Using a decision tree to predict COVID case numbers: a tutorial for beginners

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ABSTRACT

Machine learning (ML) makes it possible to analyze large volumes of data and is an important tool in biomedical research. The use of ML methods can lead to improvements in diagnosis, treatment, and prevention of diseases. During the COVID pandemic, ML methods were used for predictions at the patient and community levels. Given the ubiquity of ML, it is important that future doctors, researchers and teachers get acquainted with ML and its contributions to research. Our goal is to make it easier for students and their professors to learn about ML. The learning module we present here is based on a small but relevant COVID dataset, videos, annotated code and the use of cloud computing platforms. The benefit of cloud computing platforms is that students don't have to set up a coding environment on their computer. This saves time and is also an important democratization factor – allowing students to use old or borrowed computers (e.g., from a library), tablets or Chromebooks. As a result, this will benefit colleges geared toward underserved populations with limited computing infrastructure. We developed a beginner-friendly module focused on learning the basics of decision trees by applying them to COVID tabular data. It introduces students to basic terminology used in supervised ML and its relevance to research. The module includes two Python notebooks with pre-written code, one with practice exercises and another with its solutions. Our experience with biology students at San Francisco State University suggests that the material increases interest in ML.

KEY WORDS

Machine learning, decision tree, COVID-19, supervised learning, beginner-friendly, tutorial

INTRODUCTION

The COVID-19 pandemic made clear to many how important it is for local governments to collect and analyze data [1–3]. One particular piece of information that was of great importance

to governments, healthcare systems and citizens alike was the number of COVID cases at a specific time and location [4–6]. Because of this interest and because of the extensive availability of these types of data, COVID-19 case numbers are a great example to use when teaching data science skills to college students in health-related disciplines. Machine learning has become an extremely important data science technique with many uses in medicine [7], but many students in biology and related fields do not learn this technology in their regular curriculum. For this reason, we have created a tutorial to teach one important machine learning technique, decision trees, using COVID-19 data as the driving example. We use a small dataset that combines publicly available data from different government sites and research institutions [8–11]. The dataset has been cleaned for the purposes of this tutorial and contains observations from all 58 California counties. The goal of the tutorial is for students to learn how a decision tree can be used to predict the number of cases per 100,000 people in a county during the summer months of 2020. The variables used as possible predictors for our decision tree are: population size, vaccination rate, unemployment rate and partisan voting rates for different political parties. As the learners work through the tutorial they learn that out of these possible predictors, the unemployment rate is most important for predicting the number of Covid cases. Counties with higher unemployment rates had more Covid cases in 2020. Next, the learners will analyze data from 2021 and discover that in 2021, the best predictor for the number of Covid cases is not unemployment rate, but vaccination rate. Counties with higher vaccination rates have lower numbers of Covid cases. There are a total of four submodules, with code, written text, images and short videos tailored to the needs of a student without coding or machine learning experience.

Decision trees have been used in many research fields for a long time and they are one of the simplest, yet foundational algorithms in machine learning. Decision trees form the basis for random forest models and gradient-boosted tree models, which are some of the most popular machine learning models for supervised learning. Because of its simplicity, the decision tree is a great first algorithm to introduce to college students in order to develop a basic understanding of more advanced techniques within the field of machine learning.

We programmed our tutorial in Python, which is one of the most popular coding languages [12,13]. It is considered a good language to learn for beginners because of its relative simplicity [14]. The tutorial does not require specialized knowledge in any particular biological concept and is designed to be a friendly introduction to the decision tree algorithm for students with no prior coding or machine learning knowledge. We hope that after finishing the tutorial, students could use the provided code to analyze other datasets and research questions.

A major barrier for beginners to learn coding is to set up a development environment on their computer. Cloud computing allows students to get started with coding if they do not have the skill to set up a development environment on their own computers or if they don’t own a computer, but instead use a tablet, a Chromebook, or even their phone.

