# Singular Value Decomposition (SVD)

CS 663
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# Singular value Decomposition

- For any *m* x *n* matrix **A**, the following decomposition **always** exists:

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \mathbf{A} \in R^{m \times n},$$
$$\mathbf{U}^T\mathbf{U} = \mathbf{U}\mathbf{U}^T = \mathbf{I}_m, \mathbf{U} \in R^{m \times m},$$
$$\mathbf{V}^T\mathbf{V} = \mathbf{V}\mathbf{V}^T = \mathbf{I}_n, \mathbf{V} \in R^{n \times n},$$
$$\mathbf{S} \in R^{m \times n}$$

Diagonal matrix with non-negative entries on the diagonal – called **singular values.**

Columns of $\mathbf{U}$ are the eigenvectors of $\mathbf{A}\mathbf{A}^T$ (called the left singular vectors).
Columns of $\mathbf{V}$ are the eigenvectors of $\mathbf{A}^T\mathbf{A}$ (called the right singular vectors).
The non-zero singular values are the positive square roots of non-zero eigenvalues of $\mathbf{A}\mathbf{A}^T$ or $\mathbf{A}^T\mathbf{A}$.

# Singular value Decomposition

- For any *m* x *n* real matrix **A**, the SVD consists of matrices **U**,**S**,**V** which are always real – this is unlike eigenvectors and eigenvalues of **A** which may be complex even if **A** is real.

- The singular values are always non-negative, even though the eigenvalues may be negative.

- While writing the SVD, the following convention is assumed, and the left and right singular vectors are also arranged accordingly:

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{m-1} \geq \sigma_m$$

# Singular value Decomposition

- If only $r$ < min($m$,$n$) singular values are non-zero, the SVD can be represented in **reduced form** as follows:

$$A = USV^T, A \in R^{m \times n},$$

$$U \in R^{m \times r},$$

$$V \in R^{n \times r},$$

$$S \in R^{r \times r}$$

# Singular value Decomposition

$$\mathbf{A} = \mathbf{USV}^T = \sum_{i=1}^{r} \mathbf{S}_{ii} \boxed{\mathbf{u}_i \mathbf{v}_i^t}$$

This *m* by *n* matrix $\mathbf{u}_i \mathbf{v}^T_i$ is the product of a column vector $\mathbf{u}_i$ and the transpose of column vector $\mathbf{v}_i$. It has rank 1. Thus **A** is a weighted summation of *r* rank-1 matrices.

Note: $\mathbf{u}_i$ and $\mathbf{v}_i$ are the i-th column of matrix **U** and **V** respectively.

# Singular value decomposition

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

$$\mathbf{A}\mathbf{A}^T = (\mathbf{U}\mathbf{S}\mathbf{V}^T)(\mathbf{U}\mathbf{S}\mathbf{V}^T)^T = \mathbf{U}\mathbf{S}\mathbf{V}^T\mathbf{V}\mathbf{S}\mathbf{U}^T = \mathbf{U}\mathbf{S}^2\mathbf{U}^T$$

Thus, the left singular vectors of $\mathbf{A}$ (i.e. columns of $\mathbf{U}$) are the eigenvectors of $\mathbf{A}\mathbf{A}^T$.

The singular values of $\mathbf{A}$ (i.e. diagonal elements of $\mathbf{S}$) are square-roots of the eigenvalues of $\mathbf{A}\mathbf{A}^T$.

$$\mathbf{A}^T\mathbf{A} = (\mathbf{U}\mathbf{S}\mathbf{V}^T)^T(\mathbf{U}\mathbf{S}\mathbf{V}^T) = \mathbf{V}\mathbf{S}\mathbf{U}^T\mathbf{U}\mathbf{S}\mathbf{V}^T = \mathbf{V}\mathbf{S}^2\mathbf{V}^T$$

Thus, the right singular vectors of $\mathbf{A}$ (i.e. columns of $\mathbf{V}$) are the eigenvectors of $\mathbf{A}^T\mathbf{A}$.

