Linear Algebra review

2020. 8

References:

- Steven Skiena, The Data Science Design Manual, Springer, 2017
- Zico Kolter, CMU-388/688 Practical Data Science: Matrices, vectors, and linear algebra (review summary), 2018
- many internet sites

Matrices and Linear Algebra

- The most critical part of your data science project is reducing all the information you can find into one or more data matrices, ideally as large as possible.
  - Rows: examples, samples, or indices
  - Columns: distinct features or attributes
- Linear algebra: mathematics of matrices
  - Many machine learning algorithms are best understood through linear algebra

Matrices and Vectors

- A vector is a 1D array of values
  - By default, we use column vectors.

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

- A matrix is a 2D array of values
  - “Higher dimensional matrices” are called tensors.

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}$$

We use A_{ij} to denote the entry in row i and column j

Row and column ordering

- Matrices can be laid out in memory by row or by column

$$A = \begin{bmatrix} 100 & 80 \\ 60 & 80 \\ 100 & 100 \end{bmatrix}$$

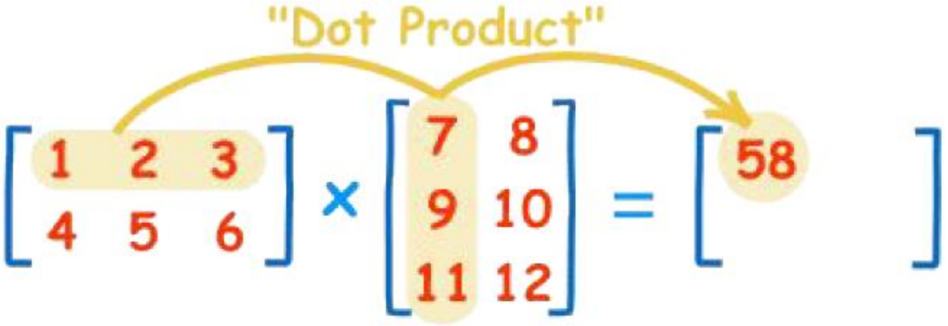
  - Row major ordering: 100, 80, 60, 80, 100, 100
  - Column major ordering: 100, 60, 100, 80, 80, 100
- Row major ordering is default for C 2D arrays (and default for Numpy), column major is default for FORTRAN (since a lot of numerical methods are written in FORTRAN, also the standard for most numerical code)

What Can n*m Matrices Represent?

- Data: rows are objects, columns features.
- Geometric point sets: rows are points, columns are dimensions
- Systems of Equations: rows are equations, columns are coefficients for each variable.
- Graphs/Networks: M[i,j] denotes the number of edges from vertex i to vertex j.
- Vectors: any row, column or d*1 matrix
- Images: pixel (x,y)

Matrix multiplication/ Dot products

- The product A*B is defined by: $C_{i,j} = \sum_{i=1}^{k} A_{i,k} \cdot B_{k,j}$
- A*B must share inner dimensions to multiply.
- Each element of the product matrix is a dot product of row/column vectors.



- It is associative, but not commutative.
- Multiplication by the identity commutes: $\mathbb{I} A = A\mathbb{I} = A$

