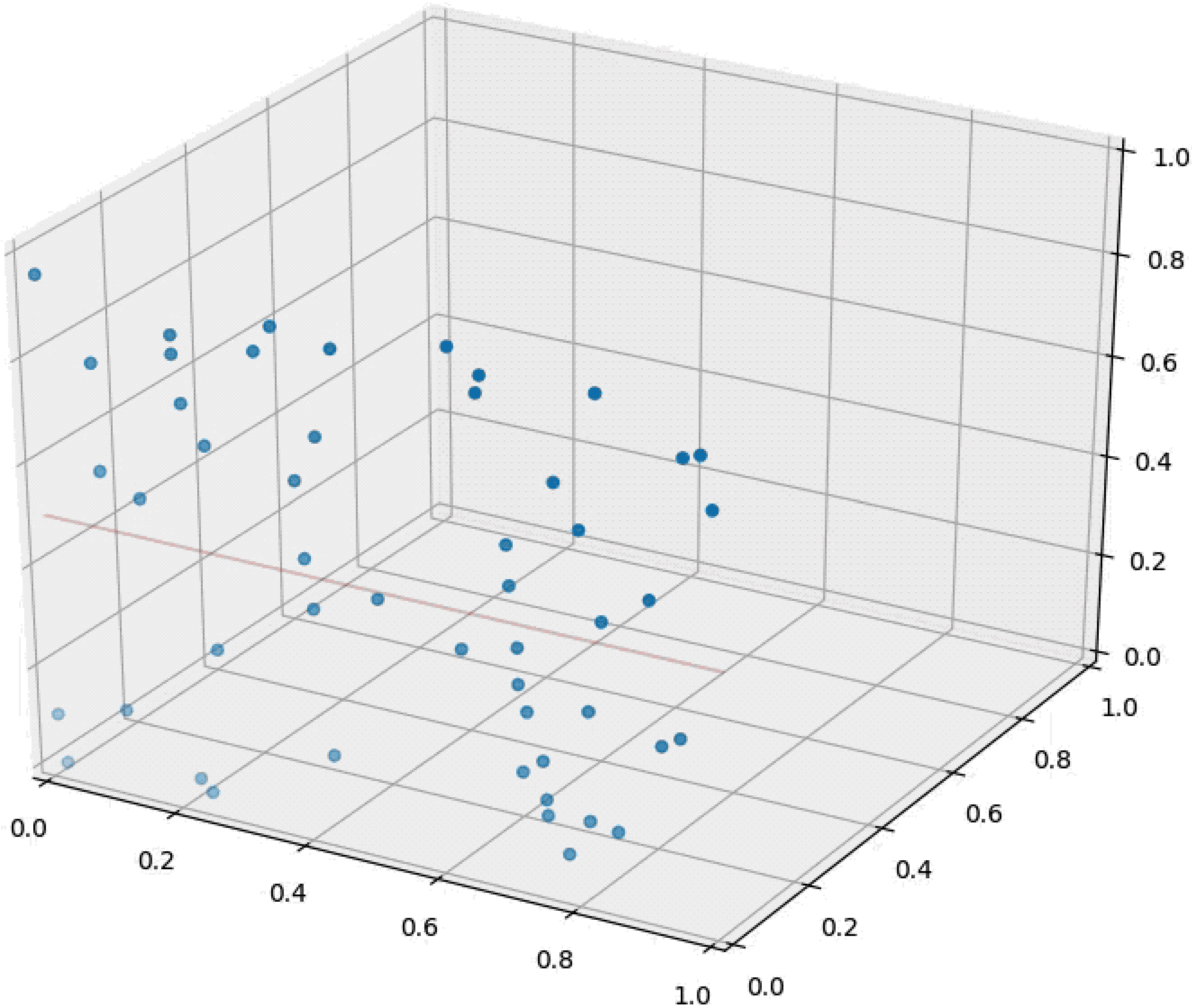
Many machine learning algorithms perform better when features are normalized. The two most common normalization methods are standardization and min-max normalization. While it is possible to implement these normalization methods from scratch, scikit-learn comes prepackaged with StandardScaler class and MinMaxScaler class for such purpose.

Back to Table of Contents

Read: The Curse of Dimensionality

High-dimensional data is data that contains a large number of features. Note that when referring to the number of dimensions, you are referring to the number of features. High-dimensional data is a particular challenge for the KNN model. As the number of dimensions increases — that is, as you include more and more features in your data set — all of your data points (or examples) become more unique and less similar to one another. Eventually, your data points are so dissimilar that the approach of finding close neighbors to predict the label of a test data point is no longer feasible. This is known as the curse of dimensionality.

To better appreciate this behavior, visualize how the high dimensionality impacts your data set. The animation below shows what happens to examples with two dimensions after adding a third dimension. This data set is randomly sampled, but a similar effect can be observed on real-world, correlated data.



In this example, let the true classification boundary be the red line (plane). Points above it are positive, and points below it are negative. Knowing this boundary, you know that the only real feature that matters is the vertical axis.

If you developed a KNN model for the data set with two dimensions, you could run it on a test data point near the boundary but still above the line. This test data point may have several close neighbors, all positive, and several nearby-but-less-close neighbors that are negative. The algorithm could predict that this data point is positive without much difficulty.

Upon adding the third dimension, however, suddenly all its neighbors are farther apart. Say you are classifying a data point just above the center of the cube. Its closest neighbors may change; suddenly, a negative data point that used to be farther away — but happened to be relatively close to your test data point along the new axis — might be the closest data point.

In general, when increasing dimensions, data points become farther away from each other and the distances between data points all become larger and less distinguishable. As the data points expand along the third dimension, their relative pairwise distances increase, but the distance to the red plane (initially a line in 2D) stays constant. This is a typical behavior in high dimensions, as randomly sampled data points in high dimensions tend to be spread out from each other (with roughly equal distances) but comparably close to separating hyperplanes.

Back to Table of Contents

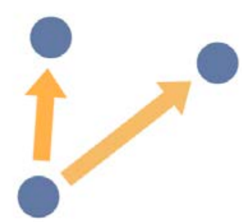
Enhancing KNN

The KNN model can be enhanced in a number of ways.

Resolving ties

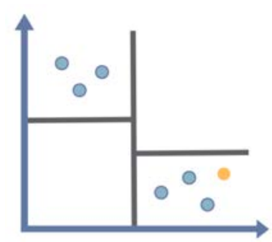
There can be cases without a unique most common label. For example, if k=4, you could retrieve two neighbors of one class and two of another. To avoid this, you typically pick odd values of k. Even in those cases (e.g., k=3), however, your neighborhood vote may result in a tie. For example, the image to the right shows our test point (a red star) and three neighbors, all from different classes. A common approach to resolve ties is to fall back onto the majority label within the k-2 closest neighbors. In the scenario on the right, since 3-NN would result in a tie, you can fall back to 1-NN and get a definitive label.

Choosing distance function



The distance function is a critical component of KNN and has a major impact on the "neighborhoods" derived from your data; how you determine the distance between two points is critical to the accuracy and performance of your classifier. Using the Euclidean distance (also known as L2 distance) with KNN is common but may be suboptimal in some settings where features follow particular structures (e.g., are normalized). Depending on your data set, there may be more suitable distance metrics, such as the L1 (taxicab) or Minkowski distance.

Data structure for speedup



One downside of KNN is that during test time, you have to compute distances from each test point to every training point. This process becomes more intensive and slower as you increase the size of the data set. One way to speed up KNN is to use data structures such as k-d trees or ball trees. In this example, you see a k-d tree structure that splits the data space into boxes. If you are trying to find the nearest neighbors for the yellow test point in the lower box, rather than computing the distance from our test point to all of the points in the upper box, you simply compute the distance to the box containing those points. You can very quickly determine that the upper box is further away than points closer to our test point, thereby ruling out any points contained in that upper box with a single calculation. Note that Scikit-learn uses this technique when fitting a KNN model.

Back to Table of Contents

Assignment: Optimizing KNN

In this exercise you will implement a KNN classification model using scikit-learn. You will train different models using different values for hyperparameter K and compare the accuracy of each model.

This exercise will be graded.

When you finish your work:

1. Save your notebook by selecting the "Save and Checkpoint" entry from the "File" menu at the top of the notebook. If you do not save your notebook, some of your work may be lost.
2. Submit your work by clicking **Education —> Mark as Completed** in the upper left of the Activity window. 

3. This assignment will be auto-graded and can be resubmitted. After submission, the Jupyter Notebook will remain accessible in the first tabbed window of the exercise. To reattempt the work, you will first need to click **Education —> Mark as Uncompleted,** then proceed to make edits to the notebook. Once you are ready to resubmit, follow steps one and two.

This exercise will be auto-graded.

Please complete this activity in the course.

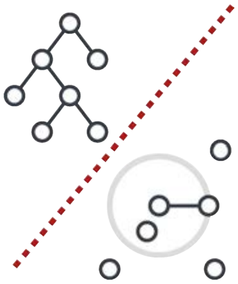
Back to Table of Contents

Module Wrap-up: Implement K-Nearest Neighbors

In this module, you explored the KNN supervised learning model and its underlying concepts. Mr. D'Alessandro explained the different distance functions that can be used with the KNN algorithm and you learned how to optimize a KNN algorithm for performance. You saw an example of KNN in practice using the Iris data set and you implemented your own KNN algorithm using the cell2cell data set.

