The Three Theorems of Data Science
UConn Math Club
April 3, 2024

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Introduction

What is Data Science/Machine Learning/AI?

An interdisciplinary field that combines theory and practice from

- Mathematics
- Computer Science
- Statistics

to extract patterns from data, predict the behavior of complex systems, and generate responses to input that capture aspects of human behavior.

The role of mathematics

Both Statistics and Computer Science grew out of Mathematics.

Mathematics seeks:

- abstraction: finding the simplest underlying framework for expressing the phenomena of interest
- generality: establishing results in the broadest possible framework
- rigor: establishing the truth of results through logical reasoning

Theorems

A *theorem* is a mathematical statement that is established by deductive proof.

Theorem: The sum of two odd numbers is even.

Proof: Let a and b be odd numbers. Then $a = 2k + 1$ and $b = 2s + 1$ where k and s are some integers. Then $a + b = 2k + 2s + 1 + 1 = 2k + 2s + 2 = 2(k + s + 1)$. Since $a + b$ is a multiple of 2, it is even.

Theorem: Let A and B be the lengths of the sides of a right triangle, and C be the length of its hypotenuse. Then $C^2 = A^2 + B^2$.

Three theorems at the heart of Data Science

- The Spectral Theorem
- Bayes's Theorem
- The Chain Rule

The spectral theorem

The spectral theorem

Theorem: Let D be a real $n \times n$ symmetric matrix. Then:

- there are real numbers $\lambda_n \geq \lambda_{n-1} \geq \cdots \geq \lambda_1$ and linearly independent vectors $v_n, \ldots, v_1$ in $\mathbf{R}^n$ such that $Dv_i = \lambda_i v_i$.
- If $\lambda_i \neq \lambda_j$, then v_i and v_j are orthogonal.
- there is an orthonormal basis $u_1, \ldots, u_n$ for $\mathbb{R}^n$ such that $Du_i = \lambda_i u_i$.
- if P is the matrix whose columns are the u_i, then $PP^\intercal = I$ and $P^\intercal DP$ is the diagonal matrix Λ whose diagonal entries are the λ_i.

Application in Data Science

Suppose that X is an $N \times k$ data matrix with N sample points each having k real valued features.

We want to generate new features by combining the existing features

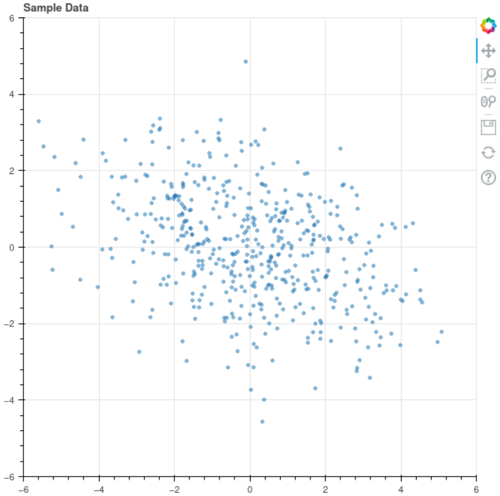
The new features are sometimes called scores

Example: class score is weighted sum of scores on individual assignments:

$$S = w_1 f_1 + w_2 f_2 + \cdots w_k f_k$$

Which scores are most informative? Those that "spread out the data" the most.

Some data



Covariance matrix

Assume that the features all have mean value zero. The *covariance matrix* of the data is

$$D = \frac{1}{N} X^{\intercal} X.$$

It is symmetric.

For the data above this matrix is

$$D = \begin{pmatrix} 4.32 & -1.2 \\ -1.2 & 2.16 \end{pmatrix}$$

Spectral theorem in this case

The λ's are $\lambda_1 = 4.85$ and $\lambda_2 = 1.63$.