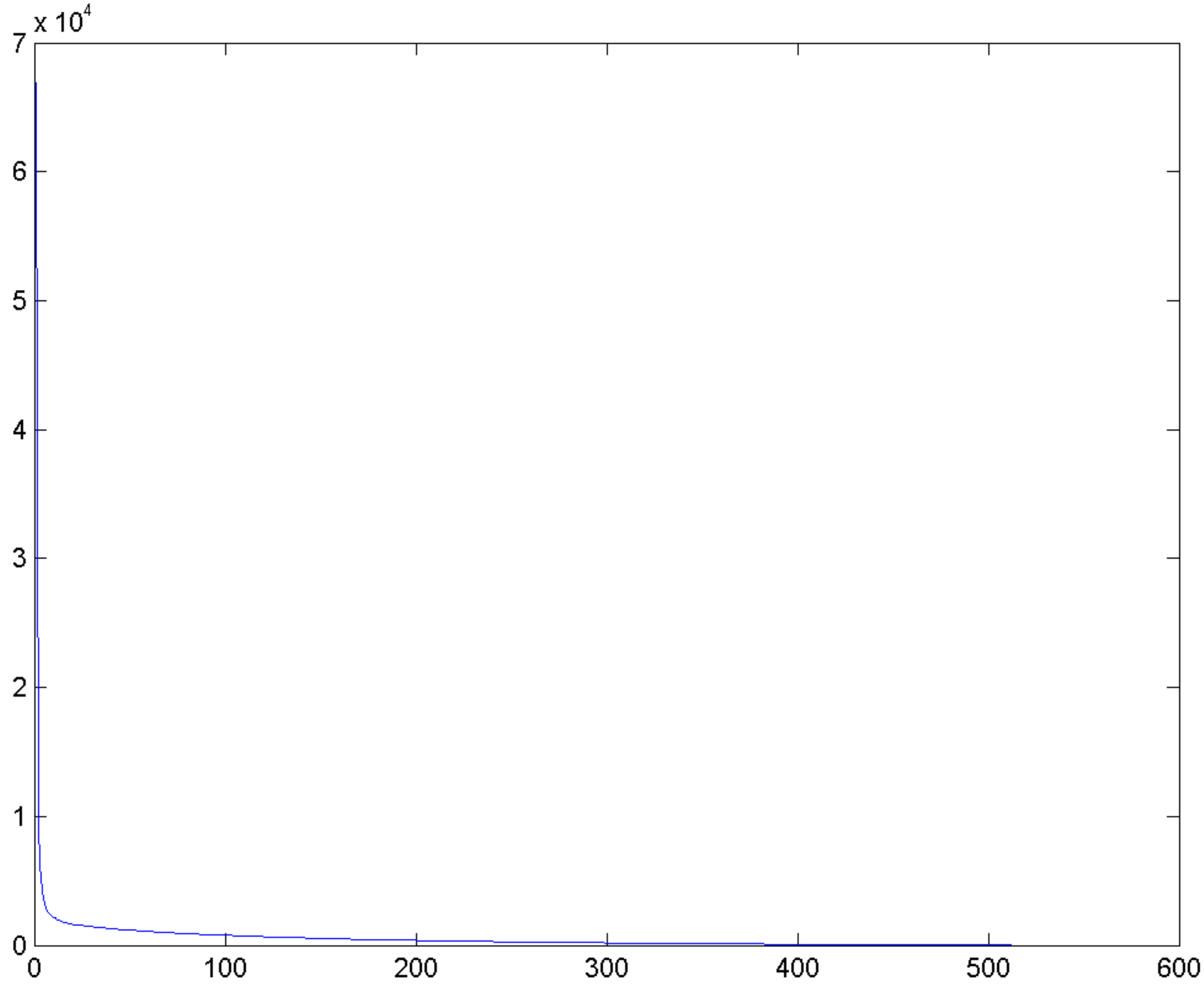
The singular values of $\mathbf{A}$ (i.e. diagonal elements of $\mathbf{S}$) are square-roots of the eigenvalues of $\mathbf{A}^T\mathbf{A}$.