Back to Table of Contents

Module Introduction: Implement Decision Trees



KNN is one of the simplest machine learning algorithms, and while it can be very useful, KNN can take a long time to make predictions on larger data sets. Splitting your data set into partitions can improve the speed of computation. You can accomplish this by using another common supervised learning algorithm: decision trees.

In this module, Mr. D'Alessandro introduces decision trees. As is the case with KNN, decision trees can be used for both regression and classification problems. You will focus on how to apply them to classification problems. In addition, you will have the opportunity to investigate how to partition the data into a tree that minimizes training error. You will also explore techniques to avoid overfitting and underfitting to the training data while maximizing your model's accuracy.

Back to Table of Contents

Watch: Information Theory Overview

In this video, Mr. D'Alessandro introduces another very popular and versatile machine learning algorithm: decision trees. In order to understand decision trees, you will first need to examine how information theory is used in the training of a decision tree. Mr. D'Alessandro also explores how information gain and entropy are used to build decision trees.

Video Transcript

Decision trees are one of the most useful algorithms in the machine learning toolkit. They have a lot of high performing properties on their own, but they're also a fundamental building block for some of the most widely used algorithms in practice. This idea of building blocks will be important, particularly in the study of decision trees. If full tree itself is built using a recursive algorithm. Once we understand the base step, we can essentially understand the entire process. At the root of decision, trees are some powerful formulas that come from a field of study called information theory. These two formulas are called entropy and information gain. These formulas are useful on their own, but they are instrumental in how decision trees are built. We'll start with entropy because this is the more fundamental of the two concepts. Here is a conceptual description along with the actual formula. First, let's start with a discrete random variable. This is the same as a categorical variable. Here are two examples of a variable with four values in different distributions. The bars just show the relative distribution across the four values. One way to think about entropy is it's a measure of dispersion or uncertainty of a discrete random variable. In the formula, each discrete value of the variable would have an associated probability or P, which is represented by the bar height. The total entropy of the variable is the sum of each P times the logarithm of P. The top chart is actually the highest entropy you can measure. This is a uniform distribution over the four values. We say this has the highest uncertainty because predicting where a particular example falls is as good as guessing at random. The bottom is different. We see more mass towards the middle two values. If you were to draw a random example and had to bet its value, you'd be better off betting one of the two middle values. Here, we quantify the entropy of each example and using the entropy formula. For each distribution, focus on the labeled probabilities. Our entropy formula again is a sum of these probabilities multiplied by their own logarithms. The negative sign means this will be a positive number and a higher number means more entropy. The upper chart is uniform or equal probability for each value. When this occurs again, we have maximum entropy. The other extreme is when all examples have the same value. This would have an entropy of zero. We often don't use entropy on its own. Instead, we use it to compute a quantity called information gain.

In words, information gain is a way to measure how much average entropy changes after we segment our data. I'll explain the motivation behind the segmentation later. For now, I want to emphasize the actual formula. We will use H as our function for entropy. The first term represents the entropy on a variable Y on a sample of data. I changed the formula to use Y instead of X here because I want to start thinking of computing entropy and information gain on a label that might be used for supervised learning. In the right-hand side of the equation, the C stands for child and represents a separate segment of the data. I use this notation of parent and child because we are building up the foundations for decision tree, and I want to use the notation common with tree based structures. Let's next assume we split the data into two or more partitions, again, with each partition being called a child of the original data. The second term is essentially a weighted average of the entropy of each partition, with the weights proportional to the amount of examples in each partition. Now, let's illustrate this graphically, this time using scatter plots that are related to binary classification. The left-hand side represents the full data: We call this the parent. The title shows the proportion of points that belong to the positive class, represented by green points, as well as the computed entropy. Now let's say we split the data into two parts to produce the plots on the right. These are what we would call the children of the parent. Notice in total, we have the same exact points, but they're organized in a specific way. To compute the information gain, we compute the entropy of each child and take a weighted average, where the weight is the proportion of points in the child. The difference between the parent entropy and this weighted average is the information gain. The most important concept is not the math here, though. Notice how in each of the children, we have a higher concentration of a specific class label. Ideally, we want the average value of Y in a child partition to be as close to zero or one as possible. When this happens, we say that the node has more purity. From a guessing perspective, imagine you had to place a bet on the value of Y for a randomly chosen point. Absent any information, your accuracy would be as good as the average value of Y on all the data. But, imagine someone gave you a piece of information. This information is the segment you sample the point from amongst the child partitions. With that information, you are guessing accuracy would dramatically increase. We call this increase in certainty the information gain, and this exact step is the base building block of decision trees.

Back to Table of Contents

Read: Information Theory Formalized

Information theory is widely utilized in the implementation of decision tree classifiers. The core concepts of information theory revolve around the idea of entropy and information gain, both of which relate to the idea of uncertainty. When building a decision tree, we want to reduce the entropy, or uncertainty about the data, and increase the information gain. You'll explore these concepts in greater detail and how they contribute to the construction of a decision tree.

☆ **Key Points**

Entropy measures the uncertainty of a random variable, with the highest uncertainty being 1 and the lowest uncertainty being 0 when the random variable is binary.

Information gain measures how much entropy has reduced once a certain condition has occurred.

Information gain in the context of a decision tree measures how much entropy has been reduced when a data set is split by some feature value.

Entropy

Entropy is a metric in information theory that is a measure of the uncertainty of a random variable. Entropy is low when the value of the random variable is predictable, and entropy is high when the value is unpredictable.

Let's consider an example. For a random variable y with n possible values, the formula for the entropy of y is:

$$H(y) = -\sum_{i=1}^{n} P(y_i)\log_2(P(y_i))$$

If the variable is a binary variable (the variable can have one of two possible values), the range of entropy is between 0 and 1. If there is no uncertainty about the value of the variable, the entropy is 0. If the variable has an equal chance of possessing either value, the entropy is 1:

$$\log_2(\text{number of possible values}) = \log_2(2) = 1$$

Let's demonstrate this with a coin toss. A fair coin toss has an entropy of 1 since the coin has an equal chance of landing on heads or tails. On the other hand, a coin toss that is somehow rigged to always result in heads has an entropy of 0 since you already know the coin will land on heads.

Mathematically, this can be explained by the entropy equation, where n is the number of values of y (two possible values: heads or tails), $H(y)$ stands for the entropy of the coin toss, and $P(y_i)$ is the probability of tossing the ith value of y (heads or tails):

$$
\begin{aligned}
H(y) &= -\sum_{i=1}^{n} P(y_i)\log_2(P(y_i)) \\
&= -\Big(P(y_1)\log_2(P(y_1)) + P(y_2)\log_2(P(y_2))\Big) \\
&= -\Big(P(\mathrm{heads})\log_2(P(\mathrm{heads})) + P(\mathrm{tails})\log_2(P(\mathrm{tails}))\Big)
\end{aligned}
$$

For a fair coin toss, there is a 50% chance of landing on heads and a 50% chance of landing on tails, so the entropy is calculated as follows:

$$H(y) = -\Big(0.50 \cdot \log_2(0.50) + 0.50 \cdot \log_2(0.50)\Big) = 1$$

If you have a coin toss that has a 30% chance of landing on heads and 70% chance of landing on tails, then the entropy is:

$$H(y) = -\Big(0.30 \cdot \log_2(0.30) + 0.70 \cdot \log_2(0.70)\Big) \approx 0.88$$

For a coin toss that always lands on heads, there is a 100% chance of landing on heads and a 0% chance of landing on tails, so the entropy is:

$$H(y) = -\Big(1 \cdot \log_2(1)\Big) = 0$$

Below is a plot of the entropy of the binary random variable y as a function of the probability of one possible outcome for y. In this case, it is the probability that y is heads. Note that the graph would be the same for $P\,(tails)$.

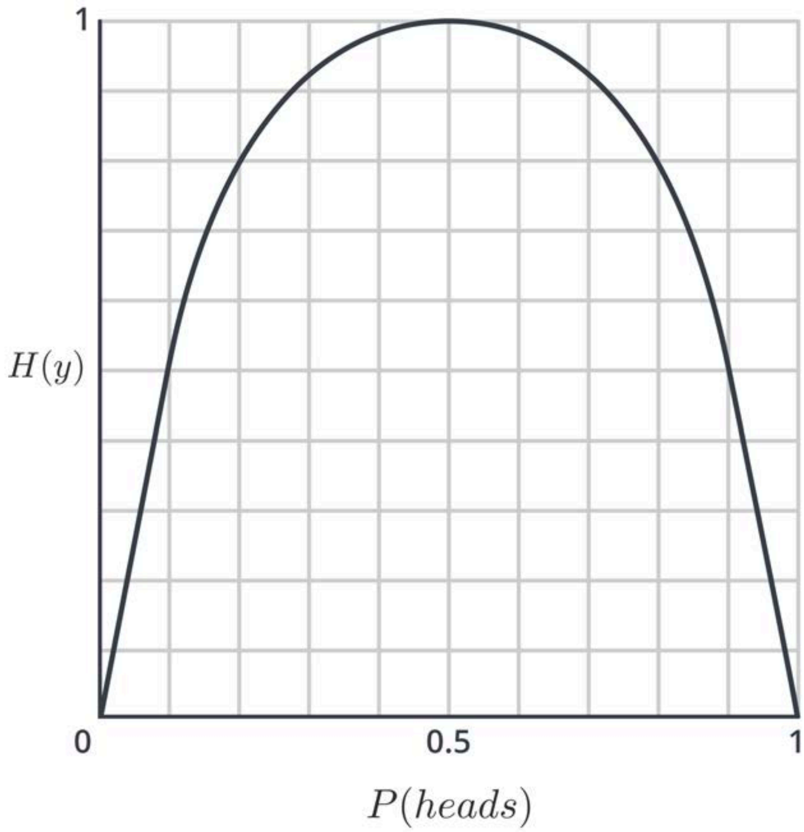


Figure 1. Entropy curve.

