THE GEORGE WASHINGTON UNIVERSITY
WASHINGTON, DC

CS 4364/6364

Machine Learning

Fall Semester 8/29/2023
Lecture 2.
Linear Algebra Review + Principal Components Analysis

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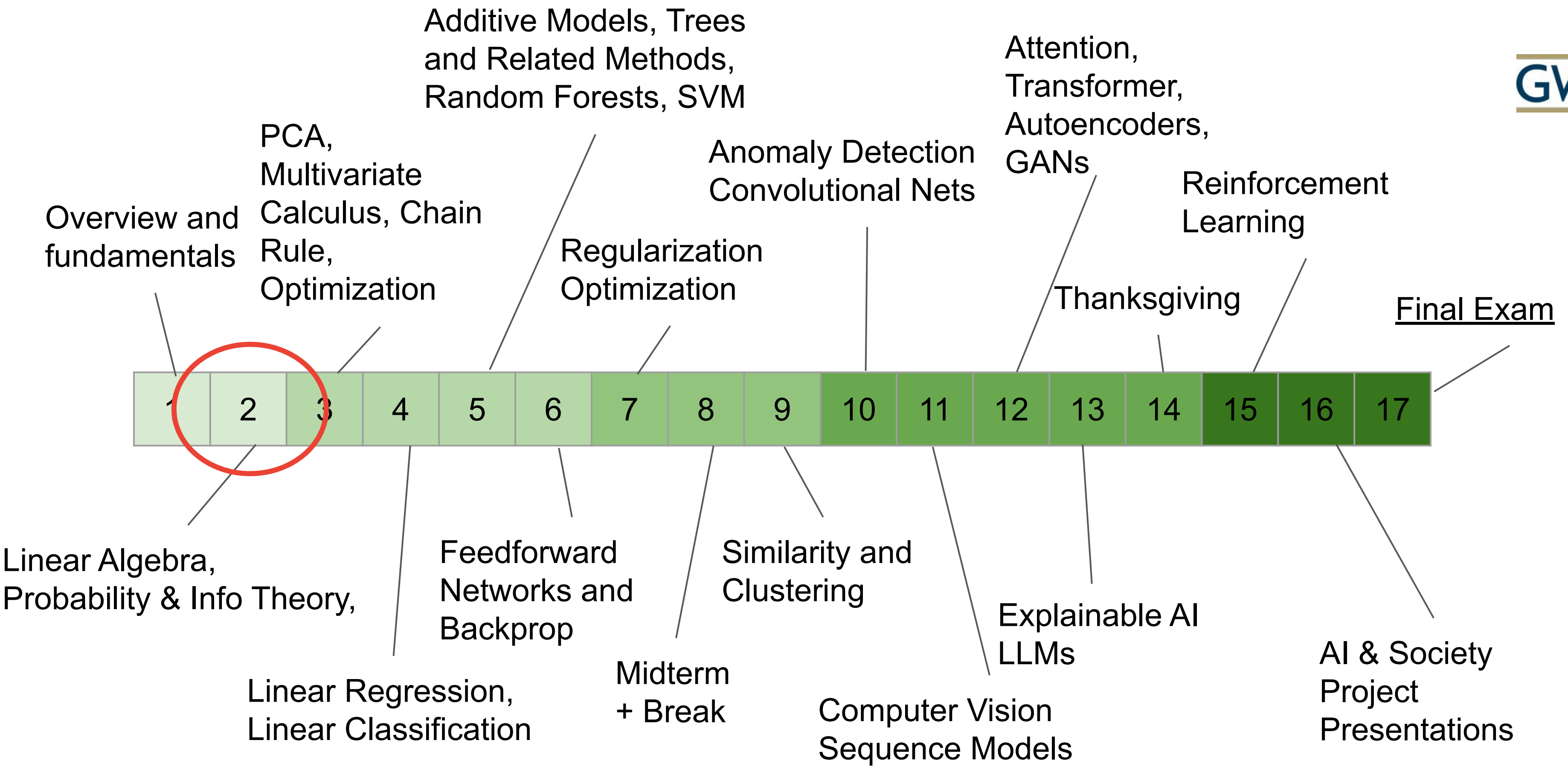
Additive Models, Trees and Related Methods, Random Forests, SVM
PCA, Multivariate Calculus, Chain Rule, Optimization
Overview and fundamentals
Regularization Optimization
Anomaly Detection Convolutional Nets
Attention, Transformer, Autoencoders, GANs
Reinforcement Learning
Thanksgiving
Final Exam
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Linear Algebra, Probability & Info Theory,
Linear Regression, Linear Classification
Feedforward Networks and Backprop
Midterm + Break
Similarity and Clustering
Computer Vision Sequence Models
Explainable AI LLMs
AI & Society Project Presentations

