Review of Linear Algebra

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Introduction to Machine Learning with Applications

Outline: Linear Algebra

- Motivating Example Eigenface
- Basics
- Dot and Vector Products
- Matrices
- Norms
- Rank and linear independence
- Range and Null Space
- Column and Row Space
- Determinant and inverse of a matrix
- Eigenvalues and Eigenvectors
- Singular Value Decomposition
- Matrix Calculus

A Motivating Example - Eigenface





predicted: Bush true: Bush



predicted: Bush true: Bush



predicted: Bush true: Bush



predicted: Bush true: Bush



predicted: Bush true: Bush



predicted: Blair true: Blair



predicted: Schroeder true: Schroeder



predicted: Bush true: Bush



predicted: Bush true: Bush



predicted: Powel true: Powell



predicted: Bush true: Bush

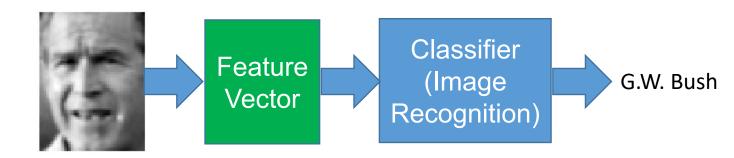




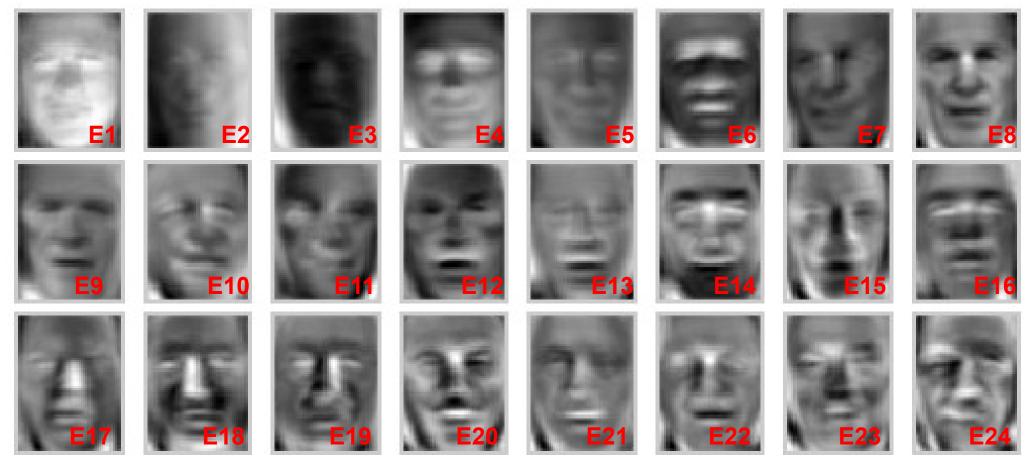
This image has 432x288 pixels

Not every pixel is equally important in classifying faces

Solution: use ideas from linear algebra to extract features from images - using eigenvectors, eigenvalues



Eigenfaces (using linear algebra)



