# EE445 Mod3-Lec1: Spectral Properties of Matrices

References:

- [CE-OptMod]: Chapter 3.3, 4, 5

# Outline

1. Review Eigenvalues & Eigenvectors
2. Symmetric Matrices
3. Introduction to Singular values and SVD

# Why are Spectral Properties Important in ML+OPT?

$$\min_{\alpha} \|K\alpha - y\|^2 + \underbrace{\frac{\lambda}{2}\|\alpha\|^2}$$

- Computational efficiency
- Analysis
- Dimensionality reduction
- Numerical stability

$$\left(\quad + \lambda I\right)^{-1}$$

**How will we see it used?**

1. Kernel methods
2. Principle component analysis (unsupervised ML)
3. Principle component regression
4. (time permitting) spectral clustering

# Reminder: Eigenvalues & Eigenvectors

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

**Some basics:** $A$ matrix, $A \in \mathbb{R}^{m \times n}$

- **Def. (Characteristic Polynomial):** $p(\lambda) = \det(A - \lambda I)$

  The roots of $p(\lambda) = 0$ are the eigenvalues of $A$.

  $$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \underline{y^* = (\bar{y})^T}$$

- **Def. (Left/Right Eigenvector-value pair):**

  A nonzero vector $x$ s.t. $Ax = \lambda x$ then $(\lambda, x)$ is a <u>right</u> eigenvalue-vec pair

  — " ——— $y$ s.t. $y^* A = \lambda y^*$ then $(\lambda, y)$ is a left eigen-pair

- **Orthogonality:** Let $\{x_1, \dots, x_n\}$ of $A$

  Orthogonal eigenvectors: $\langle x_i, x_j \rangle = x_i^T x_j = 0 \quad \forall\ i \neq j$

  Orthonormal eigvec: $\langle x_i, x_j \rangle = 0 \quad \forall\ i \neq j$ & $\|x_i\| = 1 \quad \forall\ i$

# Reminder: Eigenvalues & Eigenvectors

**Why important**?

- Many ML algorithms involve transforming the matrix $A$ into simpler, or *canonical forms*, from which it is easy to compute its eigenvalues and eigenvectors.
- These transformations are called **similarity transformations**

# Similarity transforms

$S^{-1}$, $\det(S) \neq 0$

$S^*$ : Complex conjugate transpose

- **Def. [Similarity Transform]**: The matrix $A$ is similar to $B$ if there exist a non-singular (invertible) matrix $S$ s.t. $\underbrace{B = S^{-1}AS}$
- **Proposition.** Similar matrices $A$ and $B$ has the same eigenvalues.

  $x$ is a right eigvec of $A$ $\Longleftrightarrow$ $S^{-1}x$ is a right eigvec of $B$

  $y$ is a left eigvec of $A$ $\Longleftrightarrow$ $S^*y$ is a left eigvec of $B$
- Some special matrices are similar to diagonal matrices—i.e., for some matrices $A$, there is a similarity transform $S$ such that $\Lambda = S^{-1}AS$ is diagonal, and $\Lambda$ contains the eigenvalues of $A$.
- These matrices are called diagonalizable.

# Part 2. Special Matrices [Symmetric and Positive (semi) definite]

# Symmetric Matrices

Symmetric Matrix: $A \in \mathbb{R}^{n \times n}$ is symmetric if $A = A^T$

- Symmetric matrices are one of the most important matrices in linear algebra and ML
- Mod2-L4: we often use kernel matrices $K = [K(x^{(i)}, x^{(j)})]$ and these are symmetric—i.e., $K = K^\top$—since $K(x^{(i)}, x^{(j)}) = K(x^{(j)}, x^{(i)})$
- Mod2-L2: Gram matrices $A^\top A$ and $AA^\top$ are symmetric;
  - in fact we can study all kinds of properties of a matrix $A$ such as the range and null spaces using these gram matrices (cf. Finite Rank Operator Lemma)

# Symmetric Matrices: Examples

The graph Laplacian is a symmetric matrix

$$L = \begin{bmatrix} L_{11} & L_{12} & \cdots \\ & \ddots & \\ & & L \end{bmatrix}$$

$$L_{ij} = \begin{cases} \#\text{ of edges incident to node } i, & \text{if } i = j \\ -1, & \text{if there is an edge } (i,j) \\ 0 & \text{otherwise} \end{cases}$$