Homework 1

Homework 1

Due date: 9/12/2023

Familiarization with the environment:

- Python Language and Programming Style Guide
- ML Libraries: Tensorflow, Keras, Scikit-Learn
- Google Colaboratory Notebook
- Tensorboard

Training and Evaluating Binary Classifiers

- Cross-fold validation

Hyperparameter Tuning

Comparing Linear Regression against Neural Network

Review of Linear Algebra

- High-level refresher
- Focused on the most important parts for machine learning
- Recommend dusting off your books on Linear Algebra, Calculus, and Probabilities

Scalars

- A single number
- Integers, real numbers, rational numbers
- We’ll denote them with an italic:

$$a, u, d$$

Vectors

- A vector is a 1-D array of numbers:

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Real-valued in dimension n: $\mathbb{R}^n$

- Integer/binary in dimension n: $\mathbb{Z}^n$

Matrices

- A 2-D array of numbers:

$$\begin{array}{cc} & \text{column} \\ \mathbf{A} = & \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \end{array} \quad \text{row}$$

- Example notation for type and shape:

$$\mathbf{A} \in \mathbb{R}^{m \times n}$$

Tensors

A tensor is an array of numbers that may have

- Zero dimensions → scalar
- One dimensional → vector
- Two dimensions → matrix
- And any number of dimensions…

Matrix Transpose

$$(\mathbf{A}^{\top})_{i.j} = A_{j,i}$$

$$\boldsymbol{A} = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \\ A_{3,1} & A_{3,2} \end{bmatrix} \Rightarrow \boldsymbol{A}^{\top} = \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \end{bmatrix}$$

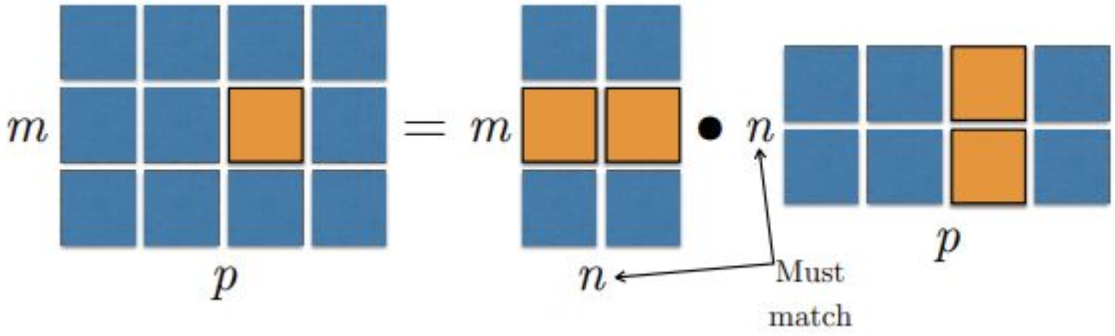
Figure 2.1: The transpose of the matrix can be thought of as a mirror image across the main diagonal.

$$(\mathbf{AB})^{\top} = \mathbf{A}^{\top}\mathbf{B}^{\top}$$

Matrix (Dot) Product

$$\mathbf{C} = \mathbf{AB}$$

$$C_{i,j} = \sum_k A_{i,k} B_{k,j}$$



Identity Matrix

$$\mathbf{I}_n = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \cdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$\mathbf{I}_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\forall x \in \mathbb{R}^n,$$
$$I_n \mathbf{x} = x$$

Systems of Equations

$$\mathbf{A}\boldsymbol{x} = \mathbf{b}$$

Expands to:

$$\mathbf{A}_{1,:}\boldsymbol{x} = b_1$$
$$\mathbf{A}_{2,:}\boldsymbol{x} = b_2$$
$$\dots$$
$$\mathbf{A}_{m,:}\boldsymbol{x} = b_m$$

Solving systems of equations

A linear system of equations can have:

- No solution (Underdetermined)

- Many solutions (Overdetermined)

- Exactly one solution → multiplication by the matrix is an invertible function

Matrix Inversion

Matrix inverse:

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}_n$$

Solving a system using an inverse:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

$$\mathbf{A}^{-1}\mathbf{A}\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

$$\mathbf{I}_n\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

Numerically unstable, but useful for abstract analysis

Matrix Invertibility

A Matrix cannot be inverted if

- More rows than columns
- More columns than rows
- Redundant rows/columns (linearly dependent or low rank)