The matrix P is

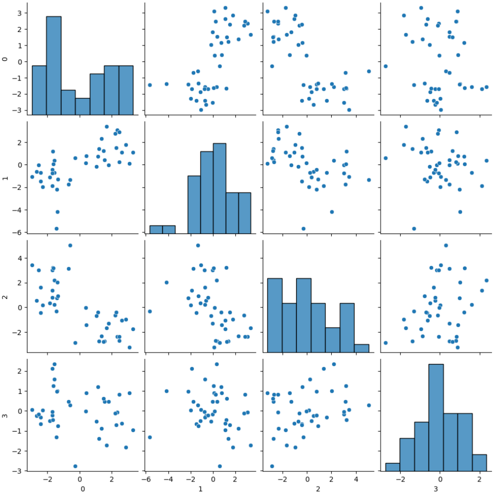
$$P = \begin{pmatrix} -0.41 & -0.91 \\ -0.91 & 0.41 \end{pmatrix}$$

The orthogonal eigenvectors

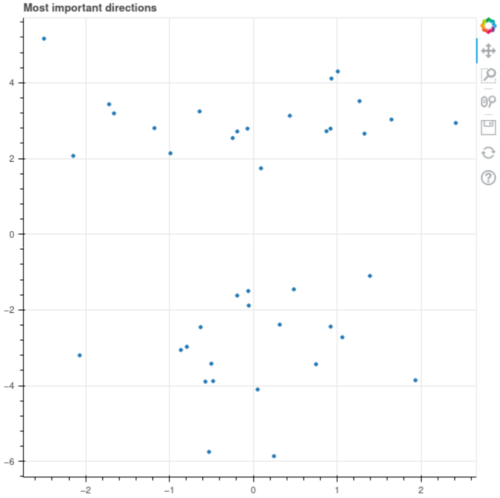
The orthonormal vectors (eigenvectors) are the "natural coordinates" for the data.

Dimensionality Reduction

The “directions” with the largest eigenvalues capture the “most interesting” part of the data. Suppose we have 40 data points with 4 features.



Use the two “directions” with largest eigenvalues



Bayes's Theorem

Bayesian perspective

Our life experiences (and maybe our genetics) give us a set of “prior probabilities” for judging truth or falsehood or evaluating likelihood in the world.

When confronted with a new event, we re-evaluate these prior probabilities and update them.

Example: I move to CT from Colorado where it is very dry. When I go on a hike, I don’t expect rain (my “prior probability for rain” is low). So I don’t bring a raincoat. But it rains a lot in CT, and each time it does, I update my sense of the chance of getting rained on to treat it as more likely; eventually I decide that when I hike in CT I need to bring a raincoat.

Bayes's Theorem

Theorem: Let A and B be events in a probability space. Then

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

where $P(A|B)$ is the conditional probability of A given B.

Bayes Theorem - a simple example

Suppose we wish to understand how something like a vaccine reduces the risk of death from (hypothetically speaking) a new respiratory virus.

In other words, we are interested in comparing:

- the probability of death from the virus in the population at large
- the difference in the probability of death between those vaccinated and those not.

The 2x2 grid

From a population of 10000 people (note: these are totally made up numbers)

	Lived	Died	Totals
Vaccinated	7450	50	7500
Unvaccinated	2470	30	2500
Totals	9820	80	10000

Here if V is the event "vaccinated" and "D" is the event died, we have $P(D|V) = 50/7500 = .6\%$ while $P(D) = .8\%$ and $P(D|\ V) = 1.2\%$.

More on the grid

Notice that:

- more vaccinated people died than unvaccinated people, but
- you are twice as likely to die if you are unvaccinated than if you are vaccinated.

Also

$$P(D|V) = \frac{P(V|D)P(D)}{P(V)} = (.625)(.008)/(.75)$$

The chance of dying is .8%; but if you "learn" that someone is vaccinated, you can improve that estimate to .6%.

Sampling methods and learning

Suppose we wish to build a system that recognizes pictures of cats; and, to begin with, we have a large data set of images marked as "cat" or "not cat". Call this our dataset D.

Our system is a mathematical model or function F that depends on a bunch of parameters Θ. We have a prior distribution $P(\Theta)$ on Θ that represents some kind of initial guess about the parameters (like, say, the Θ are clustered around zero).