We originally developed the learning module for local biology and chemistry students with limited coding experience and no machine learning experience. We wanted to demystify

machine learning concepts and their applications in biology and health-related research. The beginner-friendly learning module aims to get students acquainted with basic terminology used in machine learning with a focus on learning about decision trees. The lessons lean heavily on the practical side, are light on mathematical background and intend to build an intuitive understanding of the algorithm rather than diving into technical and theoretical details. We introduce a few simple best practices, for example, by acquainting them with making comments in the code produced. We teach students how to evaluate their decision tree model and provide them with a positive hands-on experience when they write and run ML code for the first time.

We used Jupyter notebooks in a Python kernel run in virtual machines within the Vertex AI platform. We stored the data used in the notebooks in Google Cloud Storage, both available in the Google Cloud Platform. The learning module introduces several packages for data wrangling (pandas, numpy), data visualization (matplotlib, seaborn, graphviz) and machine learning (sklearn). All packages are listed in Table 1. These packages are common and used in many other tutorials that are available online, so they provide a good start for students who are interested in learning more.

The modules serve to bridge the knowledge gaps between biology students and research practices using ML and cloud computing. Step-by-step instructions are provided to students to create their own virtual machine and access the modules. In addition, the submodules are focused on practical use of machine learning and the code can be repurposed for other datasets as well. Students get to learn about the basic workflow used in ML from loading the data to evaluating their model performance. We have used the materials presented here for different groups of biology and chemistry students in our classes and summer programs, with encouraging results (see Results section).

The learning module is split into four parts and students can work through one of them or all of them. The first submodule includes videos introducing machine learning and how it is used in research, and then each step of the tutorial is accompanied by a short video explaining what the code is accomplishing. This submodule focuses on the task of predicting the number of COVID-19 cases in counties in 2020 and provides an example of how to create a decision tree, how to visualize it and how to test how well it works. Students will see that the decision tree model works fairly well for 2020, but not for 2021. The second submodule is an optional one where we focus on data drifting and reasons why it is important to retrain our models from time to time. The third submodule provides a notebook for students to practice creating and running the code learned in the first submodule to train a model on the data from 2021. Finally, the fourth submodule is an answer key for the students who are stuck on the third submodule exercise.

METHODS

The module described in this manuscript is publicly available at https://github.com/NIGMS/Introduction-to-Data-Science-for-Biology (CGP version) and at https://github.com/MarcMachineLearning/Introduction-to-Machine-Learning (Google Colab

version). The module follows an architecture typical of many data science experiments. Tabular data is available as a CSV file in a Cloud Storage bucket and on Github, and read into several analysis pipelines. Data analysis is executed in notebooks with pre-written code. After fetching the data, the notebooks demonstrate basic data science functions such as data visualization and exploratory data analysis. Each submodule comes with written explanations and videos recorded by the authors.

The learning module was designed with students in mind who have no experience in machine learning and with little or no coding experience. For each step, we explain both the Python code that is used as well as the important machine learning concepts. Short videos, made by the authors, three of whom are graduate students themselves, make the materials more accessible. Here we will describe each of the submodules in more detail.

Submodule 1: Introduction to Decision Trees

The notebook of Submodule 1 starts by introducing the data sources used in the tutorial, followed by a video introducing students to the many applications of machine learning in everyday life and in biomedical research (13-minute video). The analysis in this submodule is split into eight steps, and each step is accompanied by a short video (1 to 13 minutes each) explaining the code and some of the concepts used in the notebook. The entire dataset of 58 counties in California, and the number of COVID-19 cases in each of these counties in the summer of 2020 are split into a training dataset of 40 counties and a test dataset of 18 counties. The objective of this submodule is to predict the number of COVID-19 cases per 100,000 people using the variables outlined in Table 1.

Table 1. List of variables (features) that are available for each of the 58 California counties.

Feature Columns	Description
`county`	Names for the 58 California counties.
`cases_per_100000`	Number of COVID cases per 100 000 people for Summer (July, August, September) 2020 and 2021.
`population`	Number of inhabitants estimated per county.
`partially_vaccinated_percent`	Percentage of partially vaccinated people.
`fully_vaccinated_percent`	Percentage of fully vaccinated people.
`2020_Unemployment_Rate`	Unemployment rate for Summer 2020 (used for 2020 and 2021).
`democrat_votes_percent`	Percentage of democrat presidential votes in 2020.
`green_votes_percent`	Percentage of green presidential votes in 2020.