Norms

Functions measure how large a vector wrt the origin

Similar to a distance between zero and the point represented by a vector (i.e., distance from zero)

$$f(\mathbf{x}) = 0 \Rightarrow \mathbf{x} = \mathbf{0}$$

$$f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$$ Triangle inequality

$$\forall \alpha \in \mathbb{R}, f(\alpha \mathbf{x}) = |\alpha| f(\mathbf{x})$$

Norms

L^p norm (*Minkowski* norm):

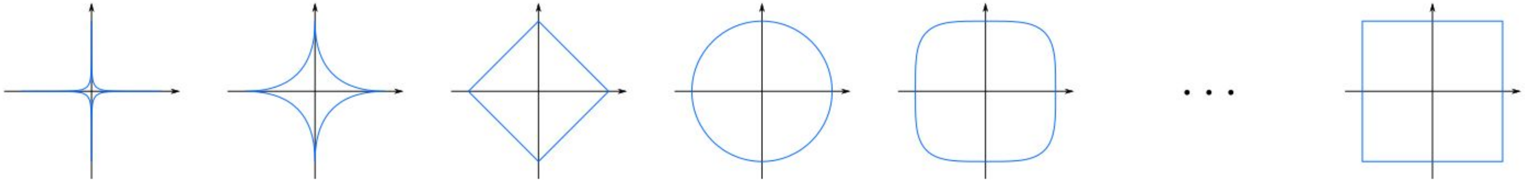
$$||\mathbf{x}||_p = \left(\sum_i |x_i|^p\right)^{\frac{1}{p}}$$

Most popular norm: $L2$ *Euclidean*, $p = 2$

$L1$ City Block norm

$$p = 1 : ||\mathbf{x}||_i = \sum_i |x_i|$$

Max norm $L_\infty : ||\mathbf{x}|| = \max_i |x_i|$



$p = 2^{-2} = 0.25$ | $p = 2^{-1} = 0.5$ | $p = 2^{0} = 1$ | $p = 2^{1} = 2$ | $p = 2^{2} = 4$ | … | $p = 2^{\infty} = \infty$

https://en.wikipedia.org/wiki/Minkowski_distance

Frobenius Norm

How large the values of a matrix are:

$$||A||_F = \sqrt{\sum_{i,j} A_{i,j}^2}$$

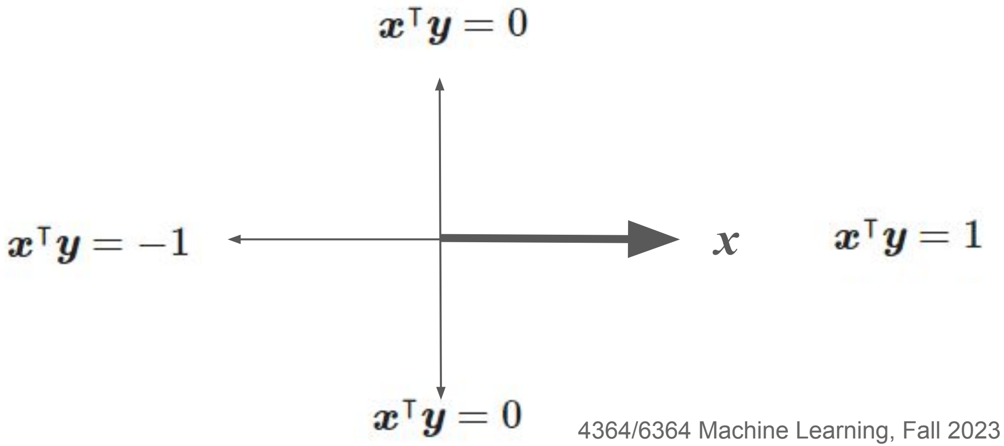
⇒ If A is an error matrix, Frobenius norm is the overall error value which we want to minimize

Dot product

The dot product of two vectors $\boldsymbol{x}, \boldsymbol{y}$ can be written in terms of norms:

$$\boldsymbol{x}^\top \boldsymbol{y} = ||\boldsymbol{x}||_2 \, ||\boldsymbol{y}||_2 \cos\theta$$

Where θ is the angle between $\boldsymbol{x}, \boldsymbol{y}$:



Special Matrices and Vectors

Unit vector:

$$||x||_2 = 1$$

Symmetric Matrix:

$$\mathbf{A} = \mathbf{A}^\intercal$$

Orthogonal Matrix:

$$\mathbf{A}^\intercal \mathbf{A} = \mathbf{A}\mathbf{A}^\intercal = \mathbf{I}$$

$$\mathbf{A}^{-1} = \mathbf{A}^\intercal$$

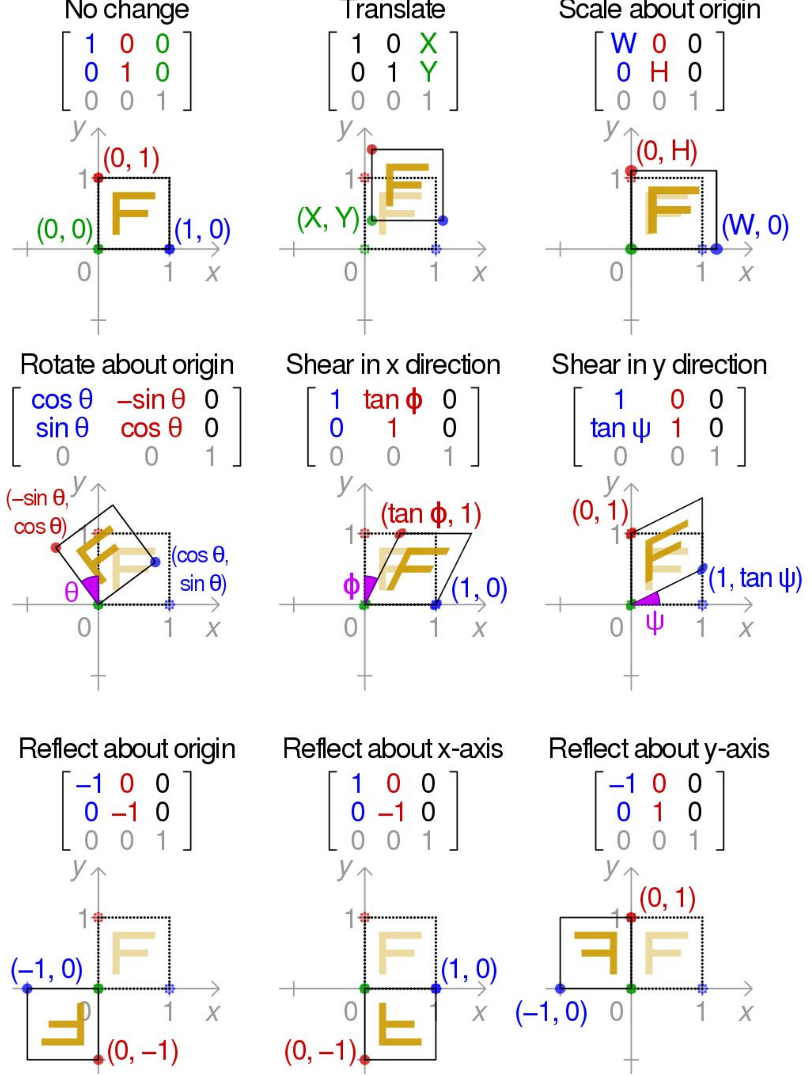
Affine Transformations

Linear matrix transformations that projects

- Points to points
- Lines to lines
- Hyperplanes to hyperplanes

Identity, Translation, Scale, Rotate, Shear and Reflection

A product of one or more affine transformations is itself an affine transformation