Sample covariance matrix

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} (x^{(i)} - \bar{x})(x^{(i)} - \bar{x})^T, \quad \bar{x} = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$$

Hessian of a function: $H = \nabla^2 f(x), \quad H_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} f(x)$ mod2-L2

$$x = (x_1, \ldots, x_n), \quad f : \mathbb{R}^n \to \mathbb{R}$$

# Quadratic Functions

$f(x) = x^\top Q x$

- Symmetric matrices play an important role not just in ML but also OPT
- We have seen how to formulate least squares regression as a optimization problem with a quadratic objective:

$$f_{1st}(x) = \|Ax - b\|_2^2 = (Ax - b)^\top (Ax - b)$$

- A quadratic function $f : \mathbb{R}^n \to \mathbb{R}$ is a second-order multivariate polynomial in $x$, that is a function containing a linear combination of all possible monomials of degree at most two—i.e.,

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j + \sum_{i=1}^{n} c_i x_i + d \iff f(x) = x^\top A x + c^\top x + d$$

$$f_{1st}(x) = x^\top A x \underbrace{- 2 b^\top A x}_{c} + b^\top b$$

# Quadratic Functions

$f(x) = x^T Q x$ ← quadratic form

$a = a^T$ for scalar $a$

- using properties of symmetric matrices, we can express any quadratic function as a quadratic form.

- Fact: $x^T A x$ is scalar $\Rightarrow$ $x^T A x = x^T A^T x$ $\Rightarrow$ $x^T A x = \frac{1}{2} x^T \underbrace{(A + A^T)}_{=: H} x$

- $A = \underbrace{\frac{1}{2}(A + A^T)}_{\text{symmetric}} + \underbrace{\frac{1}{2}(A - A^T)}_{\text{anti symmetric}}$

More in Mod 4

- Hence, $f(x) = x^T A x + c^T x + d = \frac{1}{2} x^T H x + c^T x + d$

$$= \frac{1}{2} \begin{bmatrix} x \\ 1 \end{bmatrix}^T \underbrace{\begin{bmatrix} H & c \\ c^T & 2d \end{bmatrix}}_{Q} \begin{bmatrix} x \\ 1 \end{bmatrix}$$

# Symmetric Matrices: Eigendecomposition (Spectral Theorem)

- Every symmetric matrix $A$ can be **diagonalized** as $A = V\Lambda V^\top$ with $V$ formed by the orthonormal eigenvectors of $A$ and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ a diagonal matrix of the eigenvalues of $A$

$v_i^\top v_j = 0 \;\forall\, i \neq j$

$\|v_i\| = 1$

$(\lambda_i, v_i)$

$$A = \underbrace{\begin{bmatrix} | & \cdots & | \\ v_1 & \cdots & v_n \\ | & \cdots & | \end{bmatrix}}_{V} \underbrace{\begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \lambda_{n-1} & 0 \\ 0 & \cdots & 0 & \lambda_n \end{bmatrix}}_{\Lambda} \underbrace{\begin{bmatrix} - & v_1^\top & - \\ \vdots & \vdots & \vdots \\ - & v_n^\top & - \end{bmatrix}}_{V^\top}$$

$v_i v_i^\top$

$\begin{bmatrix} | \\ v_i \\ | \end{bmatrix} \begin{bmatrix} - v_i - \end{bmatrix}$

$\Updownarrow$

or equivalently, $A = \lambda_1 v_1 v_1^\top + \cdots + \lambda_n v_n v_n^\top$ (i.e., weighted sum of dyads)

- Additionally, $VV^\top = V^\top V = I$ (i.e. $V^\top = V^{-1}$)
- This factorization property and the fact that ~~it~~ $A$ has $n$ orthogonal eigenvectors are two **important properties** for a symmetric matrix.

# Example Problem: Eigenvalues are Real

**Problem**: Consider a symmetric matrix $A$. Show that the eigenvalues of $A$ are real.

**Solution.**

[In general for a matrix $A$ eigenvalues & vectors can be complex.]