`republican_votes_percent`	Percentage of republican presidential votes in 2020.
`libertarian_votes_percent`	Percentage of libertarian presidential votes in 2020.
`other_votes_percent`	Percentage of other presidential votes in 2020.

After an introduction to machine learning and the project, we outline eight different steps, where code with extensive comments is presented to students to follow along.

1. We show what packages and functions are needed to run the code and how to import them into the notebook to use them.
2. We explain the role of training and testing data in supervised machine learning and import a CSV file with the training data into the notebook.
3. In this step we split the labels (the numbers of COVID-19 cases, which is what we would like to predict) from the features (the data we'll use to make the predictions).
4. Here we create a decision tree and train it to predict the number of COVID-19 cases per county using the DecisionTreeRegressor function from sklearn.
5. In this step we visualize the resulting decision tree and learn about the different parts of a decision tree.
6. In this step, we introduce the testing data from the 18 counties in California that were not included in the training dataset. We make predictions using the features for these 18 counties and the decision tree we created.
7. Here we provide a graphical and intuitive way to evaluate the performance of the decision tree by loading the actual testing labels and comparing them with our predictions using bar graphs.
8. Finally in step 8, we use our model, which we trained using data from 2020 to predict the number of COVID-19 cases in the following year, Summer 2021. We see that the model doesn't perform very well. We also provide a brief discussion as to the reasons why the model performed better when predicting 2020 than with 2021 data within the step 8 video. At the end of Submodule 1, there are 2 CSV files created containing the actual testing labels and the predictions made for each year by our decision tree. These files will be utilized within the (Optional) Submodule 2.