Eigendecomposition

Eigenvector $\boldsymbol{v}$ and eigenvalue λ

$$\mathbf{A}\boldsymbol{v} = \lambda\boldsymbol{v}$$

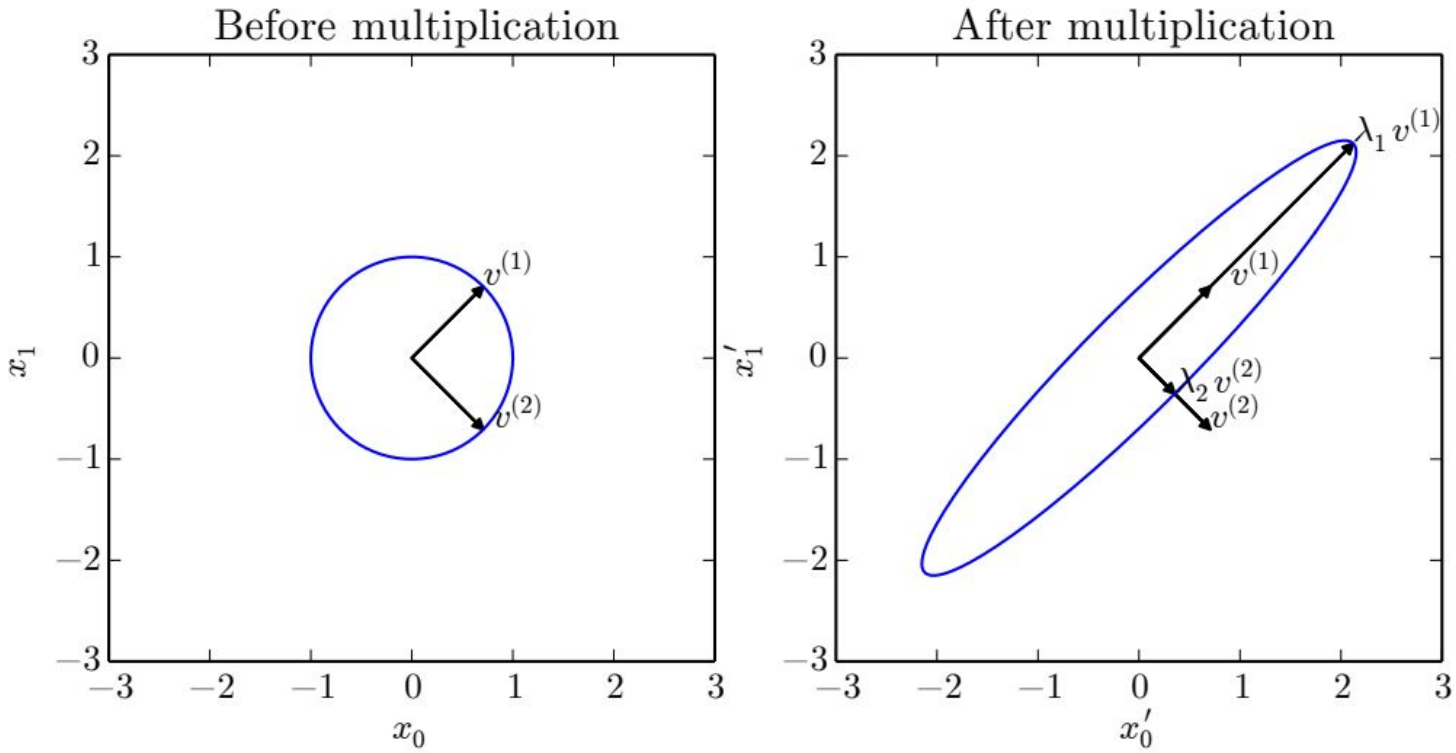
Eigendecomposition of a diagonalizable matrix:

$$\mathbf{A} = \mathbf{V}\mathrm{diag}(\lambda)\mathbf{V}^{-1}$$

Every real symmetric matrix has a real, orthogonal eigendecomposition:

$$\mathbf{A} = \mathbf{Q}\Lambda\mathbf{Q}^{\top}$$

Scaling effect of Eigenvalues



Matrix Terminology

Singular Matrix: any eigenvalue is zero (i.e., pancake)

Positive Definite Matrix: All eigenvalues are positive

Positive Semidefinite Matrix: All eigenvalues are 0 or positive

N**egative Definite Matrix**: All eigenvalues are negative

Negative Semidefinite Matrix: All eigenvalues are 0 or negative

Singular Value Decomposition

Similar to eigendecomposition

More general – matrix need not be square

$\mathbf{D}$: Singular Values (diag)
$\mathbf{U}$: Left-Singular Vectors (orthogonal)
$\mathbf{V}$: Right-Singular Vectors (orthogonal)

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$$

$m \times n$ $\quad$ $m \times m$ $\quad$ $m \times n$ $\quad$ $n \times n$

Moore-Penrose Pseudoinverse

$$\boldsymbol{x} = \mathbf{A}^{+}\boldsymbol{y}$$

If the equation has:

- Exactly one solution: same as the inverse
- No solution: this gives us the solution with the smallest error $||\mathbf{A}\boldsymbol{x} - \boldsymbol{y}||_2$
- Many solutions: this gives us the solution with the samples norm of $\boldsymbol{x}$

Computing the pseudoinverse

The SVD allows for computing the pseudoinverse

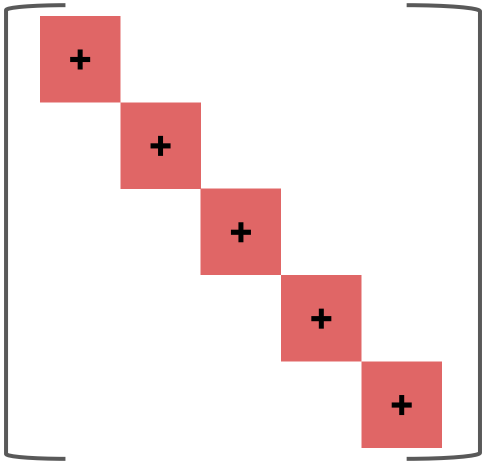
$$\mathbf{A}^{+} = \mathbf{V}\mathbf{D}^{+}\mathbf{U}^{\mathsf{T}}$$