- Consider $\underline{Ax = \lambda x}$, $x \neq 0$. $x \in \mathbb{C}^n$, $\lambda \in \mathbb{C}$
- Recall: $\langle x, x \rangle = x^* x = (\bar{x})^T x$
- WTS $\underline{\lambda = \bar{\lambda}}$ $\lambda = a + ib$ then $b = 0$
  $\bar{\lambda} = a - ib$

$$\underbrace{\lambda \langle x, x \rangle} = (\bar{x})^T (\underbrace{\lambda x}_{Ax}) = (\bar{x})^T A x = (A^T \bar{x})^T x = (A\bar{x})^T x = (\bar{\lambda}\bar{x})^T x = \underline{\bar{\lambda} \langle x, x \rangle}$$

$$\Leftrightarrow \lambda = \bar{\lambda} \Leftrightarrow \lambda \in \mathbb{R}, \; x \in \mathbb{R}^n$$

# Example Problem: Orthogonality of Eigenvectors

**Problem**: Consider a symmetric matrix $A$. Show that eigenvectors corresponding to distinct eigenvalues are orthogonal.

**Solution.**

$$\left.\begin{array}{ll}(\lambda, x) & \text{eigenpair for } A \\ (\mu, z) & \text{— '' — } A\end{array}\right\} \text{ where } \mu \neq \lambda$$

$$\lambda\langle x, z\rangle = \langle Ax, z\rangle = (Ax)^T z = x^T A^T z = x^T A z = \mu\langle x, z\rangle$$

since $\mu \neq \lambda$ we have that $(\lambda - \mu)\langle x, z\rangle = 0 \Rightarrow x^T z = 0$

# Matrix powers with eigendecomposition

- Recall from **Mod1** we saw many applications with matrix powers such as computing the number of paths of length $k$ in a graph
- For symmetric matrices, computing matrix powers is easy

$$A = V\Lambda V^T, \qquad V^TV = I$$

$$A^k = \underbrace{(V\Lambda V^T)(V\Lambda V^T)\cdots(V\Lambda V^T)}_{k \text{ times}} = V\Lambda^k V^T$$

# Positive Definite Matrices

$\langle Ax, x\rangle = x^T A^T x > 0$

- Another important class of matrices are positive definite matrices
- The matrix $A$ is **positive definite** if $\langle Ax, x\rangle > 0$; sometimes we write $A \succ 0$
- And, $A$ is **positive semidefinite (PSD)** if $\langle Ax, x\rangle \geq 0$; sometimes we write $A \succeq 0$
- Positive definite matrices need not be symmetric, but often we are interested in positive definite symmetric matrices
- Eigenvalues: let $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$ be the order set of eigenvalues of $A = A^\top$

$f(x)$ [PSD] $$\boxed{A \succeq 0 \iff \lambda_i(A) \geq 0}\ \forall i \in \{1, \ldots, n\}$$

$\frac{d}{dx} f(x^*) = 0$, $\frac{d^2}{dx^2} f(x^*) > 0$ [PD] $$A \succ 0 \iff \lambda_i(A) > 0,\ \forall i \in \{1, \ldots, n\}$$

$H = \nabla^2 f(x)$, $\nabla f(x^*) = 0$ ; eigenvalues of $H$ positive $\iff H \succ 0$

# Example Problem

$A = A^T$

**Problem**: Show that $A \succeq 0 \iff \lambda_i(A) \geq 0, \ \forall i \in \{1, \ldots, n\}$
**Solution.**

$$A = A^T \iff A = V \Lambda V^T \iff x^T A x = \underbrace{x^T V}_{=: z^T} \Lambda V^T x = \underbrace{z^T \Lambda z} = \sum_{i=1}^{n} \lambda_i(A) z_i^2 \quad (1)$$

$$\iff \left[ \underbrace{x^T A x \geq 0 \quad \forall x \in \mathbb{R}^n} \iff \underbrace{z^T \Lambda z \geq 0 \quad \forall z \in \mathbb{R}^n} \right]$$

$$\Updownarrow$$

$$\lambda_i(A) \geq 0 \quad \forall i \in \{1, \ldots, n\}$$

due to (1)

$\Rightarrow$

$\Leftarrow$

# Examples of PSD Matrices from ML and OPT

- **Mod2-L4**: we often use kernel matrices $K = [K(x^{(i)}, x^{(j)})]$ and these are symmetric and in general PSD
- **Mod2-L2**: Gram matrices $A^\top A$ and $AA^\top$ are PSD

