

Everything you wanted to know about the mathematics of dimensionality reduction and visualization but were afraid to ask: Teaching resources and activities

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Abstract

This work presents some teaching resources and activities to understand the mathematics of machine learning, unsupervised learning and visualization.

Introduction and basics

This work presents some teaching resources and activities to understand the mathematics of machine learning and unsupervised learning.

Some concepts to be covered are:

1. vector spaces

inner product

generalization of length and distance

related to norm

generalisation of angle

orthogonal

linear combination of basis

projection on to lower dimensional space

2. necker cube

3. mirror image in 4d

4. <https://www.coursera.org/learn/pca-machine-learning/lecture/svsZI/inner-product-length-of-vectors>

5. dot product

6. eigenvalues and eigenvectors of covariance matrix

7. other and probabilistic interpretations of PCA

<https://www.coursera.org/learn/pca-machine-learning/lecture/qrMP1/other-interpretations-of-pca-optional>

8. PCA resources and book

<https://hastie.su.domains/ISLR2/ISLRv2-website.pdf>

<https://www.quora.com/What-is-an-intuitive-explanation-for-PCA>

<https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues>

9. eigenvalues

<https://www.youtube.com/watch?v=PFDu9oVAE-g>

10. transformation

11. axis of rotation

12. eigenvalue 1 means just fixed in place

13. determinants

14. rotation

15. eigenvalues related to linear system of equations

<https://www.cs.unm.edu/~williams/cs530/kl3.pdf>

<https://ncert.nic.in/ncerts/l/lemh103.pdf>

16. mathematical basics of machine learning

linear algebra

<https://mml-book.github.io/book/mml-book.pdf>

17. inner product generalization of length

https://www.youtube.com/watch?v=Ww_aQqWZh8

Dot product

The dot product is defined as

$$x^T y$$

Length

The length is defined as

$$|x| = \sqrt{x^T x}$$

https://en.wikipedia.org/wiki/Dot_product#Tensors

Distance

The length/distance between two vectors is

$$|x - y| = \sqrt{(x - y)^T (x - y)}$$

<https://www.coursera.org/learn/pca-machine-learning/lecture/qQfS4/dot-product>

Angle between two vectors

The angle α between two vectors x and y is given by:

$$\alpha = \frac{x^T y}{||x|| ||y||}$$

But we know that

$$||x|| = \sqrt{x^T x} \tag{1}$$

Hence we get the following relationship for the angle

$$\alpha = \frac{x^T y}{\sqrt{x^T x} \sqrt{y^T y}}$$

Generalizations of dot product: inner product

The inner product generalizes the notion of dot product:

$$\langle x, y \rangle$$

Length: in terms of inner product

The length of the vector can be defined in terms of the inner product as

$$\|x\| = \sqrt{\langle x, x \rangle}$$

The length is also called the norm.

Distance

Distance: in terms of inner product

$$d(x, y) = \sqrt{\langle x - y, x - y \rangle}$$

This assumes we can do vector addition and subtraction.

Angle

1. Symmetric
2. Bilinear
3. Positive definite

Other properties are:

1. Triangle inequality

$$\|x + y\| \leq \|x\| + \|y\|$$

- 2.

$$\|\lambda x\| = |\lambda| \|x\|$$

3. Cauchy-Schwarz inequality

$$\| \langle x, y \rangle \|$$

What if not symmetric like K-L divergence?

[youtube.com/watch?v=lrSQH.69MTM](https://www.youtube.com/watch?v=lrSQH.69MTM)

orthogonal polynomials

inner product for polynomials

convolution as an inner product

https://www.google.com/search?q=is+convolution+an+inner+product&gs_lvs=1#tts=0

orthogonal functions

<https://www.youtube.com/watch?v=ZYf0tz9oVz8>

angle between polynomials

<https://math.stackexchange.com/questions/556291/angle-between-polynomials>

Other generalizations

Orthogonal functions

<https://www.youtube.com/watch?v=ZYf0tz9oVz8>

Fourier series is a least squares problem

<https://www.youtube.com/watch?v=u8ccubUfhKY>

polynomials as vectors

<https://www.youtube.com/watch?v=xhTciBubSfM>

Inner product can be defined for functions as well. This can be defined with integration.