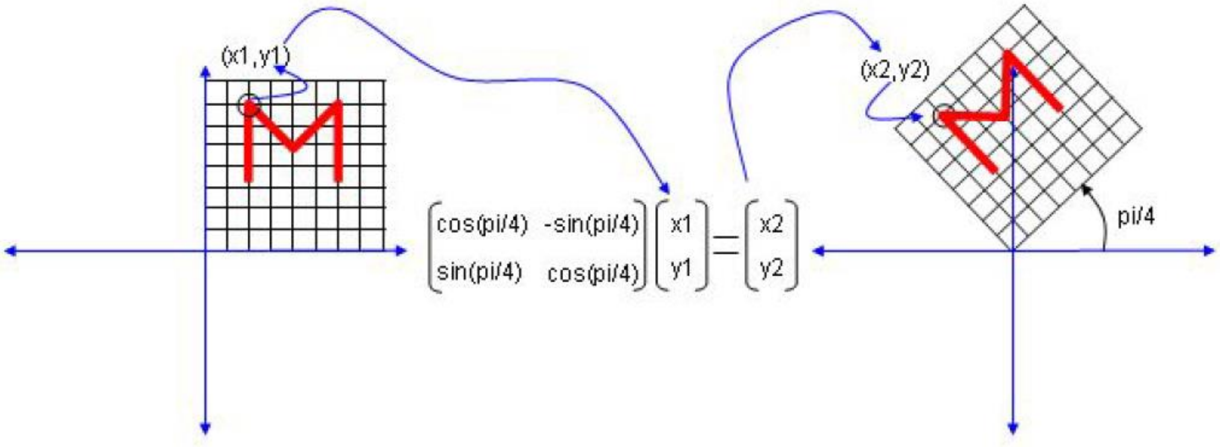
Interpreting Matrix Multiplication

- Multiplication by permutation matrices rearrange rows/columns:

$$P=\begin{pmatrix}0&0&1&0\\1&0&0&0\\0&0&0&1\\0&1&0&0\end{pmatrix}\quad M=\begin{pmatrix}m_{11}&m_{12}&m_{13}&m_{14}\\m_{21}&m_{22}&m_{23}&m_{24}\\m_{31}&m_{32}&m_{33}&m_{34}\\m_{41}&m_{42}&m_{43}&m_{44}\end{pmatrix}$$

$$PM=\begin{pmatrix}m_{31}&m_{32}&m_{33}&m_{34}\\m_{11}&m_{12}&m_{13}&m_{14}\\m_{41}&m_{42}&m_{43}&m_{44}\\m_{21}&m_{22}&m_{23}&m_{24}\end{pmatrix}$$

- Rotating point in space:



$$\begin{bmatrix}\cos(pi/4) & -\sin(pi/4)\\ \sin(pi/4) & \cos(pi/4)\end{bmatrix}\begin{bmatrix}x1\\y1\end{bmatrix}=\begin{bmatrix}x2\\y2\end{bmatrix}$$

Matrix Inversion

- *A*$^{-1}$ is the multiplicative inverse of A, if A * *A*$^{-1}$ = I, where I is the identity matrix.

$$\mathbf{A}^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

- If matrix A has an inverse, it can be computed by solving a linear system using Gaussian elimination.

$$[\mathbf{A} \quad \mathbf{I}] = \begin{bmatrix} 0 & 1 & 2 & 1 & 0 & 0 \\ 1 & 0 & 3 & 0 & 1 & 0 \\ 4 & -3 & 8 & 0 & 0 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 3 & 0 & 1 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & -3 & -4 & 0 & -4 & 1 \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 0 & 3 & 0 & 1 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 2 & 3 & -4 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & -9/2 & 7 & -3/2 \\ 0 & 1 & 0 & -2 & 4 & -1 \\ 0 & 0 & 1 & 3/2 & -2 & 1/2 \end{bmatrix}$$

$$\mathbf{A}^{-1} = \begin{bmatrix} -9/2 & 7 & -3/2 \\ -2 & 4 & -1 \\ 3/2 & -2 & 1/2 \end{bmatrix}$$

Matrix Inversion and Linear Systems

- Multiplying both sides of Ax = b by the inverse of A yields: $(A^{-1} A)x = A^{-1} b$, or $x = A^{-1} b$
- Thus solving linear equations is equivalent to matrix inversion.

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 5 & 1 \\ 2 & 3 & 8 \end{bmatrix}^{-1} \begin{bmatrix} 10 \\ 8 \\ 3 \end{bmatrix} = \frac{1}{25} \begin{bmatrix} -232 \\ 129 \\ 19 \end{bmatrix} = \begin{bmatrix} -9.28 \\ 5.16 \\ 0.76 \end{bmatrix}$$

- The inverse makes it cheap to evaluate many b vectors. However, Gaussian elimination is more numerically stable than inversion.