**Problem**: Show that Gram and Kernel matrices are PSD.

**solution.**

$$[v^T G v \geq 0 \quad \forall v]$$

$$G_{ij} = K(x^{(i)}, x^{(j)}) = \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$$

$$v^T G v = \sum_{i=1}^{n} \sum_{j=1}^{n} v_i v_j G_{ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} v_i v_j \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$$

$$= \left\langle \sum_{i=1}^{n} v_i \phi(x^{(i)}), \sum_{j=1}^{n} v_j \phi(x^{(j)}) \right\rangle = \left\| \sum_{i=1}^{n} v_i \phi(x^{(i)}) \right\|^2 \geq 0$$

# Example Problem

$A = A^\top$

**Problem**. Show that a matrix $A$ is PSD if and only if $A = B^\top B$ for some real matrix $B$.
**Solution.**

(a) (b)

$(a \Rightarrow b)$: Suppose $A = A^\top$ is PSD. eigendecomp $A = V \Lambda V^\top \iff AV = V\Lambda$

Set $B := \underbrace{\sqrt{\Lambda}\, V^\top}$ where $\sqrt{\Lambda} = \mathrm{diag}(\sqrt{\lambda_1}, \ldots \sqrt{\lambda_n})$

which exists because $\lambda_i(A) \geq 0$

Hence $B^\top B = V\sqrt{\Lambda}\sqrt{\Lambda}V^\top = V\Lambda V^\top = A \underbrace{VV^\top}_{=I} = A$

$(b \Rightarrow a)$ $A = B^\top B$. for any vector $v$ WTS $v^\top A v \geq 0$

$$v^\top A v = v^\top B^\top B v = \langle Bv, Bv \rangle = \|Bv\|^2 \geq 0 \Rightarrow A \text{ is PSD.}$$

# Part 3. SVD

# Overview

- We just talked about special classes of matrices that have a nice decomposition in terms of their eigenvalues—namely, symmetric PSD matrices.
- Now, we will talk about a matrix decomposition that every matrix has—i.e., `SVD`
- And, it is fundamentally related to a key ML analysis tool: `PCA`

# Matrix Decomposition

- Matrix decomposition, also known as matrix factorization, involves describing a given matrix using its constituent elements.
- Recall that you saw QR decomposition in **Module 1** and then its use in **Module 2** (e.g., solving least squares, in particular sparse problems)
- Perhaps the most known and widely used matrix decomposition method is the **Singular-Value Decomposition**, or `SVD`.
- All matrices have an `SVD`, which makes it more stable than other methods, such as the eigen-decomposition.
- We will see the `SVD` is useful for computing the pseudoinverse efficiently and for dimensionality reduction

# Singular Value Decomposition

# What is SVD?

- One can generalize eigenvalues/vectors to non-square matrices, in which case they are called singular vectors and singular values.
- The SVD is a unique matrix decomposition that exists for every matrix $A \in \mathbb{R}^{m\times n}$:

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

where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are *unitary* matrices, and $\Sigma \in \mathbb{R}^{m\times n}$ is a matrix with non-negative entries on the diagonal and zeros on the off diagonal.

- Unitary: $UU^\top = I$ and $VV^\top = I$

# SVD as a Dyadic Exanpsion

An equivalent way to express the SVD $A = U\Sigma V^\top$ is as a dyadic expansion:

- That is, the SVD expresses $A$ as a nonnegative linear combination of $\min\{m, n\}$ rank-1 matrices
- the singular values provide the multipliers
- the outer products of the left and right singular vectors provide the rank-1 matrices.