The inner product of two functions u and v is defined as:

$$\langle u, v \rangle = \int_a^b u(x)v(x)dx$$

Functions can be orthogonal to each other, with respect to this inner product. For example, consider the functions $\cos(x)$ and $\sin(x)$:

$$\langle \cos(x), \sin(x) \rangle = \int_{-\pi}^{\pi} \cos(x) \sin(x) dx = 0$$

Hence this is a basis.

Projecting other functions onto this basis is the idea behind Fourier series.

Basis

Basis vectors

Any other vector can be composed of a linear combination of these basis vectors

Orthogonal basis: vectors that are orthogonal to each other angle between them is 90 degrees.

$$\alpha = \frac{x^T y}{||x|| ||y||}$$

For example, consider two vectors b_1 and b_2 . They can form an orthonormal basis if their inner product is:

$$\langle b_1, b_2 \rangle = 0$$

and their length is

$$||b_1|| = 1$$

and

$$||b_2|| = 1$$

Basis of polynomials

<https://www.youtube.com/watch?v=pYoGYQOXqTk>

why $1, x, x^2$ is a terrible basis

Similarity metrics

https://www.researchgate.net/publication/372487573_Similarity_metrics_metrics_and_conditionally_negative_definite_func

Projection onto 1D

When we project x onto U , we are trying to find $\pi_U(x)$. This is the projection of x onto U . We will denote this as

$$\pi_U(x)$$

x is a vector.

Hence we want something that is closest to x . Hence the following quantity is minimal:

$$||x - \pi_U(x)||$$

$x - \pi_U(x)$ is orthogonal to U . Hence $x - \pi_U(x)$ is a basis vector of U . Let us call this basis vector b .

Hence b and $x - \pi_U(x)$ are orthogonal to each other.

By definition of orthogonality the following holds for the inner product:

$$\langle b, x - \pi_U(x) \rangle = 0$$

Also since $\pi_U(x)$ is a projection onto b , it must be a multiple of b . Hence

$$\pi_U(x) = \lambda b$$

Let us now try to find λ .

Let us start from the orthogonality condition:

$$\langle b, x - \pi_U(x) \rangle = 0$$

Substituting the value of $\pi_U(x) = \lambda b$ we get

$$\langle b, x - \lambda b \rangle = 0$$

The inner product is bilinear. Hence we get

$$\langle b, x \rangle - \lambda \langle b, b \rangle = 0$$

Rearranging we get

$$\lambda = \frac{\langle b, x \rangle}{\langle b, b \rangle}$$

Noting that $\langle b, b \rangle = \|b\|^2$ is the norm we have:

$$\lambda = \frac{\langle b, x \rangle}{\|b\|^2}$$

If the inner product is the dot product we have

$$\lambda = \frac{b^T x}{\|b\|^2}$$

For an orthonormal basis, we have $\|b\| = 1$. Hence

$$\lambda = b^T x$$

The projected vector $\pi_U(x)$ is

$$\pi_U(x) = \lambda b = \frac{b^T x b}{\|b\|^2}$$

Generalized projection onto n-dimensions

We now generalize these results to n -dimensions.

$\pi_U(x)$ is the projection and hence must be a linear combination of the basis vectors b_1, b_2, \dots

Hence we have the following condition:

$$\pi_U(x) = \sum \lambda_i b_i$$

Concretely if there are m basis vectors:

$$\pi_U(x) = \sum_i^m \lambda_i b_i$$

This can be written in matrix notation as

$$\pi_U(x) = \sum_i^m \lambda_i b_i = B\lambda$$

Now we want the closest or minimum distance. Hence the basis vector b_1 and $\pi_U(x) - x$ must be orthogonal.