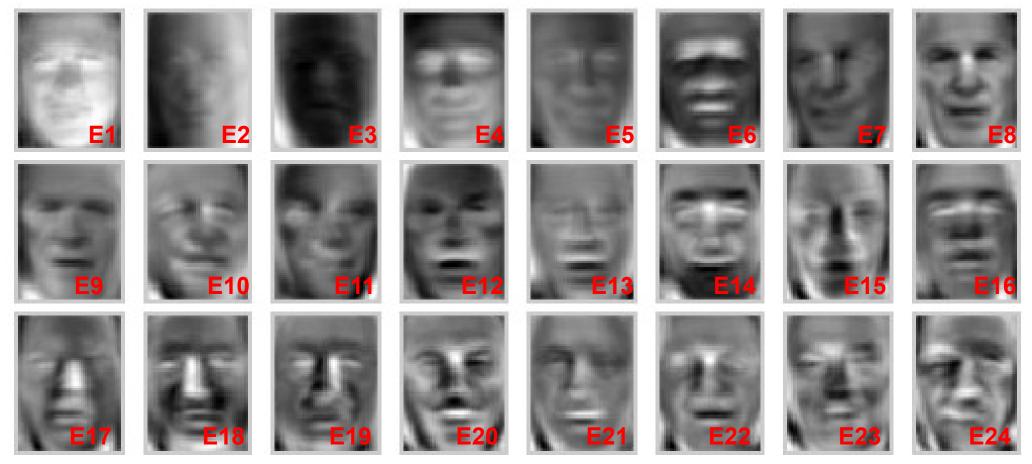


mean face

E0

$$= E0 + (-0.005) \times E1 + (-0.04) \times E2 + (0.002) \times E3 + ...$$

Eigenfaces (using linear algebra)





mean face

E0

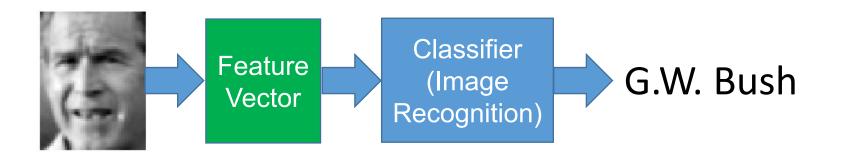
$$= E0 + (-0.015) \times E1 + (0.0037) \times E2 + (-0.01) \times E3 + ...$$

$$= E0 + (-0.015) \times E1 + (0.0037) \times E2 + (-0.01) \times E3 + ...$$

Feature Vector = [-0.015, 0.0037, -0.01, ...]

$$= E0 + (-0.005) \times E1 + (-0.04) \times E2 + (0.002) \times E3 + ...$$

Feature Vector = [-0.005, -0.04, 0.002, ...]



Use a Numerical Vector to represent an Object



"Feature Vector"

Use a Numerical Vector to represent an Object



name

agegenderheightweightoccupation

$$x_{1} = \begin{bmatrix} Homer J.Simpson \\ 35 years \\ male \\ 175 cm \\ 200 Kg \\ safety inspector \end{bmatrix}$$

How can we convert this vector to a numerical vector ? (e.g. represent the name using some number(s))

A challenging problem in Machine Learning: How can we build a good representation of data/object

Representation Learning: A Review and New Perspectives

Yoshua Bengio[†], Aaron Courville, and Pascal Vincent[†] Department of computer science and operations research, U. Montreal † also, Canadian Institute for Advanced Research (CIFAR)

https://arxiv.org/pdf/1206.5538.pdf

Note: read this paper in the middle of this semester

Linear Algebra Basics

• Linear algebra provides a way of compactly representing and operating on sets of linear equations

$$4x_1 + 5x_2 = 1$$

$$6x_1 + 7x_2 = 2$$

the above equations can be written in the form of Ax = b

$$A = \begin{bmatrix} 4 & 5 \\ 6 & 7 \end{bmatrix}, b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- $A \in \mathbb{R}^{M \times N}$ denotes a matrix with M rows and N columns, and every element of the matrix is a real number.
- $\mathbb{R}^{M \times N}$ denotes the space of M-by-N matrices (another notation $\mathcal{R}^{M \times N}$)
- $x \in \mathbb{R}^N$ denotes a vector with N elements which are real numbers
- \mathbb{R}^N denotes the space of N-dimensional vectors (another notation \mathcal{R}^N)

• $x \in \mathbb{R}^N$ denotes an N-dimensional vector

a column vector
$$\mathbf{x} = \begin{bmatrix} x_{[1]} \\ x_{[2]} \end{bmatrix}$$
 or a row vector $\mathbf{x} = \begin{bmatrix} x_{[1]} & x_{[2]} \end{bmatrix}$