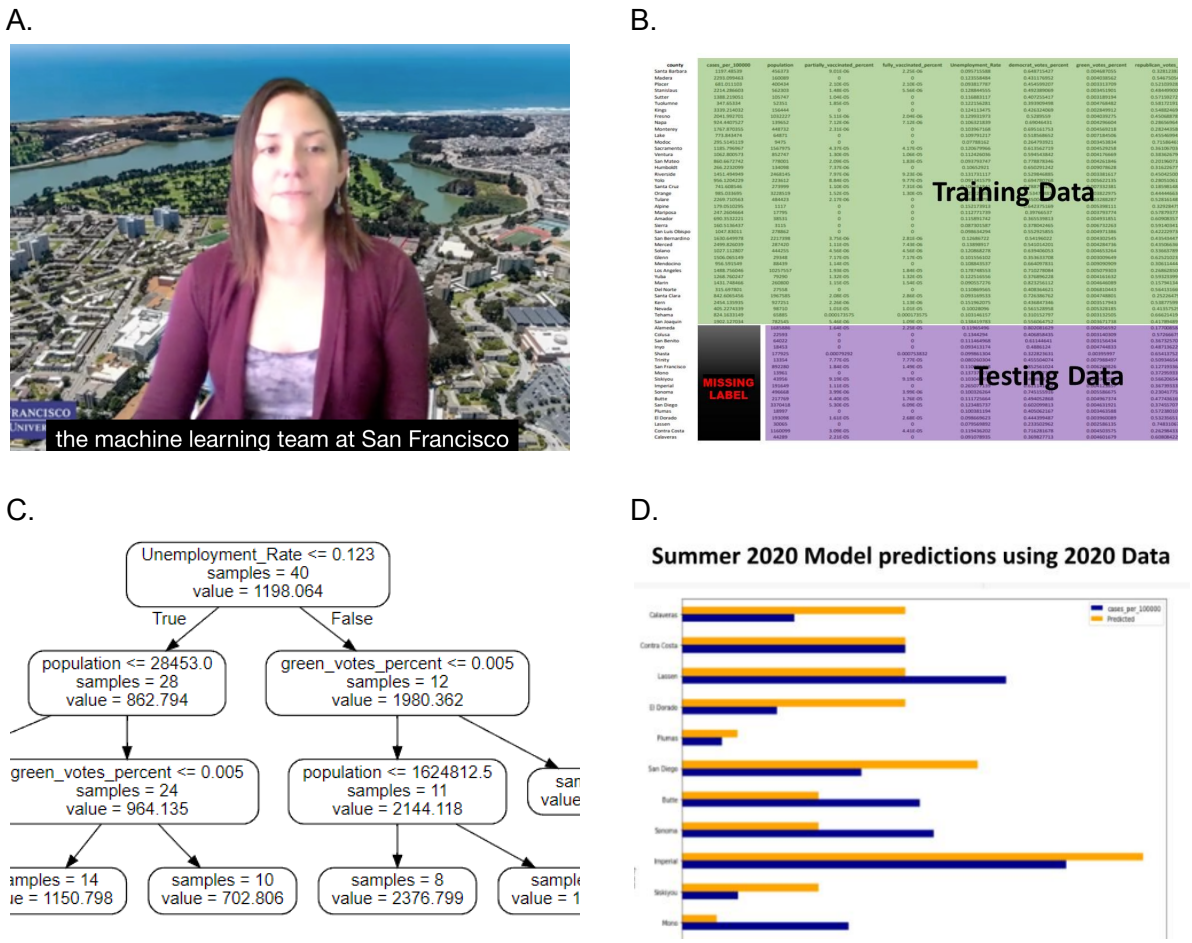

Figure 1 A. Still from one of the videos in Submodule 1, where Lorena Benitez Rivera gives a general introduction to machine learning. B. visual explanation of training and testing data. C. The trained decision tree. D. A barplot to compare predicted and actual COVID-19 numbers in 2020.

Submodule 2: (Optional) Comparing the model performance for 2020 and 2021.

At the end of Submodule 1, the students will have seen that the 2020 model does not perform as well when predicting data for 2021. Submodule 2 revisits the drop in performance of our initial decision tree model and explores some of the reasons for this performance difference. We divided this submodule into five different parts where we explore relationships between the different variables.

1. In part 1, we import packages that focus on visualization and evaluation of our models.
2. Next, we load the CSV files created at the end of Submodule 1, which contain the actual and the predicted values for Summer 2020 and Summer 2021.
3. We then go over the definition and equation of the Root Mean Square Error metric and make a comparison of the predictions made for both years.

4. Here we invite students to think about some of the reasons why the model performance differs between 2020 and 2021, and we teach them to perform some visualization of these differences through the use of descriptive statistics, histograms, correlation plots and scatterplots with trendlines.
5. Finally in part 5, we introduce the phenomenon of data drift as one of the reasons that machine learning models require retraining from time to time.

Submodule 3: Independent practice to train a model specifically for 2021

In Submodule 3, we ask students to create a new decision tree using training data from Summer 2021 to improve the performance of the previous model. The submodule contains a video showcasing how this exercise can be performed (10.5 minutes). In this hands-on exercise, we provide a notebook with empty code cells for students to create their own decision tree. Students are encouraged to copy and adapt some of the code from Submodule 1, but they can also try to write the code from scratch if they wish to do so. As a final additional exercise, we ask students to calculate the RMSE and create aggregate error histograms, similar to what we have done in Submodule 2.

Submodule 4: Answer Key for Submodule 3

Submodule 4 offers an answer key for Submodule 3 in case students get stuck. It contains the answers for all the questions posed in Submodule 3 and the video walkthrough showcased at the beginning of Submodule 3.

Packages and functions used

We used notebooks in a Python kernel run in virtual machines within the Vertex AI platform. We stored the data used in the notebooks in Google Cloud Storage, both available in the Google Cloud Platform. The learning module introduces several packages for data wrangling (pandas, numpy), data visualization (matplotlib, seaborn, graphviz) and machine learning (sklearn). All packages are listed in Table 1. These packages are common and used in many other tutorials that are available online, so they provide a good start for students who are interested in learning more.

Table 2: List of packages (or submodules of these packages) and functions or attributes used in the learning module.