Hence the inner product must be 0:

$$\langle b_1, \pi_U(x) - x \rangle = 0$$

and so on for all the basis vectors

$$\langle b_2, \pi_U(x) - x \rangle = 0$$

$$\langle b_3, \pi_U(x) - x \rangle = 0$$

and so on for all the basis vectors.

This can be written in matrix notation as:

$$\langle B, \pi_U(x) - x \rangle = 0$$

or using $\pi_U(x) = B\lambda$ we have

$$\langle B, B\lambda - x \rangle = 0$$

We have to now find λ .

For the case of the dot product this becomes

$$B^T(B\lambda - x) = 0$$

Solving we get

$$B^T B \lambda = B^T x$$

Simplifying we get

$$\lambda = (B^T B)^{-1} B^T x$$

Matrix decompositions

The determinant is the measure of volume.

The determinant is also invariant under choice of basis of a linear mapping.

Characteristic polynomial

$$\det(A - \lambda I) = c_0 + c_1 \lambda + c_2 \lambda^2 + \dots$$

The eigenvalue equation is

$$Ax = \lambda x$$

$$\det(A - \lambda I) = 0$$

Eigenvalues, determinant, and trace are key parameters of a linear mapping that are invariant under a change of basis.

<https://math.stackexchange.com/questions/507641/show-that-the-determinant-of-a-is-equal-to-the-product-of-its-eigenvalues>

You can calculate determinants in your web browser using WolframAlpha. See link below:

<https://www.wolframalpha.com/calculators/determinant-calculator>

These are a series of transformations.

Spectral theorem

As a consequence of the spectral theorem, for a symmetric matrix A , we can get:

$$A = PDP^T$$

where D is a diagonal matrix and P is a matrix such that the columns have the eigenvectors.

The determinant of a matrix A is the product of its eigenvalues

$$\det(A) = \prod_i \lambda_i$$

The trace of a matrix is the sum of its eigenvalues:

$$\text{tr}(A) = \sum_i \lambda_i$$

As a result of this, since

$$Ax_1 = \lambda x_1$$

where x_1 is the eigenvector and λ is the eigenvalue

the eigenvalue scales and stretches the original length by λ .

Hence the area increases by $\lambda_1 \lambda_2$ and the perimeter becomes $2(\lambda_1 + \lambda_2)$.

This is how the procedure transforms the original system.

CONCEPT:

A is a matrix of transformations. Eigenvectors give us the direction of transformation. Eigenvalues show us how much to stretch.

Cholesky decomposition

This is a square root like operation for matrices:

$$A = LL^T$$

Eigendecomposition

$$A = PDP^{-1}$$

where D is a diagonal matrix whose diagonal entries are the eigenvalues and P is a matrix such that the columns have the eigenvectors.

This represents a series of transformations:

1. P^{-1} performs a change of basis into the eigenbasis.
2. The diagonal matrix D scales the vectors by the eigenvalues λ
3. P scales the vectors back into the original co-ordinate system.

Singular value decomposition

$$A = U\Sigma V^T$$

where A is a rectangular matrix.

This represents a series of transformations:

1. V^T performs a change of basis.
2. The singular matrix Σ scales the vectors and performs dimensionality reduction (or augmentation).
3. U scales the vectors back into the original co-ordinate system.

Singular value equation

Similar to the eigenvalue equation, there is a singular value equation:

$$Av = \sigma u$$

Compare this to the eigenvalue equation:

$$Ax = \lambda x$$

where x is the same on both sides.

This yields $AV = U\Sigma$ which upon rearrangement gives us $A = U\Sigma V^{-1}$

Applications of SVD

SVD can be used to find structure in matrices, eg. structure in movie ratings, consumer behaviour, matrix approximation, etc.

It can be used to find the low-rank representation. The assumption is that movie preferences are linear combinations.

Other extensions and applications include multi-dimensional scaling, isomap and PCA.

Generalization of SVD to tensors

Tucker decomposition generalizes SVD to tensors (multi-dimensional arrays):

https://www.alexejgossmann.com/tensor_decomposition_tucker/

Other reading material

Non-negative matrix factorization

https://en.wikipedia.org/wiki/Non-negative_matrix_factorization

Matrix norm and Frobenius norm

PCA

PCA is the diagonalization of the covariance matrix.