Some definitions/properties

Transpose of matrix multiplication, $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}$

$$(AB)^T = B^T A^T$$

Inverse of product, $A \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times n}$ *both square and invertible*

$$(AB)^{-1} = B^{-1} A^{-1}$$

Inner product: for $x, y \in \mathbb{R}^n$, special case of matrix multiplication

$$x^T y \in \mathbb{R} = \sum_{i=1}^{n} x_i y_i$$

Vector norms: for $x \in \mathbb{R}^n$, we use $\|x\|_2$ to denote Euclidean norm

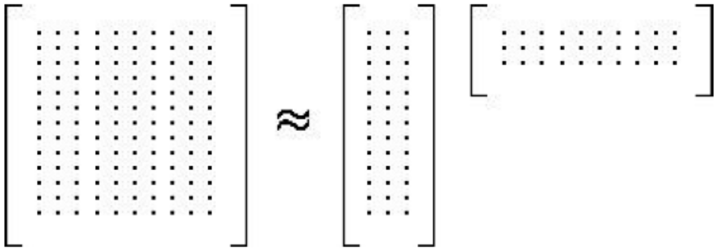
$$\|x\|_2 = (x^T x)^{\frac{1}{2}}$$

Matrix Rank

- The rank of a matrix is a measure of the number of linearly independent rows.
- An n*n matrix should be rank n for all operations to be properly defined on it.
- Some rows of the image may not be linearly independent, so it is not full rank. Adding small amounts of random noise increases rank without serious image distortion.

Factoring Matrices

- Many important machine learning algorithms can be viewed as factoring a matrix. Suppose _n*m_ matrix _A_ can be expressed as the product _B*C_, i.e an _n*k_ matrix times a _k*m_ matrix.
- (ex) factoring Word-Document Matrices
    - If A is a document/word co-occurrence matrix, and A=BC, where B is d*k and C is k*w:
    - B,C are compressed feature vectors for docs and words



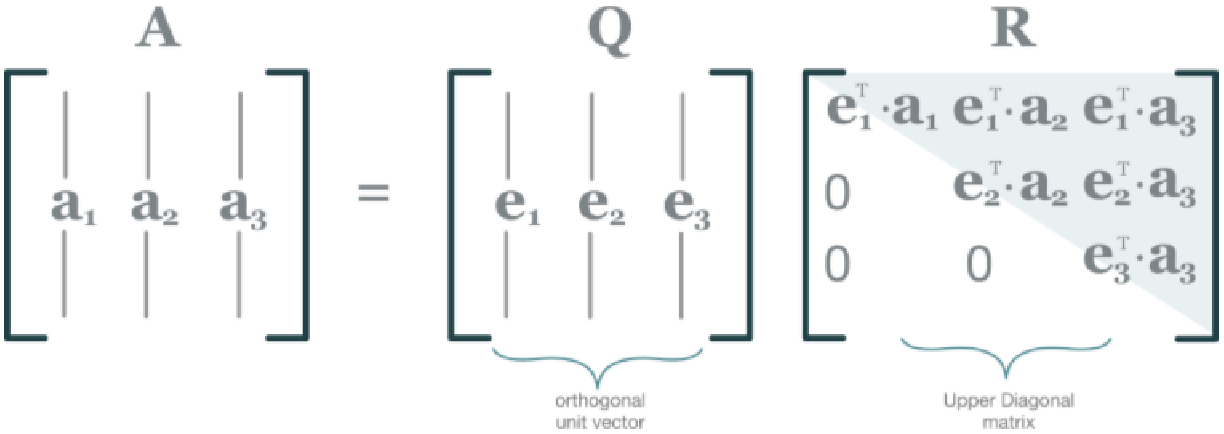
LU Decomposition (factoring)