In the context of our coin toss example, the graph shows that entropy is lowest when the coin toss is rigged to always land on heads. The entropy is highest when the coin toss is fair and there is an equal chance of landing on heads or tails.

You can also think of entropy in terms of the entropy of a collection of data. Entropy is the measure of disorder, or impurity in a data set. Let's consider a data set consisting of binary variables. Just as is the case with one binary variable, the entropy of a set consisting of many binary variables is 0 when there is no uncertainty as to the value of each variable. It is the least disordered set possible. On the other hand, the entropy is 1 in a set in which there are equal members of both classes. This set is as disordered as possible. The higher the entropy, the harder it is to draw any conclusions about the data.

Training a Decision Tree

The entropy metric is used to build a decision tree during training. Let's demonstrate this by building a binary classification decision tree. Our training data set will contain two features (x_1, x_2) and one binary class label. Note how the training data set is depicted in Figure 2; it contains ten examples and each example has a class label that is either red or blue. There is an equal amount of blue and red examples.

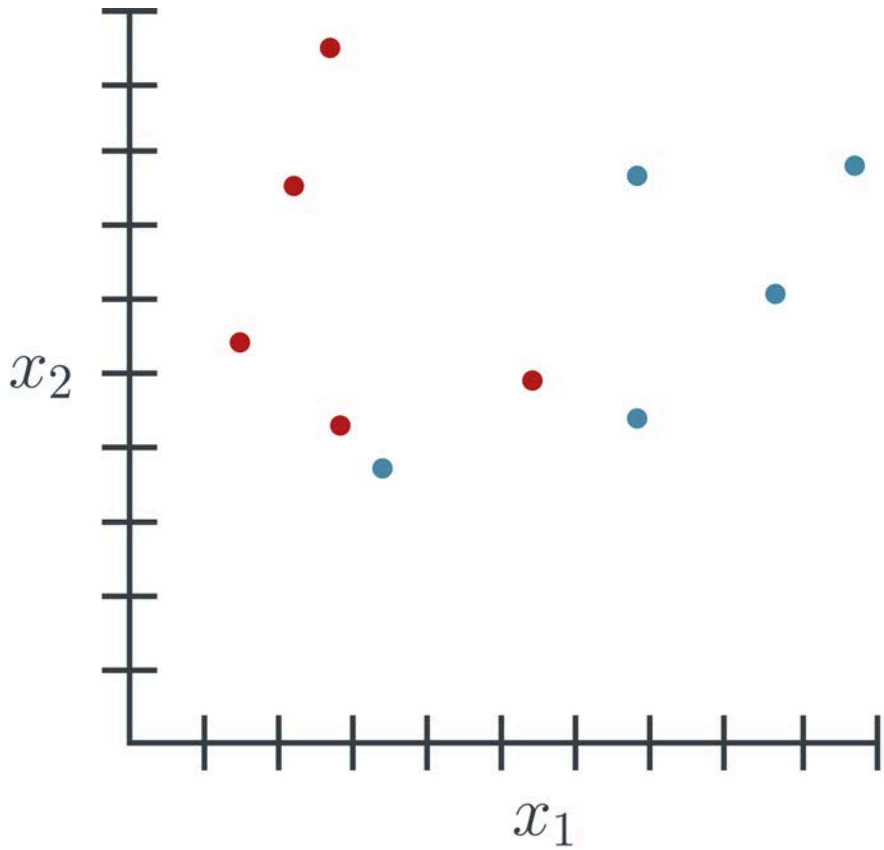


Figure 2. A training set with five red labels and five blue labels.

Without considering the positioning (feature values) of the examples, the only information we initially have is that half of the examples are red and half of them are blue. Therefore, the probability of randomly selecting an example out of the data set that is red is 50% and the probability of randomly selecting an example that is blue is also 50%. Going back to our entropy formula, we can compute the entropy of this data set to be 1 - the maximum amount of entropy:

$$
\begin{aligned}
H(y) &= -\Big(P(\text{red})\log_2(P(\text{red})) + P(\text{blue})\log_2(P(\text{blue}))\Big) \\
&= -\left(\frac{5}{10}\log_2\left(\frac{5}{10}\right) + \frac{5}{10}\log_2\left(\frac{5}{10}\right)\right) \\
&= 1
\end{aligned}
$$

The intuition behind building a decision tree during training is to reduce the uncertainty of our data set by finding the features that provide us with the most information about the class label then partitioning the data according to those features. We will effectively group examples into regions (or nodes) of the same class, thereby reducing the overall entropy of the data. In our case, we will group examples into one region in which the examples are primarily red and one region in which the examples are primarily blue.

To partition our examples into nodes, a decision tree "draws splits" based on a selected feature and a value for that feature. The aim is to split on the feature and its value that results in the lowest entropy of the new nodes. In Figure 3 below, we explore two split options and consider the reduction in entropy. The first option is to split by $\boldsymbol{x_2 = 7}$, creating two nodes of high entropies, whereby each node still has the same number of blue and red examples. The second option is to split by $\boldsymbol{x_1 = 6}$, which is a much better option as it creates a node where most examples are red and a node where all examples are blue.

Evidently, Option 2 is better as it reduces entropy by a large amount. The amount of entropy reduced is called the information gain. Information gain compares the entropy of the data set before and after the split; it tells us how much reduction in entropy (or uncertainty) has taken place. The more the entropy was reduced, the higher the information gain.

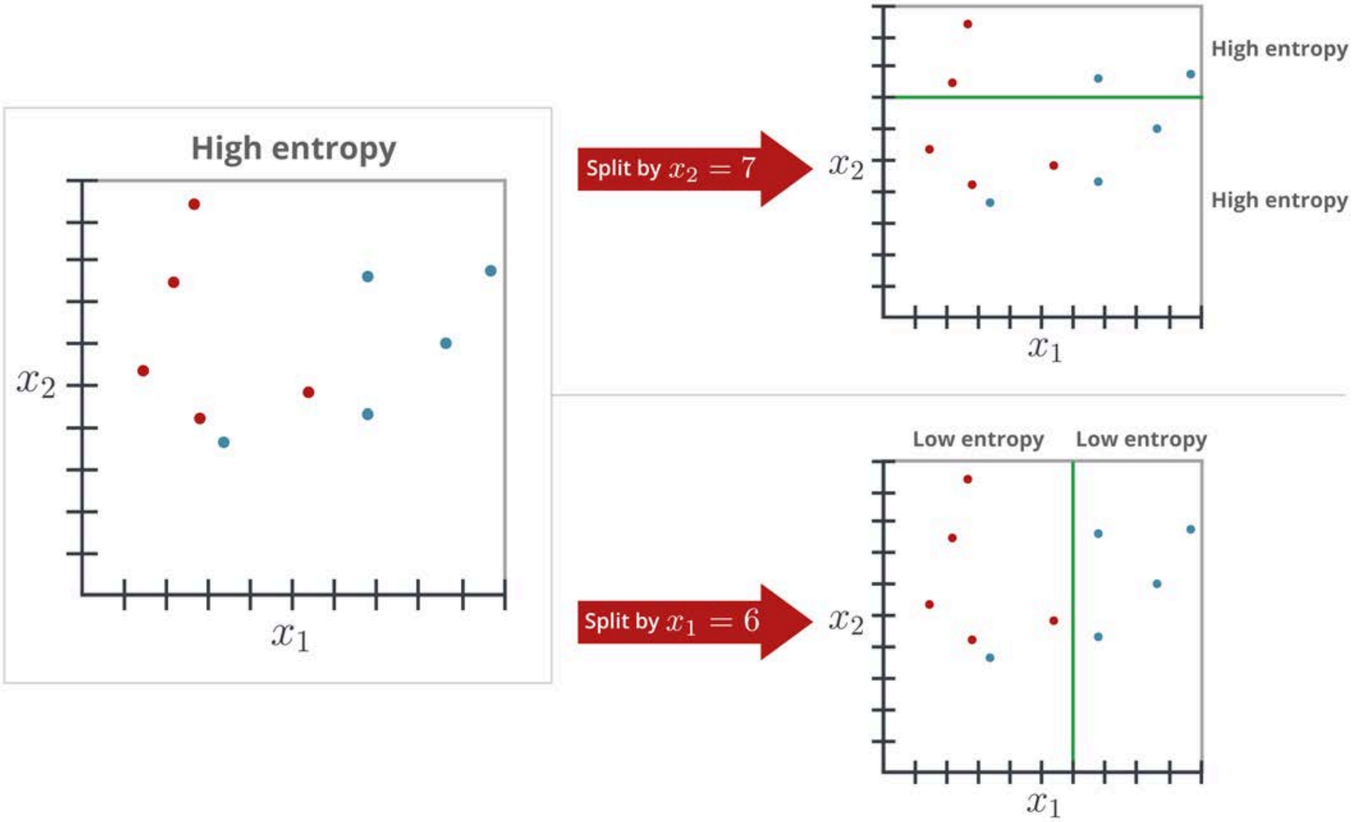


Figure 3. Two example splits to construct a decision tree.