• In the lecture notes, the statement "a vector \mathbf{x} " refers to a column vector unless we explicitly define " \mathbf{x} is a row vector"

Linear Algebra Basics

• transpose of a matrix by flipping the rows and columns.

$$A \in \mathbb{R}^{M \times N}$$
 then, $A^T \in \mathbb{R}^{N \times M}$

(A' (A-prime)) is also used to denote matrix transpose)

$$A = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$
, then $A^T = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$

• For each element of the matrix A, the transpose can be written as

$$A_{i,j}^T = A_{j,i}$$

Linear Algebra Basics

- Matrix transpose has the following properties
 - $\bullet (A^T)^T = A$
 - $(AB)^T = B^T A^T$
 - $(A + B)^T = A^T + B^T$
- A square matrix $A \in \mathbb{R}^{N \times N}$ is symmetric if $A = A^T$

• Product of two matrices $A \in \mathbb{R}^{M \times N}$ and $B \in \mathbb{R}^{N \times P}$ is a matrix $C \in \mathbb{R}^{M \times P}$

$$C_{m,p} = \sum_{n=1}^{N} A_{m,n} B_{n,p}$$

• Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$, the expression $\mathbf{x}^T \mathbf{y}$ (a.k.a $\mathbf{x} \cdot \mathbf{y}$) is called **inner product** or **dot product** of the two vectors, and it is a real number

$$\mathbf{x}^{T}\mathbf{y} = \begin{bmatrix} x_{[1]} & x_{[2]} & x_{[3]} \end{bmatrix} \begin{bmatrix} y_{[1]} \\ y_{[2]} \\ y_{[3]} \end{bmatrix} = \sum_{n=1}^{3} x_{[n]} y_{[n]},$$

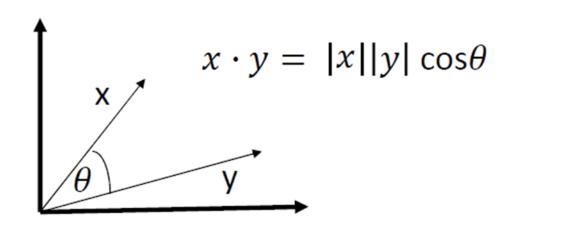
where $x, y \in \mathbb{R}^3$

vector space \mathbb{R}^N : a collection/set of all vectors that have

• Given two vectors $\mathbf{x} \in \mathbb{R}^N$ and $\mathbf{y} \in \mathbb{R}^M$, then $\mathbf{x}\mathbf{y}^T$ is called the **outer product** of the two vectors, and it is a matrix $[\mathbf{x}\mathbf{y}^T]_{n,m} = x_{[n]}y_{[m]}$

$$\boldsymbol{x}\boldsymbol{y}^{T} = \begin{bmatrix} x_{[1]} \\ x_{[2]} \\ x_{[3]} \end{bmatrix} [y_{[1]} \quad y_{[2]}] = \begin{bmatrix} x_{[1]}y_{[1]} & x_{[1]}y_{[2]} \\ x_{[2]}y_{[1]} & x_{[2]}y_{[2]} \\ x_{[3]}y_{[1]} & x_{[3]}y_{[2]} \end{bmatrix}$$

• The dot product has a geometrical interpretation, for vectors $x, y \in \mathbb{R}^2$ with angle θ between them, then



note:
$$\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y}$$

$$|\mathbf{x}| = \sqrt{x_{[1]}^2 + x_{[2]}^2}$$
'length' of the vector

• In a high-dimensional vector space \mathbb{R}^N , we can also think $\cos \theta$ is the 'angle', which measures the similarity between two feature vectors, x and y

$$\cos\theta = \frac{x \cdot y}{|x||y|}$$

Trace of a Square Matrix

• The trace of a square matrix $A \in \mathbb{R}^{N \times N}$, denoted as trace(A) or tr(A), is the sum of the diagonal elements in the matrix

$$tr(A) = \sum_{n=1}^{N} A_{n,n}$$

- Matrix trace has the following properties
 - $\operatorname{tr}(A) = \operatorname{tr}(A^T)$ for $A \in \mathbb{R}^{N \times N}$
 - tr(A+B)=tr(A)+tr(B), for $A, B \in \mathbb{R}^{N\times N}$
 - $tr(t \times A) = t \times tr(A)$ where $t \in \mathbb{R}$
 - If ABC, CBA and CAB are square matrices, then tr(ABC)=tr(CBA)=tr(CAB)