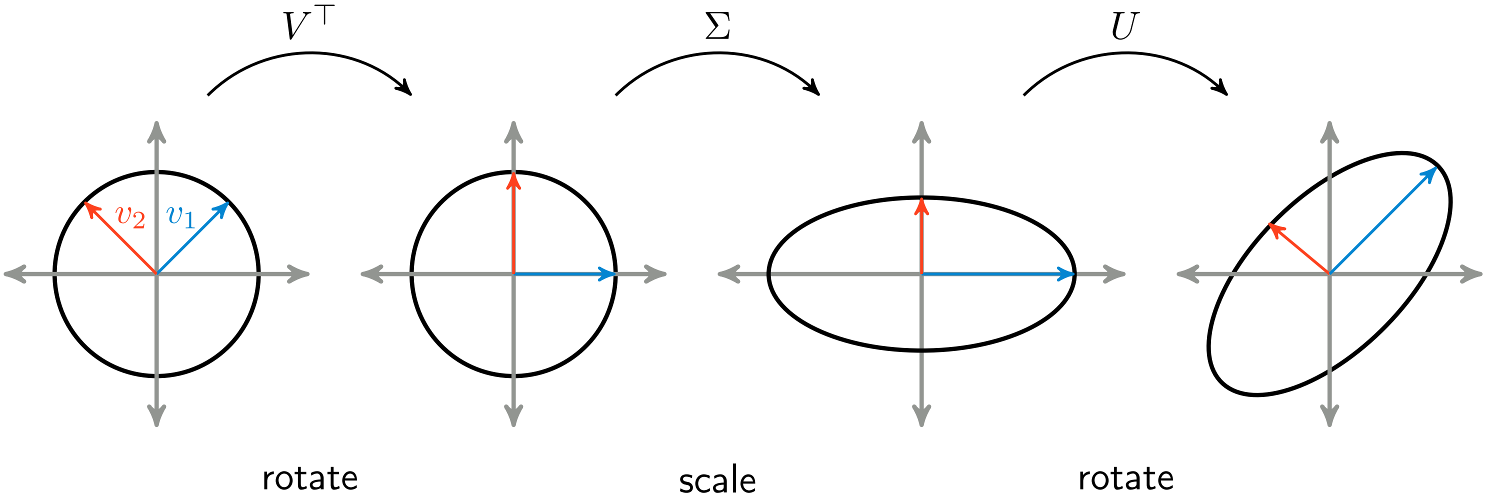
# SVD

- The diagonal entries of $\Sigma$ are called the **singular values** of $A$
- The column vectors of $V$ are called the **right singular vectors** of $A$
- The column vectors of $U$ are called the **left singular vectors** of $A$.
- The number of nonzero singular values is equal to the rank of the matrix $A$.

$$\underbrace{A}_{m \times n} = \underbrace{U}_{m \times m} \underbrace{\Sigma}_{m \times n} \underbrace{V^\top}_{n \times n}$$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_n \\ 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}$$

# Geometric View of SVD



# Unpacking the SVD

- Let $A \in \mathbb{R}^{m \times n}$
- **Fact 1**. Both $A^\top A \in \mathbb{R}^{n \times n}$ and $AA^\top \in \mathbb{R}^{m \times m}$ are symmetric square matrices:

- **Fact 2**. Both $A^\top A$ and $AA^\top$ share the same non-zero eigenvalues:

# Unpacking the SVD

- According to the othogonally diagonalizable property of symmetric matrices, the matrices $A^\top A$ and $AA^\top$ can be decomposed as following:

- **How to obtain the** SVD**?**: Compute by diagonalizing the PSD symmetric matrices $A^\top A$ and $AA^\top$

# Using the SVD to Compute Pseudo Inverses

- It turns out that using the SVD we have a very easy way to compute the pseudo-inverse of $A$—i.e., $A^\dagger = (A^\top A)^{-1} A^\top$ which we saw in **Mod1 & Mod2**

# Matrix Norms and Connections to Singular values

- Matrix norms and singular values have special relationships.
- **Forbenius Norm**:

$$\|A\|_F = \left(\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2\right)^{1/2} = (\mathsf{Tr}(A^\top A))^{1/2}$$

- **Matrix $p$-norm**: matrix $p$-Norm is defined as the largest scalar that you can get for a unit vector

$$\|A\|_p = \sup_{x\neq 0}\frac{\|Ax\|_p}{\|x\|_p} = \max_{\|x\|_p=1}\|Ax\|_p$$

- Aside: supremum $\sup(\cdot)$ is the " least upper bound" of its argument

# Matrix Norms: Spectral Norm

- **Spectral Norm** (**Matrix 2-norm**): Largest singular value of the matrix $\sigma_1(A)$

- **Fact**: show that $\|A\|_F = \sqrt{\sum_{i=1}^{\min\{m,n\}} \sigma_i^2(A)}$ using the fact that $\|A\|_F = \sqrt{\mathrm{Tr}(A^\top A)}$