Information gain

Comparing the information gain after splitting on different features and their values will help determine which feature to use to partition the data. We can view the information gain as determining how much information each feature provides about a class, thereby choosing the best feature and value to split on. As the information gain increases with each split, we can say that we have more information about the data set. The information gain value also lies within the range of 0 to 1.

The formula used to compute the information gain from one or more splits is as follows:

$$\begin{aligned} \mathrm{IG} &= \textbf{parent entropy minus the weighted average of child entropy} \\ &= H(y|\text{parent}) - \overbrace{\sum_{c \in \mathcal{C}} r(c) H(y|c)}^{\text{weighted average}} \end{aligned}$$

In the information gain formula, the symbols have the following meaning:

- $H(y|\text{parent})$ is the entropy of the parent prior to a split.
- $\mathcal{C}$ is the collection of child regions c created by a split.
- $r(c)$ is the ratio of the number of examples in a child region c divided by the number of total examples in the parent region prior to a split.
- $H(y|c)$ is the entropy of the examples within a child region c created by the split.

We essentially compute the information gain by:

1. Finding the entropies of each child node weighted by the proportion of examples from the parent node that are contained in the child node
2. Adding the entropies of the child nodes
3. Subtracting the entropies from the original entropy of the parent node

Let's demonstrate this with our binary decision tree classifier. We determined that splitting on $x_1 = 6$ was better than splitting on $x_2 = 7$. We came to this conclusion by computing the information gain of the split. Let's consider the result of the split by inspecting Figure 4 below. It shows the two child nodes c_L and c_R that were created after splitting on $x_1 = 6$. The node c_L contains examples in which their feature value for $x_1 < 6$ and the node c_R contains examples in which their feature value for $x_1 > 6$.

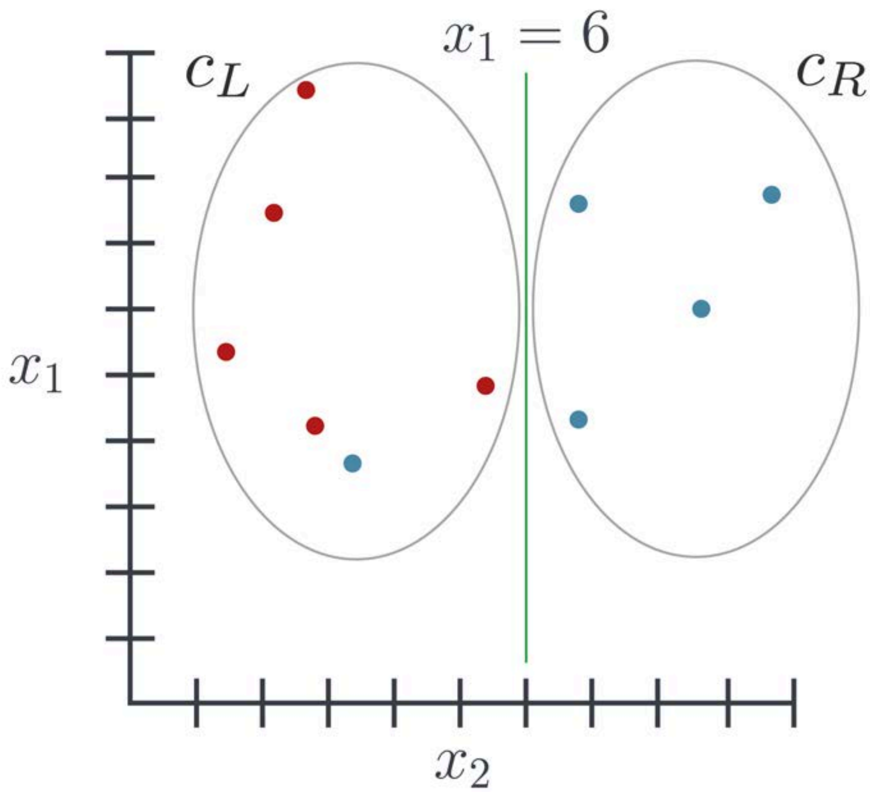


Figure 4. Split by $x_1 = 6$ to create two child regions.

Let's look at the information gain formula for our binary tree example in which we made one split. This is particularly useful, as most decision trees are constructed as binary trees.

$$\text{IG} = H(y|\text{parent}) - r(c_L)H(y|c_L) - r(c_R)H(y|c_R)$$

The symbols in the formula have the following meaning:

- $H(y|\text{parent})$ is the entropy of the parent prior to a split.
- c_L and c_R are the two child regions created by a split where L and R denote the left and right nodes.
- $r(c_L)$ and $r(c_R)$ are the ratios of the number of examples in c_L and c_R, respectively, divided by the total number of examples of the parent prior to the split.
- $H(y|c_L)$ and $H(y|c_R)$ denote the entropy of child regions c_L and c_R after the split.

Using the information gain formula above, let's compute the information gain for the split $x_1 = 6$:

$$H(y|\text{parent}) = -\left(\frac{5}{10}\log_2\left(\frac{5}{10}\right) + \frac{5}{10}\log_2\left(\frac{5}{10}\right)\right) = 1$$

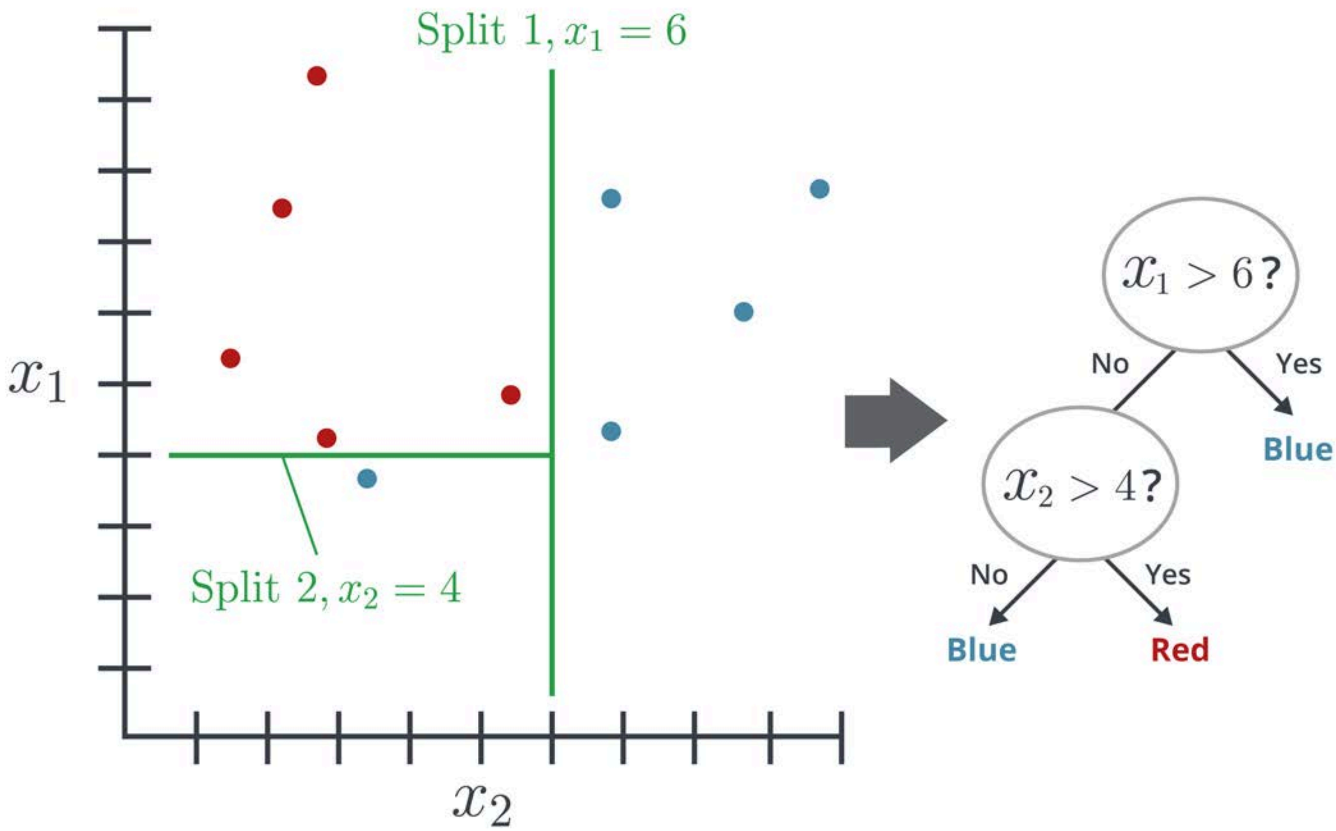
$$r(c_L)H(y|c_L) = \frac{6}{10}\left(-\left(\frac{1}{6}\log_2\left(\frac{1}{6}\right) + \frac{5}{6}\log_2\left(\frac{5}{6}\right)\right)\right) \approx 0.39$$

$$r(c_R)H(y|c_R) = \frac{4}{10}\left(-\frac{4}{4}\log_2\left(\frac{4}{4}\right)\right) = 0$$

$$\text{IG} \approx 1 - 0.39 - 0 = \boxed{0.61}$$

Based on the split above, we arrive at an information gain of 0.61, which is a fairly high number considering the highest possible information gain is 1.0. We can keep this split and continue building our tree.