- *A = LU*
  - Factoring a **square matrix** A representing lower and upper triangular matrices L and U prove useful in solving linear systems.
  - LU decomposition with partial pivoting: *PA = LU*

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

QR Decomposition (factoring)

- *A = QR*
  - A: any m*n matrix
  - Q: m*m (orthonormal matrix), R: upper triangular matrix (m*n)



ref: https://dsc-spidal.github.io/harp/docs/harpdaal/qr/

Eigenvalues and Eigenvectors

- Multiplying a vector x by a matrix A can have the same effect as multiplying it by a scalar λ.
  - $Av = \lambda v$ (x: eigenvector, λ: eigenvalue)
  - Thus the eigenvalue-eigenvector pair (λ, v) must encode a lot of information about matrix A!

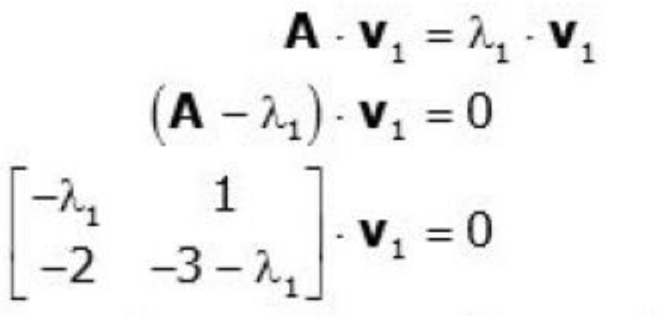
$$\begin{bmatrix} -5 & 2 \\ 2 & -2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} = -1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} \qquad \begin{bmatrix} -5 & 2 \\ 2 & -2 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -1 \end{bmatrix} = -6 \begin{bmatrix} 2 \\ -1 \end{bmatrix}$$

- The n distinct eigenvalues of a rank n matrix can be found by factoring its characteristic equation.

$$\det(A-\lambda I) = \begin{vmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{vmatrix} \qquad \begin{aligned} &= -\lambda^3 + 3\lambda + 2 \\ &= (\lambda-2)(\lambda+1)^2 \end{aligned} \qquad \lambda_1 = 2,\ \lambda_{2,3} = -1$$

Computing Eigenvectors

- The vector associated with a given eigenvalue can be computed by solving a linear system:
  - (ex)