The covariance between two random variables is the expected value of the product of the deviation from their means.

Let x_n be the data points with mean 0.

The data covariance matrix is given by

$$S = \frac{1}{N} \sum_{n=1}^N x_n x_n^T$$

The data points x_n can be compressed or projected onto a lower dimensional space z_n

$$z_n = B^T x_n$$

where B is a projection matrix.

$$B = [b_1, b_2, \dots]$$

where the columns of B are orthonormal.

$$b_i^T b_i = 1$$

$$b_i^T b_j = 0$$

if $i \neq j$.

1. PCA assumes a linear relationship between the data points and the lower dimensional representation, since $z_n = B^T x_n$.
2. PCA also assumes a squared reconstruction error (dot product).

Derivations

PCA aims to maximize the variance of the coordinates. Let z_1 be the first projected coordinate.

We aim to maximize the variance

$$\frac{1}{N} \sum_{n=1}^N z_{1n}^2$$

where $z_{1n} = b_1^T x_n$ (the projected coordinate).

Substituting this into the equation above, we get the following.

$$\frac{1}{N} \sum_{n=1}^N (b_1^T x_n)^2$$

Again we note that PCA uses the dot product. The dot product is symmetric with respect to arguments i.e.

$$b_1^T x_n = x_n^T b_1$$

Using this, we get the following

$$\frac{1}{N} \sum_{n=1}^N b_1^T x_n x_n^T b_1$$

Pulling in the summation inside (since b_1 does not depend on n), we get

$$\frac{1}{N} b_1^T \left(\sum_{n=1}^N x_n x_n^T \right) b_1$$

$$b_1^T \left(\frac{1}{N} \sum_{n=1}^N x_n x_n^T \right) b_1$$

The term in the summation (within parentheses) is the data covariance matrix S . Hence we get

$$b_1^T S b_1$$

This is the quantity we aim to maximize.

$$\max_{b_1} b_1^T S b_1$$

where we aim to find b_1 such that the quantity is maximized.

Maximizing this quantity we get the following relationships

$$S b_1 = \lambda b_1$$

which is the eigenvector/eigendecomposition equation and

$$b_1^T b_1 = 1$$

which implies that the basis vector has length 1.

Hence we choose the basis vector corresponding to the largest eigenvalue of the data covariance matrix.

λ represents the variance explained by the first coordinate b_1 . $\sqrt{\lambda}$ is called the loading.

In summary, PCA is

1. linear in its variables.
2. uses the dot product (one form of the inner product).

3. uses the squared error as the loss function.

Alternative derivation

We outline an alternative derivation here.

Let x_n be a point in the original space and z_m is the corresponding point in lower-dimensional space. z_m can be projected back into the original space. Let us call that \hat{x}_n (the corresponding point in a lower-dimensional space).

If b_m denotes the basis vectors, then since PCA is linear the point in lower-dimensional space (z_m) is a linear combination of the basis vectors:

$$\hat{x}_n = \sum_{m=1}^M z_m b_m$$

where z_m is the corresponding point in lower-dimensional space.

We intend to minimize the sum of squared error (loss function) between the original points and the reprojected points (reconstruction loss)

$$J = \frac{1}{N} \sum_{n=1}^N \|x_n - \hat{x}_n\|^2$$

This is the reconstruction loss.

We can now use gradient descent to find the minima or find an explicit formula.