Take the reciprocal of the nonzero entries and the transpose from $\mathbf{D}$ in:

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathsf{T}}$$

Matrix Trace

Sum of the diagonal elements of matrix $\mathbf{A}$



$$\mathrm{Tr}(\mathbf{A}) = \sum_i \mathbf{A}_{i,i}$$

$$\mathrm{Tr}(\mathbf{ABC}) = \mathrm{Tr}(\mathbf{CAB}) = \mathrm{Tr}(\mathbf{BCA})$$

$$\mathrm{Tr}(\mathbf{A} + \mathbf{B} + \mathbf{C}) = \mathrm{Tr}(\mathbf{A}) + \mathrm{Tr}(\mathbf{B}) + \mathrm{Tr}(\mathbf{C})$$

$$||\mathbf{A}||_F = \sqrt{\mathrm{Tr}(\mathbf{A}\mathbf{A}^\intercal)}$$

Matrix Determinant

Product of all the eigenvalues $\det(\boldsymbol{A})$ for square matrix $\boldsymbol{A}$

Scalar measure of expansion/contraction

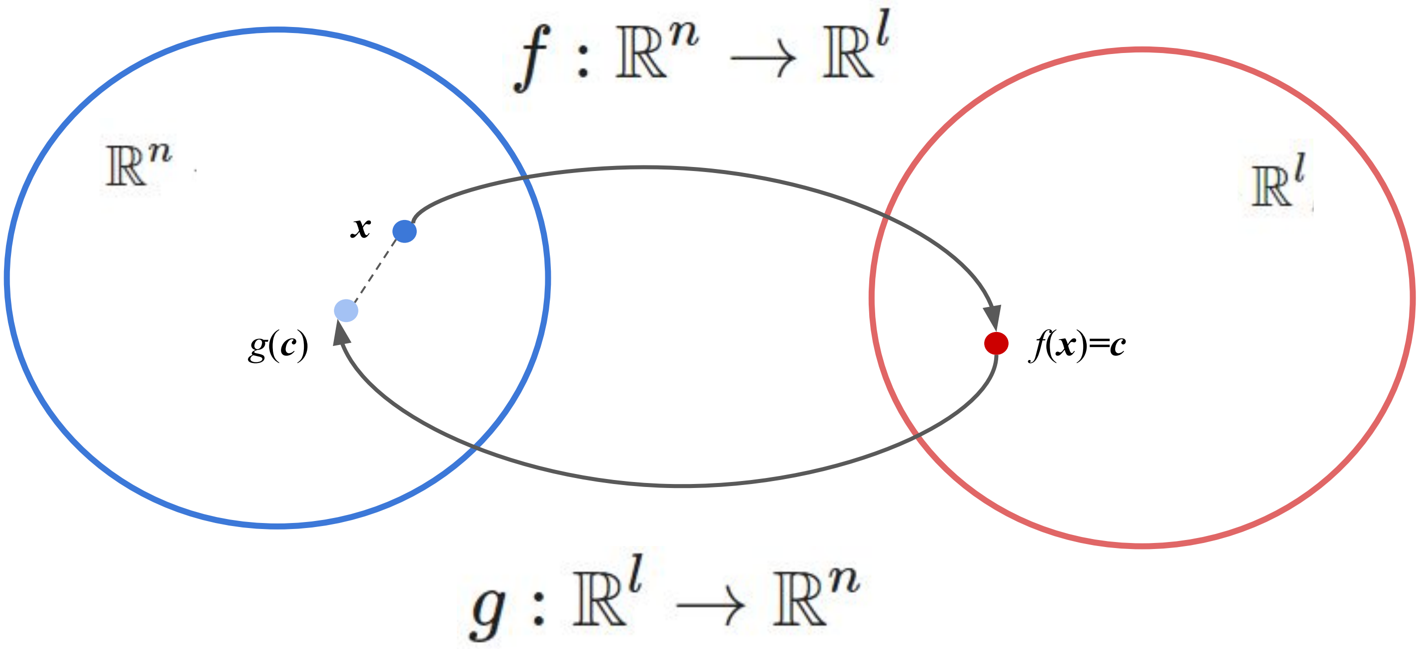
If $\det(\boldsymbol{A}) = 0$ - singular matrix, where at least one dim is 0

If $\det(\boldsymbol{A}) = 1$ - preserves volume

Principal Components Analysis

- Suppose we have m points $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ in $\mathbb{R}^n$
- We'd like to find a lower dimensional mapping: $\boldsymbol{f} : \mathbb{R}^n \rightarrow \mathbb{R}^l$, where $\boldsymbol{l} < \boldsymbol{n}$
- For every instance $\boldsymbol{x}^{(i)} \in \mathbb{R}^n$, there is a corresponding code $\boldsymbol{c}^{(i)}$
- **Encoding function** $f(\boldsymbol{x}) = \boldsymbol{c}$
- **Decoding function** $g(\boldsymbol{c}) = r(\boldsymbol{x})$, and $r(\boldsymbol{x}) = g(f(\boldsymbol{x})) \approx \boldsymbol{x}$
- Any useful application come to mind?