$$\mathbf{A} \cdot \mathbf{v}_1 = \lambda_1 \cdot \mathbf{v}_1$$

$$\left(\mathbf{A} - \lambda_1\right) \cdot \mathbf{v}_1 = 0$$

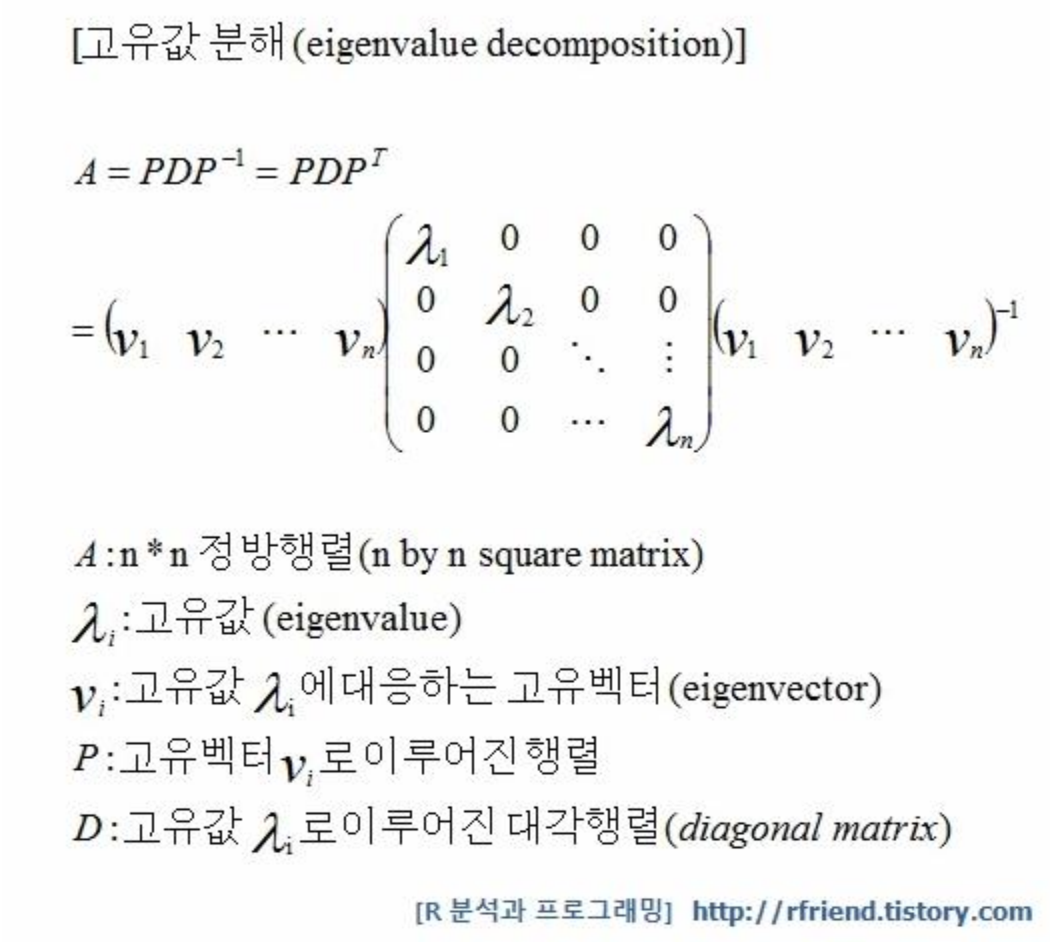
$$\begin{bmatrix} -\lambda_1 & 1 \\ -2 & -3 - \lambda_1 \end{bmatrix} \cdot \mathbf{v}_1 = 0$$

-λ1 *v1,1 + v1,2 = 0

-2 * v1,1 + (-3- λ1)*v1,2 = 0

- Another approach uses v’ = (A * v)/ λ to compute approximations to v until it converges.

Eigenvalue Decomposition



[고유값 분해(eigenvalue decomposition)]

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

$$= \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix}^{-1}$$

A : n * n 정방행렬(n by n square matrix)

λ_i :고유값(eigenvalue)

v_i :고유값 λ_i에대응하는 고유벡터(eigenvector)