Packages	functions/attributes	Description
IPython.display	YouTubeVideo()	Displays videos from a YouTube link
jupyterquiz	display_quiz()	Displays quiz questions
pandas	read_csv() DataFrame() head() drop()	Read CSV files from a link as a data frame. Organizes data into a 2-dimensional table of rows and columns. Read the first n rows. Remove rows or columns from the data frame.

	concat() plot.barh() reset_index() to_csv() describe() corr() .shape .loc	Concatenate pandas objects along a particular axis. Make a horizontal bar plot. Reset the index of the data frame, and use the default one instead. Write object to a comma-separated values (csv) file. Generate descriptive statistics. Compute pairwise correlation of columns, excluding NA/null values. Return a tuple representing the dimensionality of the data frame. Access a group of rows and columns by label(s) or a boolean array.
numpy	arange() triu() ones_like()	Return evenly spaced values within a given interval. Upper triangle of an array. Return an array of ones with the same shape and type as a given array.
sklearn.tree	export_graphviz() .fit() .predict()	Export a decision tree in DOT format to be read by graphviz (see below). Trains the algorithm on the training data, after the model is initialized. Given a trained model, it predicts the label of a new set of data.
sklearn.metrics	mean_squared_error()	Calculates the mean square error loss.
matplotlib.pyplot	title() hist() legend() show() subplots() set_title() suptitle()	Set a title for one figure plot. Computes and plots a histogram. Place a legend on the Axes. Display all open figures. Create a figure and a set of subplots. Set a title for the subplots. Add a centered subtitle to the figure.
matplotlib.lines	Line2D()	Draws a line that can have both a solid line style connecting all the vertices, and a marker at each vertex.
seaborn	heatmap() light_palette() regplot()	Plot rectangular data as a color-encoded matrix. Make a sequential palette that blends from light to a particular color. Plot data and a linear regression model fit.
graphviz	Source()	Imports and reads DOT format files so that the tree can be visualized.

Description of the datasets used in the case study/example.

The datasets used in submodules were preprocessed and already separated into training and testing data for 2020 and 2021. The datasets consist of COVID case numbers from the California Health and Human Services Agency [8] and COVID vaccination data that were collected by the data desk of the LA Times [11]. We also used unemployment data from the California Employment Development Department [9] and election data from Harvard University [10]. We used unemployment and election data from 2020 for both the 2020 model and for the 2021 model.

RESULTS

The student experience

In the summer of 2022, we let students in our summer SCIP program [15] work through the module. We found that our students had limited prior knowledge of machine learning (see Figure 2, panel A), but after doing the tutorial, 77.8% of the students were interested in learning more (the remaining students indicated they were “maybe” interested in learning more). In response to an open-ended question about what they liked about the tutorial some of the answers included: “I liked that the videos were easy to follow and straightforward.” , “I enjoyed getting to change the code myself to try and figure out how things changed in 2021” “Learning to create the decision tree model and learning to create simple visualizations of competing models with the bar plot.”