Sampling continued

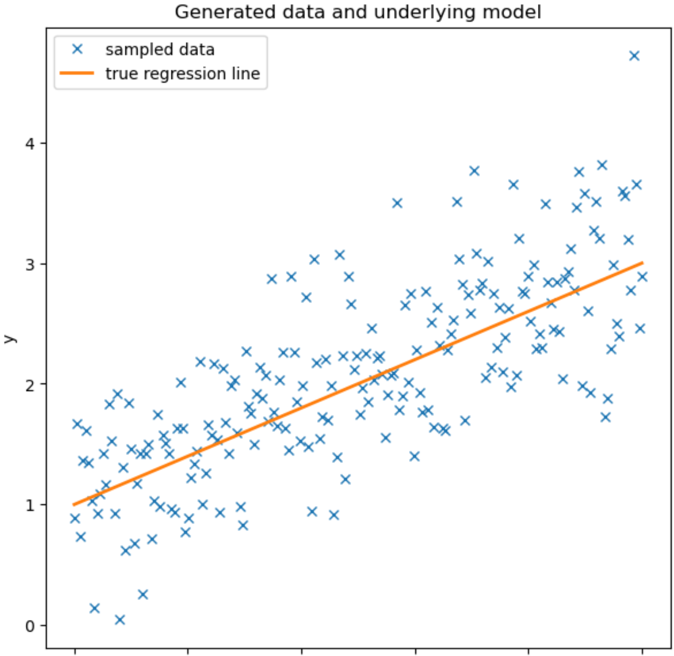
A sampling method uses Bayes Theorem in the form:

$$P(\Theta|D) \propto P(D|\Theta)P(\Theta)$$

Here $P(D|\Theta)$ is the probability that our parameters Θ predict the given data D. $P(\Theta|D)$ is the updated probability distribution on Θ taking the values D into account.

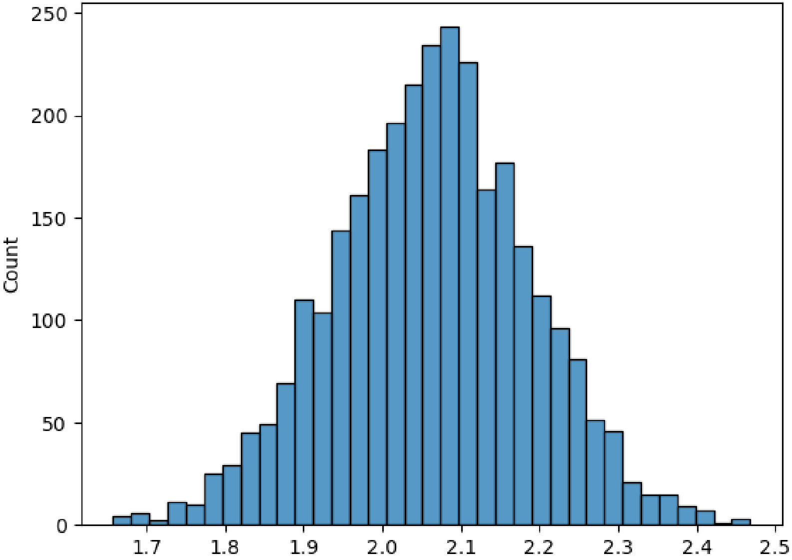
A Monte Carlo sampler draws samples from $P(\Theta|D)$ (the "posterior distribution") based on D; these give better information about Θ in light of the data.

Example



Generated data and underlying model
sampled data
true regression line
y
0
1
2
3
4

The posterior distribution on the slope



The distribution $P(\mathrm{slope}|\mathrm{data})$.

The Chain Rule

The Chain Rule

Let $F : \mathbf{R}^n \to \mathbf{R}^m$ and $G : \mathbf{R}^m \to \mathbf{R}^k$ be differentiable functions at a points $x_0 \in \mathbf{R}^n$ and $x_1 = F(x_0) \in \mathbf{R}^m$. Then

$$D_{x_0}(G \circ F) = D_{x_1}(G) D_{x_0}(F).$$

First Application

Let $F : \mathbf{R}^n \to \mathbf{R}$ be a function of n variables x_1,. . . , x_n. Then the gradient vector

$$\nabla F = \begin{bmatrix} \frac{\partial F}{x_1} & \cdots & \frac{\partial F}{x_n} \end{bmatrix}$$

points in the direction of most rapid increase of F.