Taking partial derivatives:

$$\frac{\partial J}{\partial z_m} = \frac{\partial J}{\partial x_n} \frac{\partial x_n}{\partial z_m}$$

where each term on the RHS is:

$$\frac{\partial J}{\partial x_n} = -\frac{2}{N} (x_n - \hat{x}_n)^T$$

Now we use the relationship $\hat{x}_n = \sum_{m=1}^M z_m b_m$ to find $\frac{\partial x_n}{\partial z_m}$

$$\frac{\partial x_n}{\partial z_m} = b_m$$

Setting $\frac{\partial J}{\partial z_m} = \frac{\partial J}{\partial x_n} \frac{\partial x_n}{\partial z_m}$ to 0, we get

$$-\frac{2}{N}(x_n - \hat{x}_n)^T b_m = 0$$

Rearranging we get

$$x_n b_m = \hat{x}_n^T b_m$$

On the RHS, we can write \hat{x}_n as $z_m b_m$

Hence we get

$$x_n b_m = (z_m b_m)^T b_m$$

Simplifying we get

$$x_n b_m = z_m^T b_m^T b_m$$

The basis vectors are orthonormal $b_m^T b_m = 1$. So we get

$$x_n b_m = z_m^T$$

$$z_m^T = x_n b_m$$

The optimal coordinate is a normal projection.

MDS

MDS (multi-dimensional scaling) is the diagonalization of the distance matrix (each pair).

tSNE

distance matrix

gram matrix

<https://towardsdatascience.com/t-sne-clearly-explained-d84c537f53a>

There are many pitfalls to using tSNE. See for example [1].

Other pitfalls are that distances are not preserved. For example, a 2D map is a projection from 3D.

UMAP

<https://pair-code.github.io/understanding-umap/>

<https://pair-code.github.io/understanding-umap/supplement.html>

Autoencoders

Activities

1. Activities related to PCA

<https://www.quora.com/What-is-an-intuitive-explanation-for-PCA>

<https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues>

2. Eigenvalues

<https://www.youtube.com/watch?v=PFDu9oVAE-g>

3. Play with these tools (PCA, tSNE) in the browser

<http://projector.tensorflow.org/>

4. There are many pitfalls to using tSNE. See for example [1].

Applications and case studies

Some concrete applications and case studies are outlined here.

1. removing outliers in genomic data using PCA.

Frequently in genomic data we may have to remove outliers. These outliers may be due to technical/batch effects or unknown reasons not connected to biology.

This has implications for any tests performed downstream. For example, t-tests can be performed downstream after performing PCA. If there are outliers, it may affect the results of the t-test. See [2] for an application to single-cell and bulk sequencing data.

2. tSNE can be used for hypothesis generation. There are many pitfalls to this. See for example [1].
3. Other pitfalls are that distances are not preserved. For example, a 2D map is a projection from 3D.
4. Visualizing the data (for example, time-series data) can reveal what kinds of models would be appropriate [3]. For example, if time series data has some seasonality, then a seasonal auto-regressive model (SARIMA) may be appropriate.

Visualization may also reveal if the underlying model/assumptions may have changed after a certain time. For example, in financial time-series data, there usually is a change after 2008 due to the global financial crisis.

This may suggest that a new model or more data is required [3].

Basics and pitfalls in data visualization

1. Know your audience
2. Pick visualization based on audience
3. Visualize data and then pick models
4. Add narrative

Principles of data visualization by Edward Tufte

Edward Tufte

<https://jeffhale.medium.com/five-takeaways-from-the-visual-display-of-quantitative-information-dd36dae35299>

1. <https://pudding.cool/projects/heat-records-map>

<https://pudding.cool/2022/12/yard-sale/>

power law distributions

1. Above all else show the data.
2. “Graphical excellence consists of complex ideas communicated with clarity, precision, and efficiency.” (p. 51)
3. Keep it proportional. “Lie Factor = size of effect shown in graphic divided by size of effect in data” (p.57). Keep it close to 1.
4. You do not have to use a graphic when there is not much data - a table is often better.
5. Pie charts are useless.

Minard drawing

The best statistical graphic ever drawn

<https://www.edwardtufte.com/tufte/minard>

Displaying multi-dimensional data in one plot.

Code for analysing this data

https://github.com/joannecheng/napoleon_analysis

<https://thoughtbot.com/blog/analyzing-minards-visualization-of-napoleons-1812-march>

Visualizations can be misleading

Visualizations can be misleading. Take the tSNE algorithm for example [1].