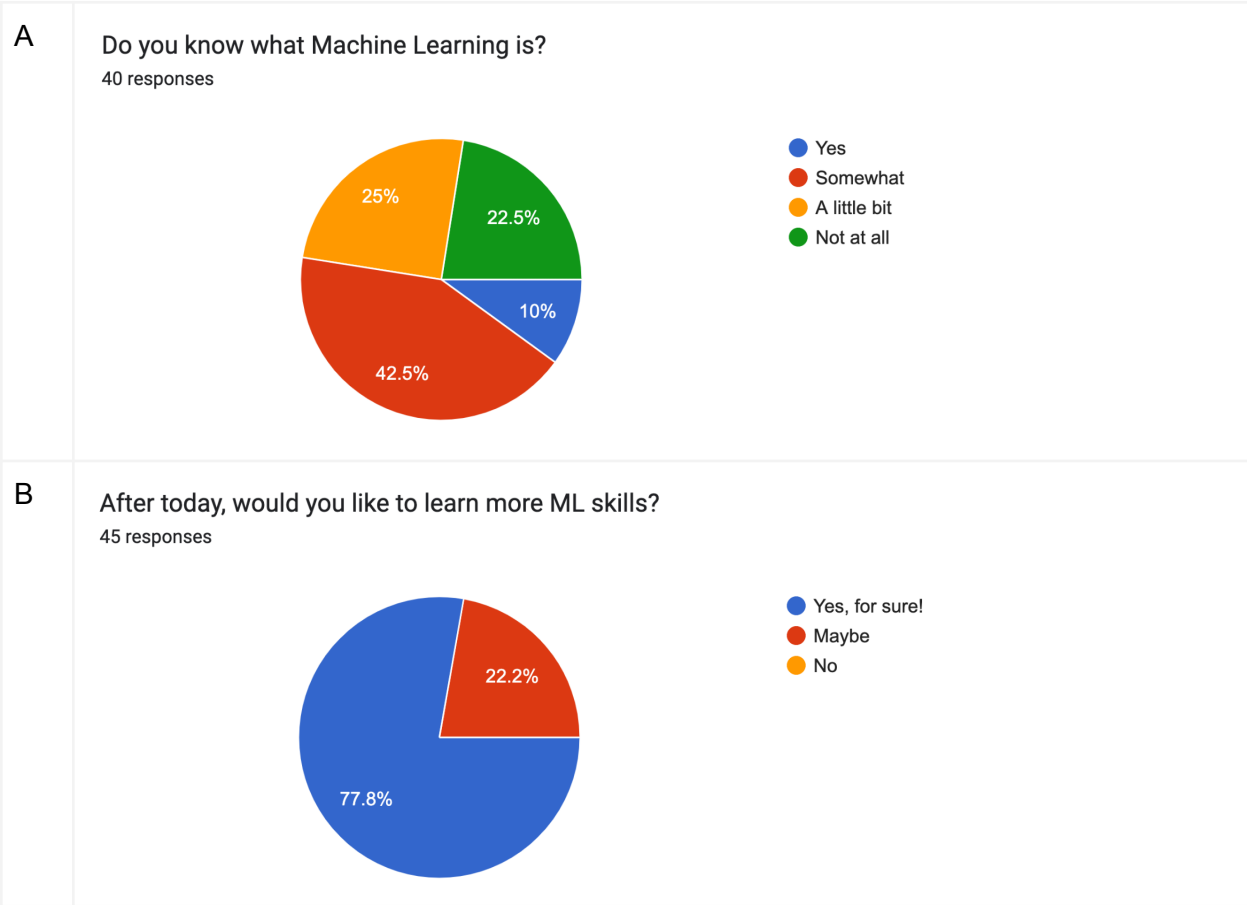

Figure 2. A: Pre-workshop survey responses. B: Post-workshop survey responses. We used the decision tree tutorial in a summer program for biology and chemistry students (Master’s level and undergraduates). These students had been in the part-time summer program for 5 weeks at this point and were learning either Python or R. They had no prior exposure to Machine Learning in their classes or in the summer program.

DISCUSSION

Our goal was to create a tutorial that could be used by students with an interest in biology or health, but with no or little coding or machine learning experience. The tutorial is designed such that faculty can have students work through the entire tutorial in a two-hour lab section. Further, we attempted to find a balance between showing students some of the tools they can use for data science and machine learning and helping them learn some of the basic concepts of supervised learning in general and decision trees specifically. We feel strongly that students should learn concepts and techniques at the same time. We hope that the users will realize that both the concepts and the techniques used are simpler than they may have expected beforehand.

Machine learning is a large field and instead of trying to give students an overview of the entire field, we focused here on just one type of supervised learning model, the decision tree. The tutorial should give students a sense of what supervised learning can do. A drawback of this approach is that many other machine learning tools are not discussed in our tutorial. Those who decide to use this tutorial in their lab or classroom may want to clarify that supervised learning is only one part of machine learning and that machine learning is only one sub-discipline of artificial intelligence.

The dataset we focused on in this tutorial is small: 58 observations (one for each county in California), an easy to understand label (number of COVID-19 cases per 100,000) and 9 features (population size, fraction partially and fully vaccinated, unemployment rate and fraction of votes in the presidential election to different parties). In fact, this dataset is so small it should be considered a toy example. Yet, we picked the topic and the dataset on purpose. Many students in biology are interested in public health and the number of COVID-19 cases was of interest to many in the early years of the pandemic.