To complete our decision tree, we will make one more split, as illustrated in Figure 5 below. After this split, our data has an information gain of 1.0 and therefore an entropy of 0.0. Our data is now pure; there is no uncertainty at any node as to which class the data belongs. Now that we have our decision tree classifier, we can use it to make class predictions for new, unlabeled data. In order to make a class prediction for a new, unlabeled example, we can just traverse down the tree. First, we can look at the value of its x_1 feature. If x_1 is greater than 6, we can classify the new example as blue. If x_1 is less than 6, we would then look at the value of its x_2 feature to determine whether the new example can be classified as red or blue.



For our very simple training data set consisting of ten examples, we only needed two splits to completely separate the examples. In practice, however, there can be thousands of examples in our training data and consequently many splits will need to be drawn.

Summary

Entropy and information gain allow you to find the best splits in your features in order to construct a decision tree. There are other criteria for splitting, such as Gini impurity and Chi-square, although information gain is the most commonly used.

Back to Table of Contents

Watch: Building a Decision Tree

Now that you have a better understanding of the basics of information theory, you are prepared to explore building a decision tree. In this video, Mr. D'Alessandro shows you the inner workings of a decision tree and how you can construct such a tree by splitting data that maximizes information gain.

Video Transcript

Now we're going to cover the fundamental steps of a decision tree. This involves taking a base segment and finding a split of the data that maximizes our information gain. We'll start with data representing a binary classification problem with just two features. Our ultimate goal is to split the data into as many partitions as we think is necessary to get the best cumulative information gain. So let's start with the basic structure of a partition. This is deliberately simple. At each step, we only want to split the data based on a single feature. This process looks like the diagram. The code shows a simple Boolean operation. If the example feature is greater than some value k, then we split to the right node. Otherwise, we split to the left. To build a good predictive model, we want to find both features and values of k that lead to the best possible increases in information gain. So the base step in the decision tree algorithm is to determine which feature to split on and what is the best split value k. The process used to answer this question is illustrated in the picture. It is somewhat of a brute force approach. We loop through each feature and range of split values for each of the features. In this case, let's assume we are using age and income to predict whether someone might default on a credit card loan. So this is binary classification with two input features. For each feature we find the split value that maximizes the information gain for that feature. This is represented by the red lines. Then we look at the feature that produces the maximum information gain. In this case, it is the left-hand side or the feature representing age. At this stage, our full sample of data has been split into a left and a right partition.

The next step is to loop through each of these partitions and apply the same exact algorithm to each partition. This would leave us with a set of partitions that look like this chart. In our first split here we split using the age feature. Now within each of the new partitions, we find we get the highest information gain with income, so we split on that. But notice how each partition splits at a different value of the feature. That's because each of these later partition steps are completely independent of each other. Our decision tree building algorithm will continue running this splitting process until some termination criteria is met. Those specific criteria are actually the input parameters we'll give to the scikit-learn when we initialize the decision tree class. The process we illustrated so far can be represented as a tree. This is of course where we get the phrase decision tree. This tree represents the conditions we use to split at each node and some key stats in each node. In this example, the f and t's represent whether the Boolean condition was met. Remember these are Boolean statements on the features. P of y here represents the average value of the label in each node. For binary classification, this is just the probability of having a positive label in that partition. When it is time to make a prediction, we follow a simple process. Starting from the top, we evaluate the new example against the splitting logic. We proceed down the tree until we reach a terminal node. The prediction here is just the average of the label at the terminal node. Since this example is a classification problem, the prediction is a probability which can be used as is or converted to a binary class prediction. You can see here that without a model, our best guess about the expected value of the label would be about 20 percent. This corresponds to the average value of the label in the dataset, which is represented in the top node. But with our well-learned tree guided by increasing information gain, we can guess that the expected value is 95 percent. Assuming this tree generalizes well, the accuracy of this prediction would be much higher thanks to this process.

Back to Table of Contents

Quiz: Check Your Knowledge: Entropy Scenarios

In this quiz, you will calculate the entropy to determine how to build the most effective decision tree given a specific scenario and data set.

Scenario

Imagine you are building a decision tree to predict whether a personal loan given to a person would result in a **payoff** (i.e., the person pays off the loan) or **default** (the person fails to pay back the loan).

- Your entire data set consists of 30 examples:
  - 16 belong to the "**default**" class.
  - 14 belong to the "**payoff**" class.
- The examples contain two features, “Balance” and "Residence."
  - "Balance" refers to the amount of money the person has in their savings and checking accounts at the time of the loan, which can take on two values: “< $50K” or “≧ $50K.”
  - “Residence” refers to whether or not the person owns their home or rents and can take on two values: “OWN” or “RENT.”

As stated, the class label for y can be either "default” or "payoff." Before splitting the parent region into child regions, the entropy of y in the parent region is:

$$\mathbf{H(y|parent) = -\frac{16}{30}\log_2\left(\frac{16}{30}\right) - \frac{14}{30}\log_2\left(\frac{14}{30}\right) \approx 0.99}$$

After splitting the parent region into two child regions c_L and c_R, the weighted average of the entropy of y over the child regions is the sum

$$r(c_L)H(y|c_L) + r(c_R)H(y|c_R)$$

where

- $r(c_L)$ is the ratio of the number of examples in child region c_L divided by the number of total examples in the parent region prior to a split.
- $r(c_R)$ is the ratio of the number of examples in child region c_R divided by the number of total examples in the parent region prior to a split.

The goal is to find a “good split” that will yield a low weighted average entropy of the partitioned child regions.

To complete the quiz:

Your task is to determine which feature — "Balance" or "Residence" — provides the lowest entropy split. There are two calculation questions to answer.

You may take this quiz up to three times.

Please complete this activity in the course.

Back to Table of Contents

Watch: Making Predictions Using the Decision Tree

The purpose of a supervised learning model is to make predictions. In this video, Mr. D'Alessandro will demonstrate how to make prediction on an unlabeled example by traversing down a decision tree. You will see how prediction is performed in both regression and classification problems. You will also touch on various hyperparameters for optimizing decision trees, such as minimum samples per leaf and maximum tree depth.

Video Transcript

Now, I want to share some practical elements regarding decision trees. We'll cover the components of a decision tree and provide an example implementation in scikit-learn. Here is a visualization of a simple decision tree. One nice property of decision trees is their inherent interpretability. The tree is defined by a set of logical conditions, which means we can trace the exact set of steps that leads to a specific prediction. However, I should share that in most realistic cases, it will be challenging to actually display the entire working tree. Most trees are produced with dozens of features or more and can easily end up with thousands of terminal nodes, so fitting them into one display will be mostly impractical. Let's dig into the components of the tree now. We can start with what we call the nodes. A decision tree is a type of graph structure, which is why the individual elements are referred to as nodes. This type of direct graph is directed in the arrows indicate the direction of some logical flow. Any starting node is called a parent node, and the endpoint of an arrow is called a child node. Once we get to the end of the tree, the terminal nodes are often referred to as the leaves of the tree. These leaves contain the information we use for predictions. Next, we'll introduce a few key components to find within the tree. The depth of the tree tells us how many splits there are down a single path. When making a prediction on a given point, this is the number of logical comparisons you would have to make. Because each split results in two child nodes, the number of nodes in the tree grows exponentially with the depth. Additionally, each note contains data, and there are a few aspects of that data that are important.

The first is the node sample size. This is simply the examples that made it to that node in the training process. Then there is the label distribution. Decision trees can be built for both binary and multiclass classification, as well as regression. The main difference between classification and regression in the algorithm is the function used to define the splits. The distribution of the labels in the leaf nodes is what determines a prediction. For classification, we can take the most common class label as the prediction, or if applicable, we can take the average value to get a probability. For regression, we would just take the average label within the leaf node. Decision trees follow the standard scikit-learn API. Here we instantiate the model. In this case, I specified values for the key input parameters. The max depth tells us how large we can grow the tree. The other two relate to the number of elements in the nodes. The split parameter says we won't split a node unless we have that many examples in the splitting node. The main sample's leaf says we won't split unless each of the child node gets at least that number of examples. These are important elements for optimizing the tree's performance, and we'll cover that in a subsequent lecture. Finally, the last two lines are for predictions. We have two choices. We can either predict the class directly, or we can predict that the probability of being in each class. You can see that there are different methods for each. The choice of whether to predict a class or a probability will be problem dependent.

Back to Table of Contents

Quiz: Check Your Knowledge: Decision Trees Part 1

To further explore how decisions trees work, you will complete two exercises that require you to review and make decisions based on some data. The example data consists of "good" and "bad" individuals and some basic characteristics that describe each individual. Using the data, you will answer a series of questions about decision trees.

Take a look at the table below, which contains training data consisting of individuals (inputs), characteristics of those individuals (features), and whether that individual is "good" or "bad" (labels). Answer the questions that follow based on the data.

Training Data

	Mask	Cape	Tie	Ears	Smokes	Height	Class
Batman	Y	Y	N	Y	N	180	Good
Robin	Y	Y	N	N	N	176	Good
Alfred	N	N	Y	N	N	185	Good
Penguin	N	N	Y	N	Y	140	Bad
Catwoman	Y	N	N	Y	N	170	Bad
Joker	N	N	N	N	N	179	Bad

You may take this quiz up to three times.