# Reduced SVD & Low Rank Approximation

- Rank of $\Lambda$ is $r \implies$ there are $r$ non-zero eigenvalues of the matrices $A^\top A$ and $AA^\top$
- Reduced `SVD`:

# Low Rank Structure

$$\underbrace{A}_{m \times n} = \underbrace{Y}_{m \times r}\,\underbrace{Z^\top}_{r \times n}$$

# Low Rank Structure

$$A = uv^\top =$$

$$A = uv^\top + wz^\top =$$

# Low Rank Approximation

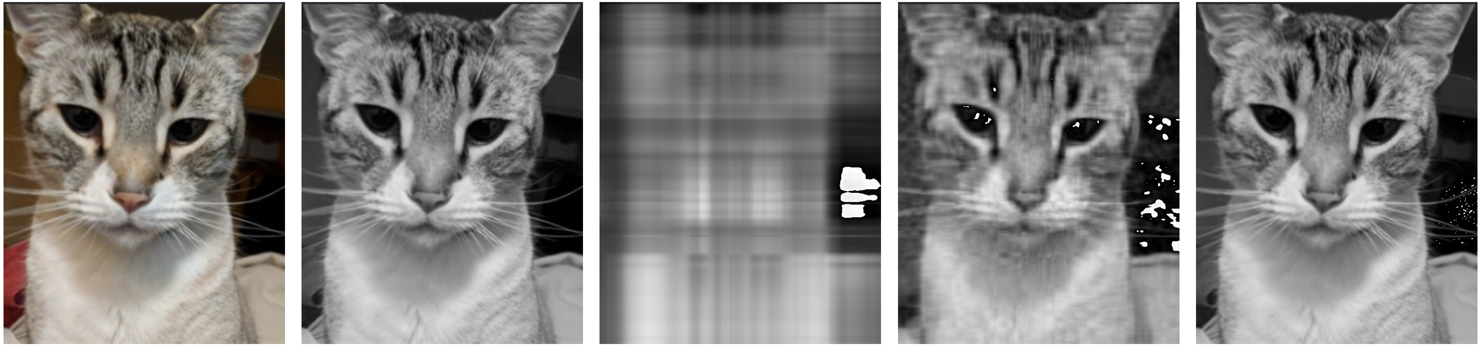
- Low Rank Approximation: take only top $k$-singular values and corresponding dyads in the dyadic expansion

- Low Rank Approximation is an important tool for many applications including
  - Linear system identification: approximating matrix is Hankel structured. (You saw this in `M2-N2.ipynb`)
  - ML: feature space dimensionality reduction
  - Recommender systems: matrix completion
  - Distance matrix completion where there is a positive definiteness constraint.
  - Natural language processing where the approximation is non-negative.
  - Image or video compression

# Example: Compression

- **Compression.** A low-rank approximation provides a (lossy) compressed version of the data matrix.
  - The original matrix $A$ is described by $mn$ numbers, while describing $Y$ and $Z^\top$ requires only $k(m+n)$ numbers.
  - When $k$ is small relative to $m$ and $n$, replacing the product of $m$ and $n$ by their sum is a big win.
  - With images, a modest value of $k$ (say 100 or 150) is usually enough to achieve approximations that look a lot like the original image.

bender in color | gray scale | rank 2 bender | rank 20 bender | rank 100 bender



# Optimality of Low Rank Approximation

- The low rank approximation obtained via SVD is optimal in the following sense.
- Recall the Forbenius norm:
- i.e., $\ell_2$-norm (i.e., usual Euclidean norm) applied to the matrix as if it were a vector
- **Theorem [Eckat-Young-Mirsky]**.

# How to choose $k$?

- When producing a low-rank matrix approximation, we have been taking as a parameter the target rank $k$.
- **Ideal Setting**: the singular values of $A$ give strong guidance
  - if the top few singular values are big and the rest are small, then the obvious solution is to take $k$ equal to the number of “big values".
- **Less Ideal Setting**: take $k$ as small as possible subject to obtaining a useful approximation, where what “useful" means depends on the application.
  - e.g., a common rule of thumb is to choose $k$ such that the sum of the top $k$ singular values is at least $c$ times as big as the sum of the other singular values, where $c$ is a domain-dependent constant (like 10, say).

# Next Up

- Next lecture we will talk about PCA, and show that PCA reduces to SVD and is fundamentally connected to low rank approximations.