In addition to the fact that COVID-19 numbers will be of interest to many biology students, we hope that by using a public health topic for a machine learning tutorial, students will realize that computer science and machine learning can be relevant to topics they care about. To those who are already familiar with machine learning, it may seem obvious that the tools from machine learning can be used in almost any field that is data-heavy, but for undergraduate students, this may not be clear. We were happy to see that a large majority of biology and chemistry students in our summer program were interested in learning more about machine learning after doing the tutorial (see Figure 2).

Python is a great language for undergraduate students in biology to learn computing skills. Python is one of the most common computer languages at the moment [12,13]. Importantly, it is used often in biology and in computer science departments. The other option for biology students would be R, which also has good data science and machine learning capabilities. However, R is almost never used in computer science departments and is not the best stepping stone for students to get ready to take classes in a computer science department.

The tutorial described here is the result of a collaboration between San Francisco State University, the NIH NIGMS, and a team from Google and Deloitte. This collaboration combined

didactic and technical skills of different team members, as well as a variety of backgrounds including biology, CS and statistics. As a result, the tutorial should be of interest to those who teach college students with a biology background, while it uses approaches and tools that are valued in industry.

The tutorial is available on the Google Cloud Platform [16] and also on Github as a set of Google Colab notebooks [17]. There are several benefits of having students use Google Cloud Platform or Google Colab notebooks. The most important practical reason is that students can get started more quickly and don't need to install any software on their computers. In fact, students could use a tablet or library computer if they don't own their own computer. Because of the availability in the cloud, this material will benefit the research community, especially students and faculty in (Institutional Development Awards) IDeA states and at less research-intensive universities in non-IDeA states.

An additional benefit of having this and related tutorials available on cloud platforms is that students can become familiar with different cloud platforms. For this particular tutorial, the barrier to entry would be lowest if students use the Google Colab version, but if they are interested in using the Google Cloud Platform, then this tutorial is available there too. The Google Cloud Platform also allows each student to store their own data in a secure way using Cloud Storage options, that prevent data loss and have advanced security options that control data sharing and enable better cross-institutional collaboration. The cloud platform also allows them to have access to many other datasets from official research and/or government institutions to test what they have learned.

Limitations of the approach we took are that at several steps we chose simplicity over completeness. For example, students learn about test and training data, but not validation. Also, students learn about decision trees, but not related methods such as random forests and gradient-boosted trees, and not other common supervised learning methods such as logistic regression, support vector machines, and neural networks. Another limitation is the barrier to entry if students want to use the Google Cloud Platform, which requires a separate login. The Google Colab version would currently be easier to access since most students in the US have a Google account.

In conclusion, we hope that the tutorial we have created will be used by many faculty and students to get started with data science and machine learning.

KEY POINTS

1. Machine learning is an increasingly important field, but it is usually not taught in biology departments.
2. We have created a beginner-friendly introduction to machine learning focused on a simple but relevant COVID dataset from counties in California.
3. The material is made accessible by using cloud-computing platforms which means that all a student needs to participate is a browser window.

4. The tutorial includes pre-written code, practice material, an answer key, all accompanied by a series of videos by the makers.
5. Surveys at San Francisco State University showed that after doing the tutorial, biology and chemistry students were interested to learn more about machine learning.

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DATA AND CODE AVAILABILITY

Code is available in the NIH GitHub site and data was stored in Google Cloud Storage. The code is also available as Google Colab notebooks in this GitHub repository.

AUTHOR CONTRIBUTIONS

1. Lucy Moctezuma: Notebook development: coding, testing, graphics, notebook videos, manuscript writing.
2. Megumi Fuse: Conceptualization and supervision of the project.
3. Pleuni Pennings: Conceptualization and supervision of the project. Writing and reviewing the paper.
4. Lorena Benitez: Notebook videos and contribution to manuscript writing.
5. Florentine van Nouhuijs: Notebook videos and contribution to manuscript writing.
6. Faye Orcales: Original data collection and the idea to use California COVID data to teach machine learning.
7. Allen Kim: Notebook development, coding, and testing.
8. Ross Campbell: Notebook development, coding, and testing.

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