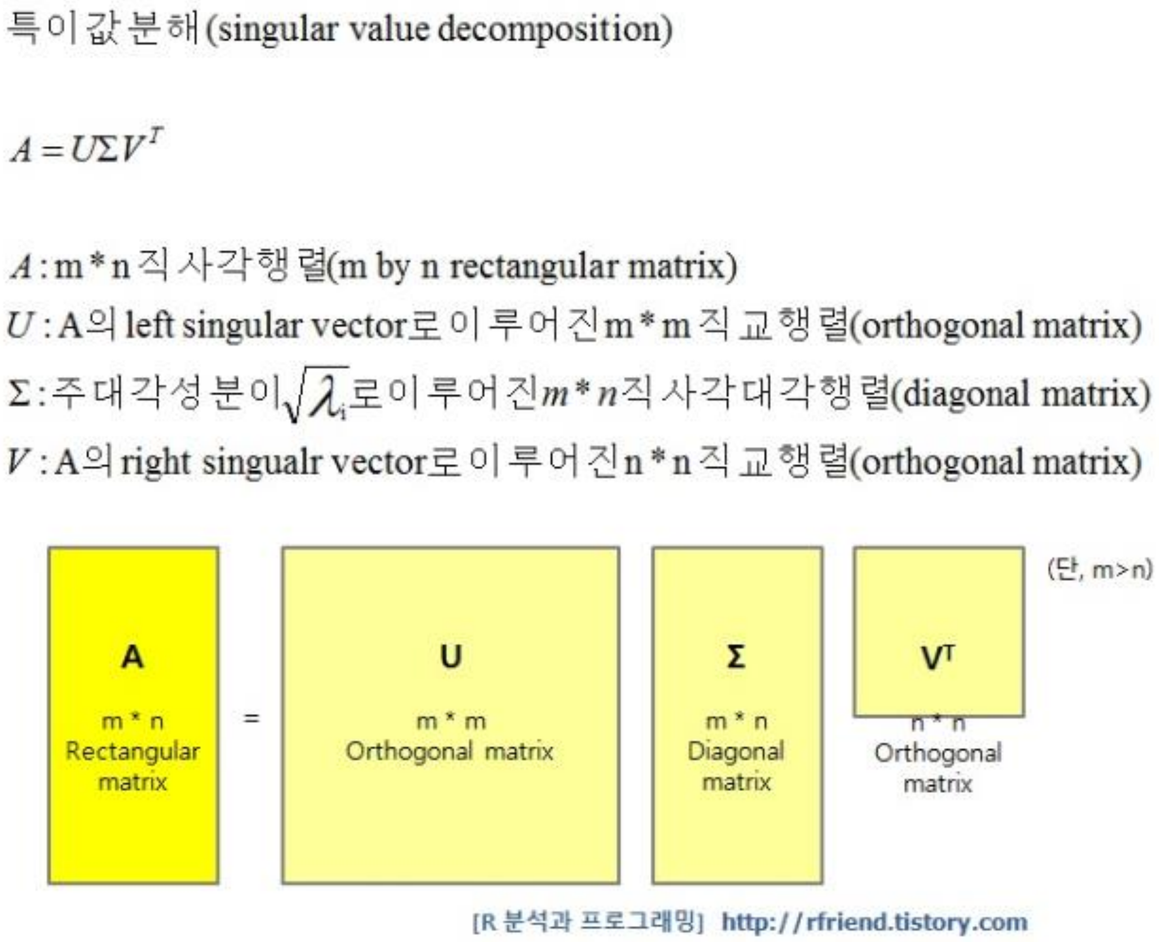
P :고유벡터 v_i로이루어진행렬

D :고유값 λ_i로이루어진 대각행렬(*diagonal matrix*)

[R 분석과 프로그래밍] http://rfriend.tistory.com

- Larger eigenvalues correspond to more important vector products.

Singular Value Decomposition



특이값분해(singular value decomposition)

$A = U\Sigma V^T$

A : m*n 직사각행렬(m by n rectangular matrix)

U : A의 left singular vector로 이루어진 m*m 직교행렬(orthogonal matrix)

Σ : 주대각성분이 $\sqrt{\lambda_i}$ 로 이루어진 $m*n$ 직사각대각행렬(diagonal matrix)

V : A의 right singualr vector로 이루어진 n*n 직교행렬(orthogonal matrix)

A
m * n
Rectangular matrix
=
U
m * m
Orthogonal matrix
Σ
m * n
Diagonal matrix
V^T
n * n
Orthogonal matrix
(단, m>n)

[R 분석과 프로그래밍] http://rfriend.tistory.com

- AA^T 의 eigenvalue 의 square root – singular value
- Retaining only the rows/column with large weights permits us to compress m features with relatively little loss.