Linear Independence and Rank

• A set of vectors $\{x_1, x_2, ..., x_N\} \subset \mathbb{R}^M$ are linearly independent if no vector can be represented as a linear combination of the remaining vectors

$$\mathbf{x}_n = \sum_{k \neq n} \alpha_k \mathbf{x}_k$$

linearly dependent if some α_k is not zero

Linear Independence and Rank

- The **column rank** of a matrix $A \in \mathbb{R}^{M \times N}$ is the size of the largest set of linearly independent columns of A
- e.g., the column rank of A is 2 means 2 columns in A are linearly independent.
- The **row rank** of a matrix $A \in \mathbb{R}^{M \times N}$ is the size of the largest set of linearly independent rows of A
 - e.g., the row rank of A is 3 means 3 rows in A are linearly independent.
- matrix rank = row rank = column rank

Span

• The span of a set of vectors $\{x_1, x_2, ..., x_N\}$ is the set of all vectors that can be expressed as a linear combination

$$\mathrm{span}(\{\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_N\}) = \{\boldsymbol{v} \mid \boldsymbol{v} = \sum_{n=1}^N \alpha_n \boldsymbol{x}_n \,,\, \alpha_n \in \mathbb{R}\}$$

• If $\{x_1, x_2, ..., x_N\} \subset \mathbb{R}^N$ is a set of linearly independent vectors, then span $(\{x_1, x_2, ..., x_N\}) = \mathbb{R}^N$

Range (column space)

• The range of a matrix $A \in \mathbb{R}^{M \times N}$, denoted as $\mathcal{R}(A)$, is the span of the columns of A

it is also called column space

Column Space and Row Space

• row space and column space are the linear subspaces generated by row and column vectors of a matrix

- For a matrix $A \in \mathbb{R}^{M \times N}$,
 - col space of A = span (cols of A)
 - row space of A = span (rows of A)
 - rank(A) = dim (row space of A) = dim (col space of A)

note: column is col, dimension is dim

dim of a space is the size of the largest set of linearly independent vectors in the space

Null Space

• The nullspace of a matrix $A \in \mathbb{R}^{M \times N}$, denoted as $\mathcal{N}(A)$, is the set of all vectors defined in

$$\mathcal{N}(A) = \{ \boldsymbol{x} \mid A\boldsymbol{x} = 0, \boldsymbol{x} \in \mathbb{R}^N \}$$

• Norm of a vector ||x|| is a measure of the 'length' of the vector x, and $x \in \mathbb{R}^N$

• Common norms used in machine learning are

•
$$\ell_2$$
 norm $||\mathbf{x}||_2 = \sqrt{\sum_{n=1}^N x_{[n]}^2} = \sqrt{\mathbf{x}^T \mathbf{x}}$ (Euclidean norm)

Vector Norm of $x \in \mathbb{R}^N$

- Common norms used in machine learning are
 - ℓ_1 norm $||x||_1 = \sum_{n=1}^N |x_{[n]}|$ (sum of the absolute values of the elements)
 - ℓ_2 norm $\|\mathbf{x}\|_2 = \sqrt{\sum_{n=1}^N x_{[n]}^2} = \sqrt{\mathbf{x}^T \mathbf{x}}$ (Euclidean norm)

• ℓ_{∞} norm $||x||_{\infty} = \max\{|x_{[1]}|, ..., |x_{[N]}|\}$ (max of the absolute values)