Proof: Consider

$$\frac{d}{dt} F(\mathbf{x} + t\mathbf{v})|_{t=0} = \nabla F \cdot \mathbf{v}$$

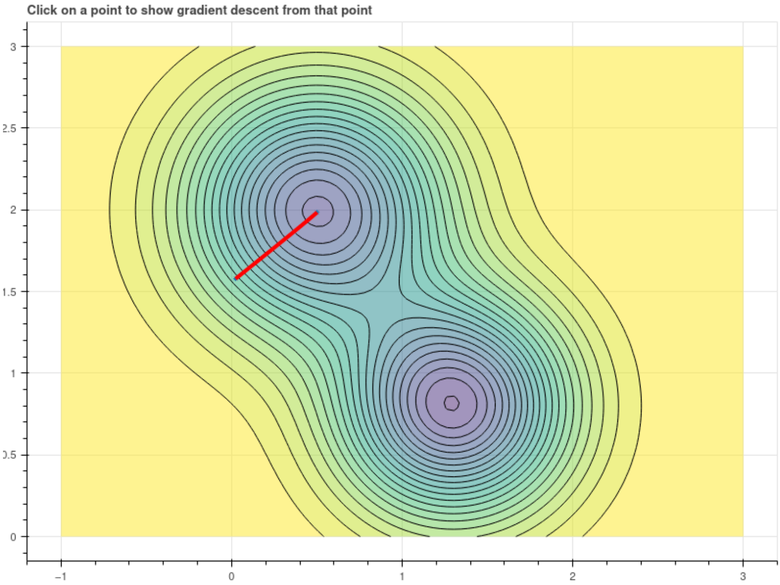
which measures the rate of change of F as you travel in with velocity v. If $\|\mathbf{v}\|^2 = 1$ (so you travel at speeed one) this is maximal when $\mathbf{v}$ points in the direction of ∇F.

Gradient Ascent/Descent

Similarly, F decreases most rapidly if you move in the direction of $-\nabla F$.

A machine learning algorithm is typically a complicated function $F(x; u)$ where x is the data and u are a set of unknown parameters. The "goodness" of our function is controlled by a "loss" or "error" function $L(x; u)$. We try to adjust the weights u to minimize this.

Algorithm: (Gradient Descent) Iteratively compute the gradient ∇L of L with respect to the variables u, and then repeatedly modify u by a small multiple of the gradient, reducing L at each step, until this process stabilizes.


Click on a point to show gradient descent from that point
3
2.5
2
1.5
1
0.5
0
−1
0
1
2
3

Animation

Gradient Descent in Deep Learning

A deep learning algorithm is a composition of a sequence of linear and nonlinear operations:

$$F(x; u) = L_1(u_1) \circ L_2(u_2) \circ \cdots \circ L_n(u_n)$$

To optimize $F(x; u)$ we apply some version of gradient descent to minimize the "loss" function by varying the u_i.

Deep learning software like pytorch can compute the chain rule "automatically".

Example

Least Squares Via Torch

- Loss is MSE
- Model is z=wx+b
- Derivative of MSE with respect to w is

$$\frac{-2}{10}\sum_{i=1}^{10}(z_i - wx_i - b)x_i$$

Code

```
x_data = torch.tensor(x.reshape(10,1))
w=torch.rand(1,1,dtype=torch.float64,requires_grad=True)
b=torch.rand(1,1,dtype=torch.float64,requires_grad=True)
y_data = torch.tensor(y.reshape(10,1))
z_data=torch.matmul(x_data,w)+b
loss = torch.nn.functional.mse_loss(z_data,y_data)
```

Results

```
print(torch.sum(-2*(z_data-y_data)*x_data)/10)
```

and

```
loss.backward()
print(w.grad)
```

are the same.