Singular Value Decomposition

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

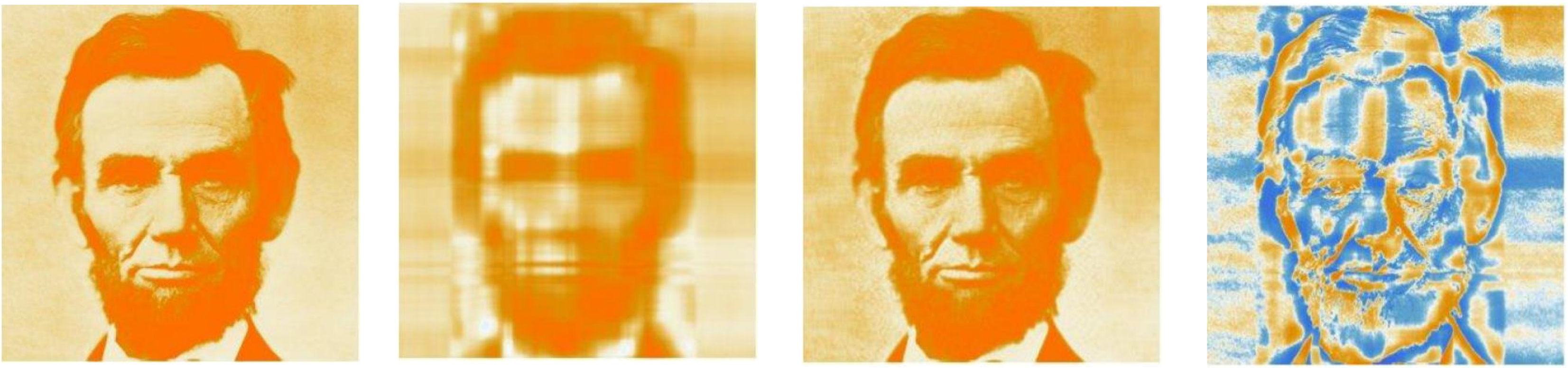
$$AA^T = \begin{pmatrix} 17 & 8 \\ 8 & 17 \end{pmatrix}$$

$$A = U\Sigma V^T = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{18} & -1/\sqrt{18} & 4/\sqrt{18} \\ 2/3 & -2/3 & -1/3 \end{pmatrix}$$

ref: https://www.d.umn.edu/~mhampton/m4326svd_example.pdf

Reconstructing image from SVD

- Lincoln’s face from 5 and 50 singular values, a substantial compression of the original matrix.
  - (a) original (b) k=5 © k=50 (d) error for k=50



Sparse matrices

- Many matrices are *sparse* (contain mostly zero entries, with only a few non-zero entries)
- Examples: matrices formed by real-world graphs, document-word count matrices (more on both of these later)
- Storing all these zeros in a standard matrix format can be a huge waste of computation and memory
- Sparse matrix libraries provide an efficient means for handling these sparse matrices, storing and operating only on non-zero entries (memory and storage-efficient)

Coordinate format

- There are several different ways of storing sparse matrices, each optimized for different operations
- Coordinate (COO) format: store each entry as a tuple (row-index, col-index, value)

$$A = \begin{bmatrix} 0 & 0 & 3 & 0 \\ 2 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 4 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{aligned} \text{data} &= [2\ 4\ 1\ 3\ 1\ 1] \\ \text{row-indices} &= [1\ 3\ 2\ 0\ 3\ 1] \\ \text{col-indices} &= [0\ 0\ 1\ 2\ 2\ 3] \end{aligned}$$

- A good format for constructing sparse matrices

Compressed sparse column format

- Compressed sparse column (CSC) format

$$A = \begin{bmatrix} 0 & 0 & 3 & 0 \\ 2 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 4 & 0 & 1 & 0 \end{bmatrix}$$

$$\text{data} = [2\ 4\ 1\ 3\ 1\ 1]$$

$$\text{row-indices} = [1\ 3\ 2\ 0\ 3\ 1]$$

~~$\text{col-indices} = [0\ 0\ 1\ 2\ 2\ 3]$~~

$$\Downarrow$$

$$\text{col-indices} = [0\ 2\ 3\ 5\ 6]$$

- *Ordering is important (always column-major ordering)*
- Faster for matrix multiplication, easier to access individual columns
- Very bad for modifying a matrix, to add one entry need to shift all data