• In general, we can define a ℓ_p norm with $p \ge 1$

$$\|x\|_p = \left(\sum_{n=1}^N |x_{[n]}|^p\right)^{\frac{1}{p}}$$

• $\|x\|_p$ is not a norm when 0 because triangle inequality may not hold. an example:

$$||[1,0]||_p = 1$$

 $||[0,1]||_p = 1$

$$||[1,0] + [0,1]||_p = ||[1,1]||_p = 2^{\frac{1}{p}} > 2 = ||[1,0]||_p + ||[0,1]||_p$$

• ℓ_0 norm: a special norm of $\mathbf{x} \in \mathbb{R}^N$ $||\mathbf{x}||_0 = \sum_{n=1}^N |x_{[n]}|^0$

$$|x_{[n]}|^0 = 1 \text{ if } |x_{[n]}| > 0$$

 $|x_{[n]}|^0 = 0 \text{ if } |x_{[n]}| = 0$

Thus, $||x||_0$ is the number of non-zero elements in x

$$\sum_{n=1}^{N} |x_{[n]}|^p \to ||x||_0 \text{ when } p \to 0$$

||x|| is the same as $||x||_p$

$$p \ge 1 \text{ or } p = 0$$

- Norm of a vector ||x|| is a measure of the 'length' of vector x
- $x \in \mathbb{R}^N$
- norm ||x|| is a function $f: \mathbb{R}^N \to \mathbb{R}$ that satisfies
 - For every $x \in \mathbb{R}^N$, $f(x) \ge 0$ (non-negativity)
 - f(x) = 0 if and only if (iff) x = 0 (definiteness)
 - For every $\mathbf{x} \in \mathbb{R}^N$, $t \in \mathbb{R}$ $f(t\mathbf{x}) = |t| f(\mathbf{x})$ (homogeneity)
 - For every $x, y \in \mathbb{R}^N$, $f(x + y) \le f(x) + f(y)$ (triangle inequality)

Matrix Norm

Norms can be defined for matrices

• Frobenius Norm (F Norm) for $A \in \mathbb{R}^{M \times N}$

$$||A||_F = \sqrt{\sum_{m=1}^M \sum_{n=1}^N A_{m,n}^2} = \sqrt{tr(A^T A)}$$

other norms:

http://mathworld.wolfram.com/MatrixNorm.html

Identity Matrix

• The identity matrix, denoted by $I \in \mathbb{R}^{N \times N}$ is a square matrix with ones on the diagonal and zeros everywhere else.

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

Diagonal Matrix

• A diagonal matrix, $D = diag(d_1, d_2, ..., d_N) \in \mathbb{R}^{N \times N}$, is a square matrix where all non-diagonal elements are zeros

$$D = \begin{vmatrix} d_1 & 0 \\ 0 & d_2 \end{vmatrix} = diag(d_1, d_2)$$

Orthogonal Matrix

- Two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$ are orthogonal (e.g., perpendicular) to each other if $\mathbf{x} \cdot \mathbf{y} = 0$.
- two vectors \mathbf{x} , \mathbf{y} are orthonormal to each other if they are orthogonal and $\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = 1$
- A matrix $U \in \mathbb{R}^{N \times N}$ is called orthogonal if $U^T U = I = U U^T$
 - the columns are orthonormal to each other
 - the rows are orthonormal to each other
 - a property: $||Ux||_2 = ||x||_2$

Determinant of a Matrix

• The determinant of a square matrix $A \in \mathbb{R}^{N \times N}$ us a function $f: \mathbb{R}^N \to \mathbb{R}$, denoted by |A| or $\det(A)$, and is calculated as $|A| = \sum_{i=1}^{N} (-1)^{i+j} A_{i,i} |B|$, for any $j \in \{1, 2, ..., N\}$