Please complete this activity in the course.

Back to Table of Contents

Tool: Decision Trees Cheat Sheet

The tool linked to this page provides an overview of classification and regression trees for your reference. You'll find information about the applicability, underlying mathematical principles, assumptions, and other details of this algorithm.

Download the Tool

Use this **Decision Trees Cheat Sheet** as a quick way to review the details of how the algorithm works.

Back to Table of Contents

Ask the Expert: Mehrnoosh Sameki on Decision Trees

Depending on the problem you are trying to solve, you may want to build a regression decision tree or a classification decision tree. In this video, Dr. Sameki compares a regression decision tree with a classification decision tree.

Note: The job title listed below was held by our expert at the time of this interview.

Mehrnoosh Sameki	Product Manager, Microsoft	Dr. Mehrnoosh Sameki is a Senior Technical Program Manager at Microsoft, responsible for leading the product efforts on machine learning interpretability and fairness within the Open Source and Azure Machine Learning platforms. Dr. Sameki also co-founded Fairlearn and Responsible-AI-widgets and has been a contributor to the InterpretML offering.

Can you compare DT for regression vs. DT for classification?

Video Transcript

Both regression tree and decision tree are tree-based models, obviously, and they are used for different purposes. A regression tree is used for predicting a continuous target variable. It essentially recursively splits the data into different branches based on the value of the input features and, of course, the target variable that it's predicting. And the target variable that is being predicted is the mean or median of the value in each leaf node of that decision tree.

Versus in a classification case, you're predicting obviously categorical target variables, and so it recursively splits the data into different branches based on the values of the input features. And in this particular case, the target variable is predicted based on the majority class of the samples in each leaf node. So both create a tree form or tree-like structure where each internal node represents a feature and each leaf node represents a predictive value or class. But the main difference is the type of target variable they're used to predict. A regression tree is used for continuous a target variable, whereas decision tree is used for a categorical target variable.

Back to Table of Contents

Quiz: Check Your Knowledge: Decision Trees Part 2

To further explore how decisions trees work, you will complete two exercises that require you to review and make decisions based on some data. The example data consists of "good" and "bad" individuals and some basic characteristics that describe each individual. Using the data, you will answer a series of questions about decision trees.

Take a look at the table below, which contains a few test examples consisting of individuals (inputs) and characteristics of those individuals (features) but without labels. Based on the training data, there is a simple decision tree below that accurately classifies the training data. Use the data and tree to answer the following questions.

Testing Data

	Mask	Cape	Tie	Ears	Smokes	Height	Class
Batgirl	Y	Y	N	Y	N	165	?
Riddler	Y	N	N	N	N	182	?
Fred	N	N	Y	Y	Y	181	?

You may take this quiz up to three times.

Please complete this activity in the course.

[Back to Table of Contents](#)

Watch: Optimizing a Tree

Just as K is the hyperparameter to optimize KNN, the hyperparameters to optimize a decision tree are minimum samples per leaf, maximum tree depth, and minimum samples split. In this video, Mr. D'Alessandro goes over in detail how each of these hyperparameters is used to control the model complexity of a decision tree.

Finding the ideal hyperparameters helps control the model complexity, which in turn reduces model estimation errors due to bias and variance. Bias error arises when a model is too simple, and is therefore not capable of learning patterns and relationships from the training data — a condition known as underfitting. On the other hand, when a model is too complex, it fits the training data too closely. It learns patterns and relationships that are very specific to the training data, making it difficult to generalize to new data — a condition known as overfitting. This will result in a high variance error. Mr. D'Alessandro discusses the bias-variance tradeoff and how the ideal tradeoff between bias and variance lies in finding the right hyperparameters, leading to a model with balanced complexity.

Video Transcript

Now we'll discuss how to tune a decision tree to get optimal performance. Remember, every supervised learning algorithm has hyperparameters that determine its complexity. With a decision tree, the complexity is related to the size of the tree. Each leaf of the tree is a separate and distinct partition of the feature space. The more leaves or partitions we use, the more the tree is able to learn the nuances of the data. For us, tuning the size of the tree leads to the best generalization. A bigger tree results in more complexity; with more complexity we have a higher likelihood to overfit, and the model will have what we call model estimation variance. With less complexity, we have a higher likelihood to underfit, and the model will have what we call model estimation bias. High variance in a model means it is sensitive to slight variations of the data. For instance, if you were to randomly split your data into two training sets and train a model on each data set, a model algorithm that has high estimation variance will produce very different models between the two training sets. Although each random subset comes from the same distribution, the process of sampling will cause slight variations in those two distributions. This is even worse when you have small sample sizes. On the other hand, a model with higher bias tends to not fit the data well. An example is with curve fitting where you're trying to fit a parabola with a straight line. The right complexity is always a balance between these two extremes of high and low complexity. The main thing to remember and consider when tuning your tree is how to get more or less complexity with each of the main hyperparameters. In this case, we'll cover: "max_depth," where higher values lead to larger trees and higher complexity; "min_sample_split," where higher values lead to smaller trees and lower complexity; and "min_samples_leaf," where higher values lead to smaller trees in lower complexity. Max_depth, again, controls how many splits we can make, and min_sample_split controls the minimum number of samples and a parent node required to split it. Then, min_samples_leaf dictates how many samples can be in the leaf nodes. Given a large tree will usually be difficult to actually visualize the complexity of the tree, or basically visualize the entire tree, since each leaf of a tree represents a specific partition of the data, we can instead visualize the tree by showing how it partitions the feature space. The graph here shows three different output scenarios for trees trained on the same data. The left-most chart shows the original data for your reference. Each subsequent chart shows what we call the decision surface.

The colors of these plots represent how new examples will be predicted. This is binary classification, so we're predicting two classes, represented by the two colors. Essentially, when a new point comes in, we can see its corresponding color and the decision surface, and use that to assign it a label. This visualization is aimed at showing the typical complexity trade off. At a high max_depth, we can see a lot of very small partitions where neighboring partitions predict different classes. Meanwhile, on the left with a very small tree, there isn't much nuance. As a general rule, when looking at decision surfaces like this, we want to see curved, but smooth lines, without having many alternating colors in a small region. When we spend time optimizing our models, we'll empirically test different values of the input hyperparameters and try to test both low and high complex models to find the right fit. Now, I want to make one last point about decision trees that is separate from hyperparameter optimization. This relates to optimizing the performance of the tree in general, but can also be leveraged for learning general insights from the data. The decision tree algorithm in scikit-learn automatically computes an attribute that they call feature importance. The technical definition of feature importance, here, is the cumulative information gain that feature contributes in the learning process. Here's an example of feature importance on some real data. The data and learning problem doesn't matter so much, so I won't get into that, but the plot here shows what the above array stores. By looking at this data, we can quickly determine which features are contributing the most to our predictions. The plot is sorted, and we can see that features on the right-hand side have little to no predictive value. We can use information like this to better explain the process we're trying to model, as well as to drop features we think aren't adding any value.

Back to Table of Contents

Ask the Expert: Mehrnoosh Sameki on Overfitting and Underfitting

A possible cause of poor performance in machine learning can be from a model overfitting or underfitting the training data. Here, Dr. Sameki uses videos to explain what it means to have a model that is overfitting or underfitting. She also provides insight on how you can tell when your model is overfitting or underfitting.

Note: The job title listed below was held by our expert at the time of this interview.

Can you explain what overfitting and underfitting is? And can you provide examples?

Video Transcript

So let's start with overfitting. Usually, it happens when we train a machine learning model; almost too much tuned to the training set that you're providing to your model. And so specifically as a result, the model learns the training data little too well.

But when you want it to generalize to other data sets -- specifically, unseen data that you're throwing at your model -- then it is going to generate really bad predictions. And so it is going to have a very low accuracy result for unseen data but a very good accuracy result, obviously, on the patterns that it has seen. And so that could lead to suboptimal, nonoptimal decisions.

And for underfitting, it's kind of the other side of the spectrum in that sense that it occurs when the machine learning model is not well tuned to the training data, and so the resulting model is not capturing the complexities and the relationship between inputs and outputs well enough. And so it doesn't produce accurate predictions, even for the training set.

And so resultantly, an underfit model generates poor results that lead to super-high error decisions, like an overfitted model. So in both cases, we're talking about super-high error rates on test data. But in one, the model almost learns the training data too well, which is overfitting. In some other case, the model is not understanding the nuances and complexities of the relationship between inputs and outputs and so still generates a very high error rate.

As far as examples for overfitting, assume that you're performing fraud detection on credit card application on folks from United States. And so just pretend that there are tens of thousands of examples that are available to you in order to train your machine learning model in fraud detection.

Now, when you explore further, you only have seven examples from folks in South Boston, imagine, and two of the seven examples are part of validation set, whereas five of them are part of the training set. And imagine all seven of these examples are classified as fraudulent. And so as a result, your algorithm will most likely learn that all South Boston residents are fraudsters because it has nothing else for that particular subpopulation to draw conclusions from.

And so it will confirm this hypothesis it just formed using those two cases that you have in validation set, because they had also fraud prediction -- or fraud ground truths, so that hypothesis is confirmed. And so as a result, no one from South Boston will be approved for a credit card or loan or whatever depends on that outcome of the model.