Principal Components Analysis



Principal Components Analysis

- Let's choose a very simple decoder based on matrix multiplication

$$g(\boldsymbol{c}) \equiv \mathbf{D}\boldsymbol{c}$$

  where $\mathbf{D} \in \mathbb{R}^{n \times l}$
- Let's add the following constraints (*orthonormal basis*):

1. Columns of $\mathbf{D}$ are orthogonal to each other.
2. Columns of $\mathbf{D}$ have unit norm.

Principal Components Analysis

Need to choose the optimal code point $\boldsymbol{c}^*$ for any input $\boldsymbol{x}$

- Minimize the distance *reconstructon loss* between $\boldsymbol{x}$ and $g(\boldsymbol{c}^*)$ using the L^2 norm:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2$$

- Is equivalent to minimizing the squared L^2 norm:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2^2$$

- By defintion of the L^2 norm, function simplifies to:

$$\begin{aligned} &(\boldsymbol{x} - g(\boldsymbol{c}))^\top(\boldsymbol{x} - g(\boldsymbol{c})) \\ &= \boldsymbol{x}^\top\boldsymbol{x} - \boldsymbol{x}^\top g(\boldsymbol{c}) - g(\boldsymbol{c})^\top\boldsymbol{x} + g(\boldsymbol{c})^\top g(\boldsymbol{c}) \\ &= \boldsymbol{x}^\top\boldsymbol{x} - 2\boldsymbol{x}^\top g(\boldsymbol{c}) + g(\boldsymbol{c})^\top g(\boldsymbol{c}) \end{aligned} \tag{2.57}$$

Principal Components Analysis

- We can drop the first term $\boldsymbol{x}^\top \boldsymbol{x}$ in (2.57) since it doesn't depends on $\boldsymbol{c}$

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top g(\boldsymbol{c}) + g(\boldsymbol{c})^\top g(\boldsymbol{c})$$

- Substitute in the defintion of $g(\boldsymbol{c}) = \mathbf{D}\boldsymbol{c}$:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \mathbf{D}\boldsymbol{c} + \boldsymbol{c}^\top \mathbf{D}^\top \mathbf{D}\boldsymbol{c}$$

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \mathbf{D}\boldsymbol{c} + \boldsymbol{c}^\top \mathbf{I}_l \boldsymbol{c}$$

(since D is orthogonal and unit norm)

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \mathbf{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c}$$

Principal Components Analysis

- Using **vector calculus** we can replace $\arg\min_{\boldsymbol{c}}$ with gradient $\nabla(\cdot) = \mathbf{0}$:

$$\nabla_{\boldsymbol{c}}\left(-2\boldsymbol{x}^\top \mathbf{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c}\right) = \mathbf{0}$$

$$-2\mathbf{D}^\top \boldsymbol{x} + 2\boldsymbol{c} = \mathbf{0}$$

$$\boldsymbol{c} = \mathbf{D}^\top \boldsymbol{x}$$

- We can optimally encode $\boldsymbol{x}$ with just matrix-vector operation!

$$f(\boldsymbol{x}) = \mathbf{D}^\top \boldsymbol{x}$$

- PCA reconstruction operation:

$$r(\boldsymbol{x}) = g(f(\boldsymbol{x})) = \mathbf{D}\mathbf{D}^\top \boldsymbol{x}$$

Principal Components Analysis

- We want to choose $\mathbf{D}$ that minimizes the reconstruction error $\boldsymbol{x} - r(\boldsymbol{x})$ for all m points
- Apply the **Frobenius norm** of the error matrix $\mathbf{X} - r(\mathbf{X})$ for all n dimensions and m points:

$$\mathbf{D}^* = \arg\min_{\mathbf{D}} \sqrt{\sum_{i,j} \left(x_j^{(i)} - r(\boldsymbol{x}^{(i)})_j \right)^2} \text{ subject to } \mathbf{D}^\top \mathbf{D} = \mathbf{I}_l \qquad (2.68)$$