You can go through this resource which is also an interactive notebook:

<https://distill.pub/2016/misread-tsne/>

1. Distances not preserved in tSNE
2. Cluster sizes do not matter.
3. You can sometimes see some shapes.
4. random does not always look random.

Now read the plots in the paper [2]. What pitfalls do you see in communicating these insights to experimentalists?

Visualization for help with picking models

Visualization of data can help us pick the right models. For example, many models assume that the data or noise come from some underlying distribution (such as a Gaussian).

We can and should visualize the distribution of the data. The model residuals should also be visualized [4].

Most models come with a number of assumptions. These assumptions should be tested [4]. Some of them are:

1. Linearity
2. Normality of residuals. Use q-q plot (quantile-quantile plot).

<https://www.youtube.com/watch?v=okjYjClSjOg>

Code in Python

<https://stackoverflow.com/questions/13865596/quantile-quantile-plot-using-scipy>

Code in R [4]

```
hist(residuals(xmdl))
```

```
qqnorm(residuals(xmdl))
```

3. Collinearity
4. Homoskedasticity

More details and code in R is available in [4] and the following repository:

https://bitbucket.org/neelsoumya/anova_linear_mixed_effects_examples/

Code for visualization in R, model diagnostics and linear mixed effects models is available here:

https://github.com/neelsoumya/anova_linear_mixed_effects_examples

https://github.com/neelsoumya/anova_linear_mixed_effects_examples

Data transformations

Other cases:

Log-log plot. Check these for normality. For example, if the distribution is not normal, then maybe you can transform the data somehow.

See the following resource:

<https://statisticsbyjim.com/regression/log-log-plots/>

Time series data and autocorrelations

Time series data. We need to consider:

1. Autocorrelations.
2. Seasonality.

Visualizing the data (for example, time-series data) can reveal what kinds of models would be appropriate [3]. For example, if time series data has some seasonality, then a seasonal auto-regressive model (SARIMA) may be appropriate.

Visualization may also reveal if the underlying model/assumptions may have changed after a certain time. For example, in financial time-series data, there usually is a change after 2008 due to the global financial crisis.

This may suggest that a new model or more data is required [3].

Other principles of data visualisation

From Edward Tufte

1. Design effect vs. data effect
2. The number of information carrying dimensions depicted should not exceed the number of dimensions of the data. Area and volumes.

Resources and Activities

Here are some resources for students to browse through.

Thinking outside the 10 dimensional box:

<https://www.youtube.com/watch?v=zwAD6dRSVyI>

<https://www.popularmechanics.com/science/math/a27737/visualize-higher-dimensions/>

Different kinds of cartographic projections

<https://whereexactlymaps.com/blogs/articles/an-introduction-to-map-projections>

<https://www.viewsoftheworld.net/?p=752>

Tufte's principles in R

<https://jtr13.github.io/cc19/tuftes-principles-of-data-ink.html>

Data visualization excellence

<https://classes.engr.oregonstate.edu/eecs/winter2018/cs519-400/modules/4-data-visualization/1-excellence-integrity/>

Great talks on visualization and how to do it right

https://www.youtube.com/watch?v=iipVIV4I_Vg&list=PLB2SCq-tZtVnXalwtfVPcjwy0xJbu-btN&index=4

Minard drawing (The best statistical graphic ever drawn)

<https://www.edwardtufte.com/tufte/minard>

code for analysing this data

https://github.com/joannecheng/napoleon_analysis

<https://thoughtbot.com/blog/analyzing-minards-visualization-of-napoleons-1812-march>

Resources

All resources are available here:

https://github.com/neelsoumya/visualization_lecture

Declarations

Acknowledgements

We acknowledge the help and support of the Accelerate team.

Funding statement

This work was funded by Accelerate Research Fellowship. The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript. The views expressed are those of the authors and not necessarily those of the funders.

Conflicts of interests

All authors declare they have no conflicts of interest to disclose.

Ethics

No ethics approval was necessary.

Data accessibility

This study does not generate any clinical data.

Author contributions

SB carried out the analysis and implementation, participated in the design of the study and wrote the manuscript. All authors gave final approval for publication.

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