And so obviously, this is an issue. And while this is not overfitting in general, I just wanted to conclude that this is overfitting for some group -- in this case, South Boston residents -- because you draw some conclusion from training data, and you confirmed your hypothesis in the validation data, but when you bring it back -- bring it out in the wild, obviously it's going to cause harm, and that's what overfitting is.

In terms of an example of underfitting, there is no tangible example from the machine learning world that I can share because it's about not understanding the complexities of your data. But it's very similar to if you're working with some students and you're giving them less study materials, and so they're not appropriately trained on the subject that you want to test them on, and so obviously, they're going to not perform; they're not going to perform well in the exams. And so the solution would be simply like train them well and provide the right training materials and the right patterns you're going to create an exam on. And so that's an example of underfitting, when the model is underprepared to understand the nuances in data.

How can you tell if a model is overfitting?

Video Transcript

So you can tell your model is overfitting when, on your training data, you see that the model performs really well, but then you take it and you try to run it on some unseen evaluation data, and then you suddenly see super-poor performance results; maybe your accuracy is suddenly dropping or any other metric, like error rate, is suddenly going high. And so that will give you a hint that, wow, my model is memorizing the data that it has seen in the training data but it is not able to generalize to some unseen data and the patterns that exist there. So always try to take a look at your performance across your training data and then try to see whether that rough performance range holds when you are taking it to some unseen evaluation data.

How can you tell if a model is underfitting?

Video Transcript

So usually you can look at the performance of your model on your training data and evaluation data. And one of the hints for underfitting is when the model is also performing very poorly on training data. So even the data that you provided to it to train it, the model wasn't able to learn the relationships between input and output. And so that is usually your first hint.

Back to Table of Contents

Read: Model Complexity Revisited

To revisit, there are two equally problematic cases which can arise when training a model: underfitting and overfitting. If the model isn't able to distinguish important aspects of the training data, it will fail to classify new data accurately. On the other hand, if the model learns the idiosyncrasies that are particular to only the training data set, it will fail to generalize to new data.

An overfit model is too complex; it has captured the idiosyncrasies of the training data and will not generalize to unseen data.

An underfit model is too simple; it has not captured the predictive nuances present in the data and will perform poorly on new data.

Finding the ideal hyperparameters helps control the model complexity, which, in turn, reduces model estimation errors due to bias and variance.

Underfitting: The model is too simple. The model has not captured the relevant relationships and details among features and labels that are necessary to make proper predictions. In this case, both the training error and the test error will be high and the model will not be able to make predictions about new, unseen data.

Overfitting: The model is too complex. The model has learned relationships and details among features and labels that are too specific to the training data only. The model therefore cannot be used to accurately infer anything about new, unseen data. Although training error may be low, test error will be high, as the model can make decisions based on patterns which exist only in the training set and not in unseen data.

Bias-variance tradeoff

Finding the ideal hyperparameters helps control the model complexity, which, in turn, reduces model estimation errors due to bias and variance.

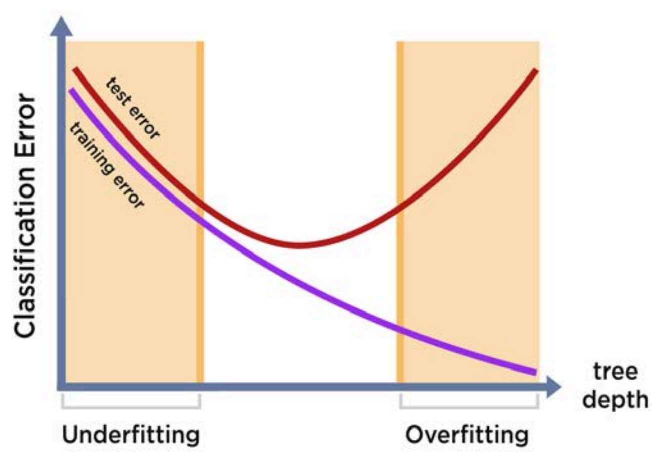
- **Bias**: Model bias expresses the error that the model makes (how different is the prediction from the training data). Bias error arises when a model is too simple and

is underfitting.
- **Variance**: Model variance expresses how consistent the predictions of a model are on different data. High variance is a sign that the model is too complex and is overfitting to the particular data set on which it is trained.
- The ideal **tradeoff** between bias and variance lies in finding the right hyperparameters, leading to a model with balanced complexity.

Hyperparameter tuning to manage complexity

To ensure your model is not susceptible to overfitting or underfitting, you want to tune the model's hyperparameters to some optimal values. As a refresher, hyperparameters are tune-able properties to control the behavior of a model. Most models have some kind of hyperparameter to control a model's complexity. For a decision tree, it can be the maximum allowable depth of the tree. Note in the graph below how changing the tree depth of a decision tree can affect underfitting and overfitting.

A machine learning engineer's job is to experiment with various hyperparameter values to ensure that the models developed are not overfitted or underfitted.



[Back to Table of Contents](#)

Ask the Expert: Annie Wong on Bias and Variance Errors

There are different types of errors when it comes to machine learning: bias error and variance error. Ms. Wong defines both errors in these videos.

Note: The job title listed below was held by our expert at the time of this interview.

	**Mehrnoosh Sameki**	Product Manager, Microsoft	Dr. Mehrnoosh Sameki is a Senior Technical Program Manager at Microsoft, responsible for leading the product efforts on machine learning interpretability and fairness within the Open Source and Azure Machine Learning platforms. Dr. Sameki also co-founded Fairlearn and Responsible-AI-widgets and has been a contributor to the InterpretML offering.
	**Annie Wong**	Senior Manager - Data Science, Verizon Wireless	Annie Wong is a Senior Manager leading a team of data scientists at Verizon. Ms. Wong works with the business to utilize data more in their day-to-day decision making. Technology is exciting for her because it is constantly growing and that enables her to learn every day!

What is a bias error in machine learning?

Video Transcript

In general, bias can come when your datasets aren't diverse enough or don't cover enough bases to get a full understanding of the full population base that you're looking at. Typically, adding more data can be helpful here. Data prep is also really important. Being able to normalize the data, the scaling of your information, imputing data whenever needed. Then really that second piece is when you look at feature engineering, you can really identify these issues or patterns in the data. Feature engineering is something that is very important and definitely you want to spend multiple iterations on as you're training your model. Then the last piece, just the model complexity with some of the different diversity in data. Simple models might under fit data, while complex models might over fit data. Really important to, again, choose that model that strikes the balance between being complex and simple enough.

What is a variance error in machine learning?

Video Transcript

Really quick, high variance can lead to a lot of differences in data, which could also lead to over fitting a model. Essentially what that means is you might be training your model on a data set that has a lot of different information. Then when you apply it to actual real data, you may find that the model isn't able to generalize information you have because of the high-variance in the data set. That's where over fitting fits in with the variance.

Back to Table of Contents

Assignment: Optimizing Decision Trees

In this exercise you will implement a decision tree classification model using scikit-learn. You will train different models using different values for hyperparameter max depth and compare the accuracy of each model.

This exercise will be graded.

When you finish your work:

1. Save your notebook by selecting the "Save and Checkpoint" entry from the "File" menu at the top of the notebook. If you do not save your notebook, some of your work may be lost.
2. Submit your work by clicking **Education —> Mark as Completed** in the upper left of the Activity window. 

3. This assignment will be auto-graded and can be resubmitted. After submission, the Jupyter Notebook will remain accessible in the first tabbed window of the exercise. To reattempt the work, you will first need to click **Education —> Mark as Uncompleted,** then proceed to make edits to the notebook. Once you are ready to resubmit, follow steps one and two.

This exercise will be auto-graded.

Please complete this activity in the course.

Back to Table of Contents

Assignment: Unit 3 Assignment - Train Decision Trees After Data Preparation

In this assignment, you will practice the modeling phase of the machine learning life cycle. You will perform data preparation techniques to prepare your data for modeling and train decision tree models using scikit-learn. You will train a few different decision tree classifiers using different hyperparameter values, and you will plot the resulting accuracy scores. You can accomplish this assignment by using all of the techniques you practiced and implemented in the different exercises and activities in this unit and the previous one.

This assignment will be graded.

When you finish your work:

1. Save your notebook by selecting the "Save and Checkpoint" entry from the "File" menu at the top of the notebook. If you do not save your notebook, some of your work may be lost.
2. Submit your work by clicking **Education —> Mark as Completed** in the upper left of the Activity window. 

3. Note: This assignment will be manually graded by your facilitator. You cannot resubmit.

This assignment will be graded by your facilitator.

Please complete this activity in the course.

[Back to Table of Contents]

Assignment: Unit 3 Assignment - Written Submission

In this part of the assignment, you will answer six questions about building and evaluating your models using algorithms such as decision trees and k-nearest neighbors.

The questions will prepare you for future interviews as they relate to concepts discussed throughout the unit. You've practiced these concepts in the coding activities, exercises and coding portion of the assignment.

Completion of this assignment is a course requirement.

Instructions:

1. Download the **Unit 3 Assignment document.**
2. Answer the questions.
3. Save your work as one of these file types: .doc or .docx. No other file types will be accepted for submission.
4. Submit your completed Unit 3 Assignment document for review and credit.
5. Click the **Start Assignment** button on this page, attach your completed Unit 3 Assignment document, then click **Submit Assignment** to send it to your facilitator for evaluation and credit.