B is obtained by eliminating the *i*-th row and the *j*-th col of A

Inverse of a Matrix

- The inverse of a square matrix $A \in \mathbb{R}^{N \times N}$ is denoted A^{-1} such that $A^{-1}A = I = AA^{-1}$
- For some square matrices, A^{-1} may not exist, those matrices are called singular or non-invertible. A^{-1} exists if and only if A is full rank (rank(A) = N)

Inverse of a Matrix

• For non-square matrices, $A \in \mathbb{R}^{M \times N}$, the inverse, denoted by A^+ , is given by

$$A^{+} = (A^{T}A)^{-1}A^{T}$$
 which is called pseudo inverse

assuming the square matrix $A^T A$ is invertible (usually N < M)

$$A^{+}A = (A^{T}A)^{-1}A^{T}A = I, A^{+}$$
 is the left-inverse of A

Note:
$$AA^+ = A(A^TA)^{-1}A^T \neq I$$
, A^+ is NOT the right-inverse of A

• Given a square matrix $A \in \mathbb{R}^{N \times N}$, the scalar λ is an eigenvalue and \boldsymbol{x} is an eigenvector of A if

$$Ax = \lambda x$$
, and $x \neq 0$

 $\lambda \in \mathbb{C}$ (it could be a complex number)

• Given a square matrix $A \in \mathbb{R}^{N \times N}$, $\lambda \in \mathbb{C}$ (could be a complex number) is an eigenvalue and $\mathbf{x} \in \mathbb{C}$ is an eigenvector of A if

$$Ax = \lambda x$$
, and $x \neq 0$

obtain x and λ by solving the linear equations:

$$(A - \lambda I)x = 0$$
, and $|A - \lambda I| = 0$

Eigenvalues may not be unique

Eigenvalues could be complex numbers

• Eigen Decomposition Theorem

http://mathworld.wolfram.com/EigenDecompositionTheorem.html

http://mathworld.wolfram.com/Eigenvector.html

• Given a square matrix $A \in \mathbb{R}^{N \times N}$, $\lambda \in \mathbb{C}$ (could be a complex number) is an eigenvalue and $\mathbf{x} \in \mathbb{C}$ is an eigenvector of A if

$$Ax = \lambda x$$
, and $x \neq 0$

• Eigen Decomposition Theorem

if we can obtain N linearly independent eigenvectors, then

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

every column of $P \in \mathbb{R}^{N \times N}$ is an eigenvector of A

$$D = \operatorname{diag}(\{\lambda_1, \dots, \lambda_N\})$$

if the number of linearly independent eigenvectors < N

A can be written using a so-called singular value decomposition.

- Symmetric matrix $A \in \mathbb{R}^{N \times N}$
 - eigenvalues are **real** numbers, $\{\lambda_1, ..., \lambda_N\}$, $D = \text{diag}(\{\lambda_1, ..., \lambda_N\})$
 - eigenvectors are **orthogonal**, $\{x_1, ..., x_M, M \le N\}$, $x_n^T x_k = 0$ if $k \ne n$ (usually set $||x_n||_2 = 1$ to achieve orthonormal)

Singular Value Decomposition (full)

• A matrix $A \in \mathbb{R}^{M \times N}$ $(M \ge N)$ can always be decomposed as

$$A = UDV^T$$

$$A = [u_1, u_2, ..., u_M]D[v_1, v_2, ..., v_N]^T$$

- $D \in \mathbb{R}^{M \times N}$, and main diagonal elements of D are $[\lambda_1, ..., \lambda_N, 0, ..., 0]$
- the columns of $U \in \mathbb{R}^{M \times M}$ are orthonormal: $U^T U = I$
- the columns of $V \in \mathbb{R}^{N \times N}$ are orthonormal: $V^T V = I$
- singular values $\{\lambda_1, ..., \lambda_N\}$ are real numbers
- every column of U, denoted by u_m , is called a left-singular vector of A
- every column of V, denoted by v_n , is called a right-singular vector of A