Principal Components Analysis

- To get to $\mathbf{D}^*$, let's start by considering one-dimensional projection, $l = 1$, and later expand to $l > 1$
- This makes $\mathbf{D}$ just a 1-dimensional matrix (i.e., vector) $\boldsymbol{d}$ simplifying (2.68):

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} \sum_i ||x^{(i)} - \boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{x}^{(i)}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1$$

- Rearrange the terms into standard formatting, noting that a scalar and its transpose are equal:

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} \sum_i ||x^{(i)} - \boldsymbol{d}^\top \boldsymbol{x}^{(i)} \boldsymbol{d}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1$$

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} \sum_i ||x^{(i)} - \boldsymbol{x}^{(i)\top} \boldsymbol{d}\boldsymbol{d}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1$$

Principal Components Analysis

- Now, we'll rewrite this in terms of the design matrix: $\mathbf{X} = \left[\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\right]^\top \in \mathbb{R}^{m \times n}$

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} ||\mathbf{X} - \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top||_F^2 \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1$$

- Ignoring the constraint for a moment, and focusing on the Frobenius norm:

$$\arg\min_{\boldsymbol{d}} ||\mathbf{X} - \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top||_F^2$$

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}\left(\left(\mathbf{X} - \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top\right)^\top\left(\mathbf{X} - \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top\right)\right) \quad (2.74)$$

Principal Components Analysis

- Rewriting (2.74):

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}\left(\mathbf{X}^\top \mathbf{X} - \mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top - \boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X} + \boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top\right)$$

- Trace of a sum is the sum of the traces:

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\mathbf{X}^\top \mathbf{X}) - \operatorname{Tr}(\mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top) - \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X}) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top)$$

- Drop $\operatorname{Tr}(\mathbf{X}^\top \mathbf{X})$ because it doesn't affect $\boldsymbol{d}$:

$$= \arg\min_{\boldsymbol{d}} -\operatorname{Tr}(\mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top) - \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X}) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top)$$

- We can rearrange order of a matrix product inside trace:

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top)$$

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\mathbf{X}^\top \mathbf{X} \boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top)$$

Principal Components Analysis

- Now, let's bring the constraint back and apply it to simplify further:

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

- Adding two identical terms:

$$= \arg\min_{\boldsymbol{d}} -\operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

- Drop the minus and make a maximization problem:

$$= \arg\max_{\boldsymbol{d}} \operatorname{Tr}(\mathbf{X}^\top \mathbf{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

- Rearrange terms inside the Trace:

$$= \arg\max_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{d}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{d}) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

Principal Components Analysis

- The optimization problem is solved via eigendecomposition
- The optimal $\boldsymbol{d}$ is given by the eigenvector of $\mathbf{X}^\intercal\mathbf{X}$ corresponding to the largest eigenvalue: $\max(\Lambda)$:

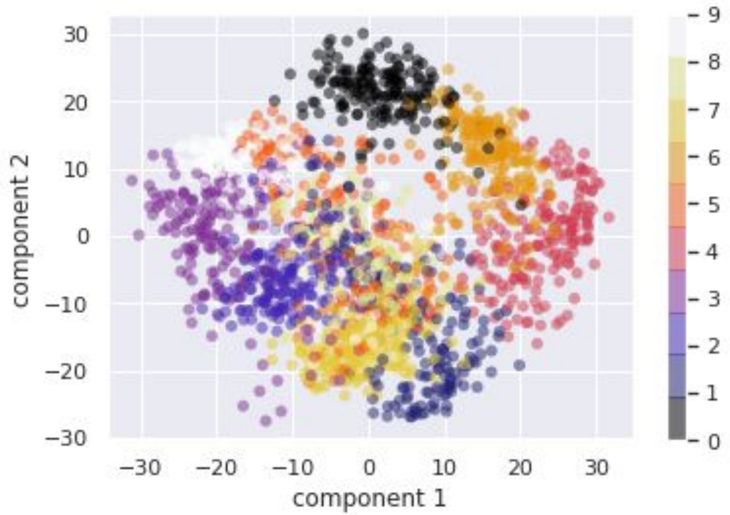
$$\mathbf{X}^\intercal\mathbf{X} = \mathbf{Q}\Lambda\mathbf{Q}^\intercal$$

- For $l > 1$, choose $\mathbf{D}$ using the eigenvectors in $\mathbf{Q}$ corresponding to the l largest eigenvalues
- Can be proven via induction.

PCA Demo

Source:

https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.09-Principal-Component-Analysis.ipynb#scrollTo=NKCCssS-tNR-



Great colab tutorial on linear algebra

https://github.com/jonkrohn/ML-foundations/blob/master/notebooks/2-linear-algebra-ii.ipynb

Discussion about your final project