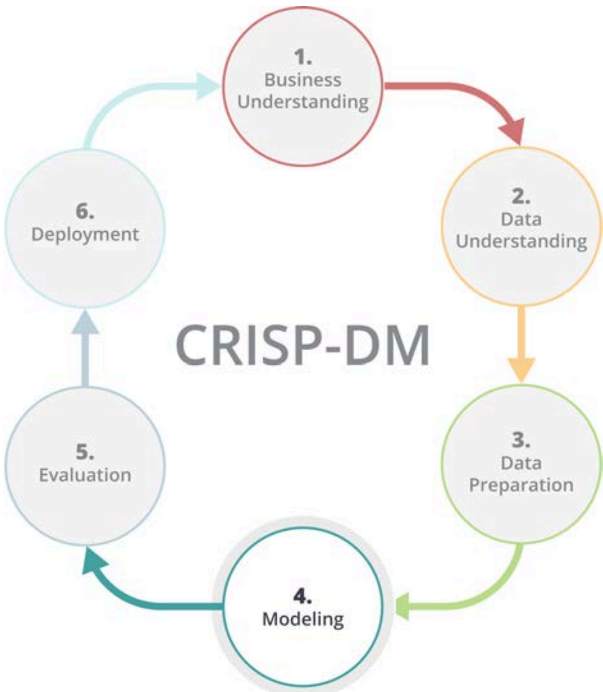
Back to Table of Contents

Module Wrap-up: Implement Decision Trees

Now that you've completed this module, you can see how building a decision tree by repeatedly dividing data into partitions allows you to predict labels in larger data sets more efficiently. You continued to explore hyperparameter tuning and talked about the different hyperparameters for a decision trees. Remember that regulating the complexity of a model by using the correct hyperparameters avoids both overfitting and underfitting, improving the likelihood that your model performs well on new data.

Back to Table of Contents

Lab 3 Overview: ML Life Cycle: Modeling



In this lab, you will practice the fourth step of the machine learning life cycle: modeling. You will practice training KNNs and decision trees then optimizing them by tuning their hyperparameters to find the best-performing model for your predictive problem. You will be working in a Jupyter Notebook.

This three-hour lab session will include:

- **10 minutes** - Icebreaker
- **30 minutes** - Week 3 Overview and Q&A
- **20 minutes** - Breakout Groups: Big-Picture Questions
- **10 minutes -** Class Discussion
- **10 minutes - Break**
- **30 minutes** - Breakout Groups: Lab Assignment Working Session 1
- **15 minutes** - Working Session 1 Debrief
- **30 minutes** - Breakout Groups: Lab Assignment Working Session 2
- **15 minutes** - Working Session 2 Debrief
- **10 minutes -** Concluding Remarks and Survey

In Lab 3, you will:

- Define your ML problem and build your DataFrame.
- Prepare your data:
  - Perform feature engineering by converting categorical features to one-hot encoded values.
- Train multiple decision trees and evaluate their performances:
  - Train decision tree classifiers with various hyperparameter values.
  - Visualize and evaluate the accuracy of the models' predictions.
- Train multiple KNN classifiers and evaluate their performances:
  - Train KNN classifiers with various hyperparameter values.

    - Visualize and evaluate the accuracy of the models' predictions.
- Determine the best-performing model for your predictive problem.

[Back to Table of Contents]

Ask the Expert: Mehrnoosh Sameki on Comparing DTs and KNNs

In this video, Dr. Sameki describes the difference between a decision tree and a k-nearest neighbors model, as well as the advantages and disadvantages of using each model.

Note: The job title listed below was held by our expert at the time of this interview.

Mehrnoosh Sameki

Product Manager, Microsoft

Dr. Mehrnoosh Sameki is a Senior Technical Program Manager at Microsoft, responsible for leading the product efforts on machine learning interpretability and fairness within the Open Source and Azure Machine Learning platforms. Dr. Sameki also co-founded Fairlearn and Responsible-AI-widgets and has been a contributor to the InterpretML offering.

Can you compare DTs and KNNs? What are the advantages and disadvantages of using each model?

Video Transcript

Both of these techniques are non-parametric methods. Decision tree supports automatic feature interaction much better than KNN -- or KNN, I should say, they can't. And so when we say feature interaction, if you think about the decision tree branch, if there are interaction or correlation between multiple features leading to a particular decision, obviously decision tree allow you to take that pattern into the consideration versus KNN can't. Decision tree is also much faster due to KNN's expensive real-time execution.

Now I can also dive a little bit deeper with talking about advantages and disadvantages of each of these algorithms. So for instance, for advantages, decision trees are very effective in capturing nonlinear relationship, which can be very difficult to achieve with other algorithms like support vector machines and others.

They're super easy to explain to other people, and some people say they're actually mimicking the way that humans are making decisions. And so if you are having a certain scenario where explainability and interpretability is a huge part, say in a regulated space, decision trees seem to be very, very effective in making sure that everyone understands how the AI has come up with its decision. They can also handle qualitative or categorical features without the need to create advanced dummy variables really well.

The disadvantages are they don't have the same level of predictive accuracy as some of the other classification or regression approaches. Sometimes trees could be unrobust or non-robust, meaning small changes in the data can cause a large change in the final estimated tree. Also, as the tree grows, it becomes prone to overfitting. And so there is a technique, pruning, that might be required in order to avoid that overfitting.

In other words, or on the other hand, KNN, the advantages are they are also simple and intuitive in a way similar to decision tree. It's also easy to give a sense or give a picture to your stakeholders and laypeople and try to explain how they have come up with the particular decisions.

Similarly, they are non-parametric so that they are not holding or having any assumptions on the data distribution. One other good thing about them is they're easy to implement for multi-class scenarios as well. And for hyperparameters when working with KNN, you just need to provide two parameters, which is k, the number of neighbors to consider, and also the choice of distance function, which often is Euclidean or Manhattan distance.

They could be used for both classification and regression, just like decision trees. They are also really great for lazier learning or instance-based learning. You don't need to fit a model in advance. Just you can provide a data point, and it will give you the prediction.

Now, the disadvantages are it is quite slow with a larger data set. That's where a decision tree could play a role and kind of complement that scenario. It could suffer from curse of dimensionality. It's way more appropriate to use when you have a smaller number of inputs. If the number of variables grow, then the KNN algorithm will have a super hard time predicting the output of a new data point.

Feature inputs need to be scaled. As I mentioned, KNN use distance criteria like Euclidean or Manhattan to come up with this prediction. Therefore, it's very important that all the features have the same scale.

It is quite sensitive to outliers because as you know, it's an instance-based algorithm. And so in the distance scenarios when there are outliers that are super far from the rest of the data points, then it is liable to create a very, very biased outcome.

It's also capable of treating -- it's not capable of treating or dealing with missing values. So unfortunately, missing values could cause a problem if they're not treated there. And eventually, class imbalance could be a huge issue for KNNs. If you have imbalanced class data, the algorithm might wrongly pick the majority class, which is the wrong prediction.

Back to Table of Contents

Ask the Expert: Kathy Xu on Using DTs vs. KNNs

How do you know when to implement a decision tree or k-nearest neighbors model to solve your problem? In this video, Kathy Xu explains when you should use one over the other.

Note: The job title listed below was held by our expert at the time of this interview.

	**Kathy Xu**	Analytics Extensibility Lead, Pfizer	Kathy (Qingyu) Xu leads a team responsible for extending analytics capabilities across Pfizer. Her team helps create machine learning-powered products (web apps, plugins, and dashboards) for use across the enterprise and provides guidance for fellow data scientists and analysts to optimize their usage of data and analytical technologies that are a part of the enterprise analytics platform. In particular, Ms. Xu has an interest in MLOPs and industrializing machine learning models. Outside of work, she is an avid art history lover and frequently visits the museums around NYC, such as the Cooper Hewitt and Brooklyn Museum. Ms. Xu received her Master and Bachelor of Science in Statistics from Cornell University.

When should you use DTs vs. KNNs?

Video Transcript

The difference between a KNN, when I would use a k-nearest neighbor type of model versus a decision tree, might depend on the overarching problem at hand. For example, if I'm looking at a clustering algorithm, one of the methods that I would leverage is probably the k-nearest neighbors because I want to understand what different data points are closest to one another or can actually cluster together. A use case where I might look at leveraging a decision tree is understanding what different types of subpopulations I have for an overarching data set. For example, if I'm trying to figure out, from a marketing perspective, what are the subgroups that I particularly want to target, I might want to look at a decision tree that will help me provide those tree-like structures or split up based off of if-then statements. It's really helpful for me to understand if, for example, a particular variable performs as X, then it's more likely for this next variable to perform as Y and so on and so forth, to provide very specific subsets and sub-units of a particularly larger group.

Back to Table of Contents

Assignment: Lab 3 Assignment

In this lab, you will continue working with the Airbnb NYC "listings" data set.

This assignment will be graded.

When you finish your work:

1. Save your notebook by selecting the "Save and Checkpoint" entry from the "File" menu at the top of the notebook. If you do not save your notebook, some of your work may be lost.
2. Submit your work by clicking **Education —> Mark as Completed** in the upper left of the Activity window. 

3. Note: This assignment will be manually graded by your facilitator. You cannot resubmit.

This lab assignment will be graded by your facilitator.

Please complete this activity in the course.