Matrix Calculus (basic concepts)

scalar by vector

For vectors
$$\mathbf{x}, \mathbf{b} \in \mathbb{R}^N$$
, let $f(\mathbf{x}) = \mathbf{b}^T \mathbf{x}$, then $\frac{\partial f}{\partial \mathbf{x}} = \nabla_{\mathbf{x}} f = \mathbf{b}$

$$\nabla_{x} f = \begin{bmatrix} \frac{\partial f}{\partial x_{[1]}} \\ \dots \\ \frac{\partial f}{\partial x_{[N]}} \end{bmatrix} \text{ where } \mathbf{x} = \begin{bmatrix} x_{[1]} \\ \dots \\ x_{[N]} \end{bmatrix}$$

We need this to understand back-propagation in neural networks

Matrix Calculus (basic concepts)

scalar by vector

Quadratic function $f(x) = x^T A x$ with $A \in \mathbb{R}^{N \times N}$ and A is symmetric

then: $\nabla_x f = 2Ax$

References for self study

http://cs229.stanford.edu/section/cs229-linalg.pdf

https://atmos.washington.edu/~dennis/MatrixCalculus.pdf

If you want to be a machine learning researcher, then read:

Mathematics for Econometrics (chapter 1 to 5) https://www.springer.com/us/book/9781461481447

Matrix Cookbook by KB Peterson

Singular Value Decomposition (Economy-Size)

• A matrix $A \in \mathbb{R}^{M \times N}$ $(M \ge N)$ can always be decomposed as $A = UDV^T$

$$A = [\boldsymbol{u}_1, \boldsymbol{u}_2, \dots, \boldsymbol{u}_N] \begin{bmatrix} \lambda_1 & & \\ & \dots & \\ & & \lambda_N \end{bmatrix} [\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_N]^T$$

- the columns of $U \in \mathbb{R}^{M \times N}$ are orthonormal: $U^T U = I$
- the columns of $V \in \mathbb{R}^{N \times N}$ are orthonormal: $V^T V = I$
- $D = diag(\lambda_1, ..., \lambda_N)$
- singular values $\{\lambda_1, \dots, \lambda_N\}$ are real numbers
- every column of U, denoted by u_n , is called a left-singular vector of A
- every column of V, denoted by v_n , is called a right-singular vector of A
- $A \boldsymbol{v}_n = \lambda_n \boldsymbol{u}_n$ and $A^T \boldsymbol{u}_n = \lambda_n \boldsymbol{v}_n$, for n=1 to N

Singular Value Decomposition (SVD) and Eigen Decomposition

• A matrix $A \in \mathbb{R}^{M \times N}$ $(M \ge N)$ can always be decomposed as (SVD)

$$A = UDV^T$$

$$A = [\boldsymbol{u}_1, \boldsymbol{u}_2, ..., \boldsymbol{u}_N] \begin{bmatrix} \lambda_1 & & \\ & ... & \\ & & \lambda_N \end{bmatrix} [\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_N]^T$$

- $AA^T = UDV^T (UDV^T)^T = UDV^T VDU^T = U(DD)U^T$ U contains N linearly independent eigenvectors of AA^T λ_n^2 is an eigenvalue of AA^T
- $A^T A = (UDV^T)^T UDV^T = VDU^T UDV^T = V(DD)V^T$ V contains N linearly independent eigenvectors of $A^T A$ λ_n^2 is an eigenvalue of $A^T A$

Pseudo Inverse and SVD

$$A = UDV^T$$

$$D = diag(\lambda_1, \lambda_2, ... \lambda_r, 0, 0, 0)$$
, where $\lambda_1 > 0$... and $\lambda_r > 0$

$$D^{+} = diag\left(\frac{1}{\lambda_{1}}, \frac{1}{\lambda_{2}}, \dots, \frac{1}{\lambda_{r}}, 0, \dots, 0\right)$$

$$A^+ = VD^+U^T$$