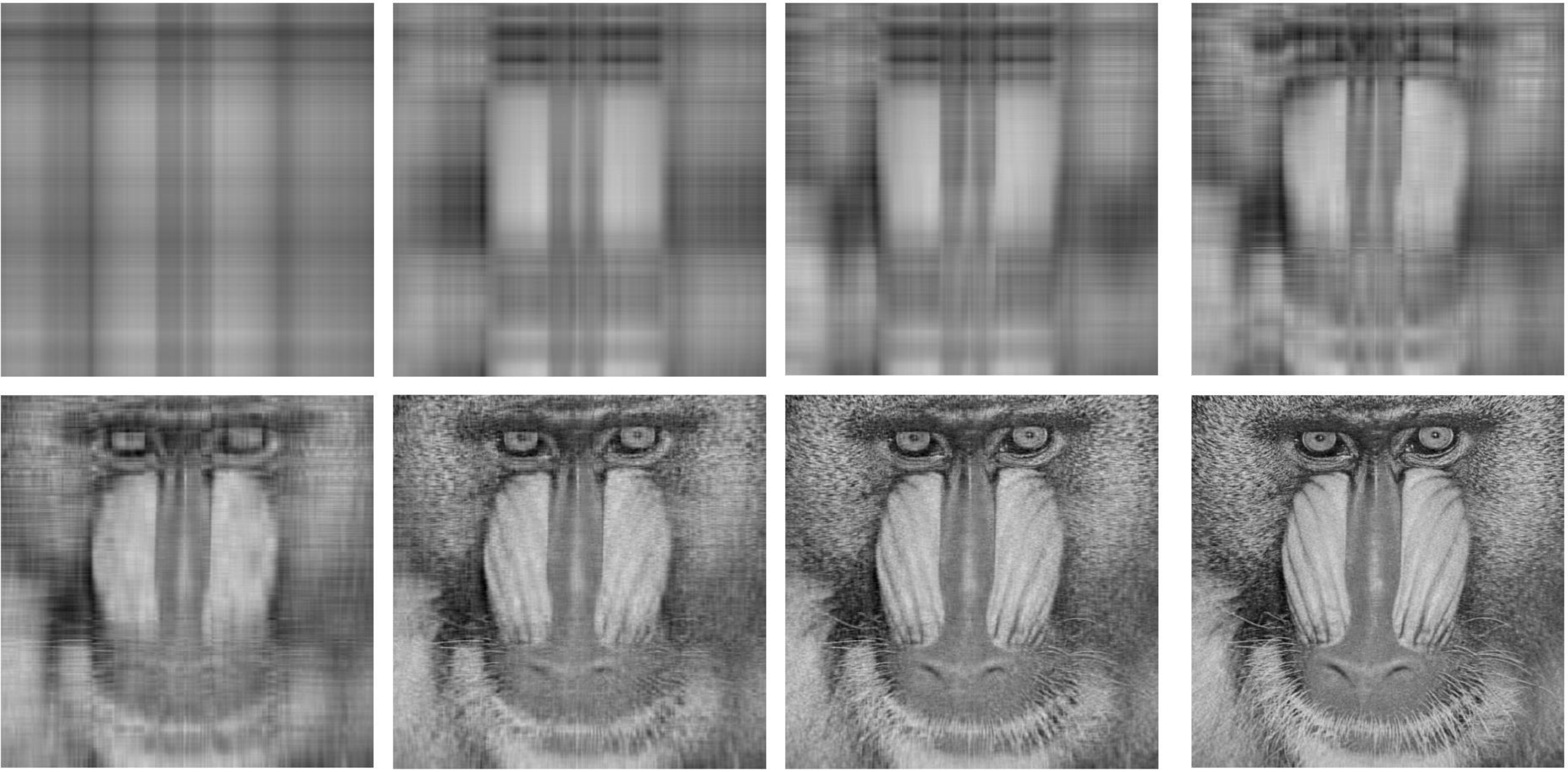
# Application: SVD of Natural Images

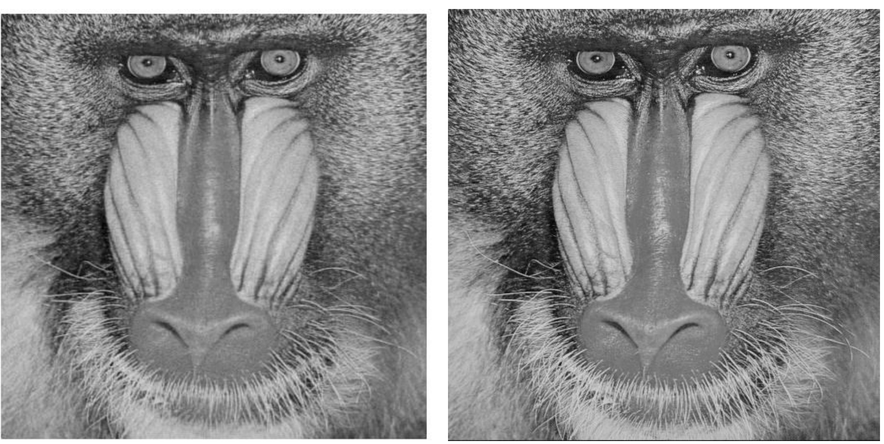
- An image is a 2D array – each entry contains a grayscale value. The image can be treated as a matrix.
- It has been observed that for many image matrices, the singular values undergo rapid decay (note: they are always non-negative).
- An image can be approximated with the *k* largest singular values and their corresponding singular vectors:

$$\mathbf{A} \approx \sum_{i=1}^{k} \mathbf{S}_{ii} \mathbf{u}_i \mathbf{v}_i^t, k < \min(m,n)$$

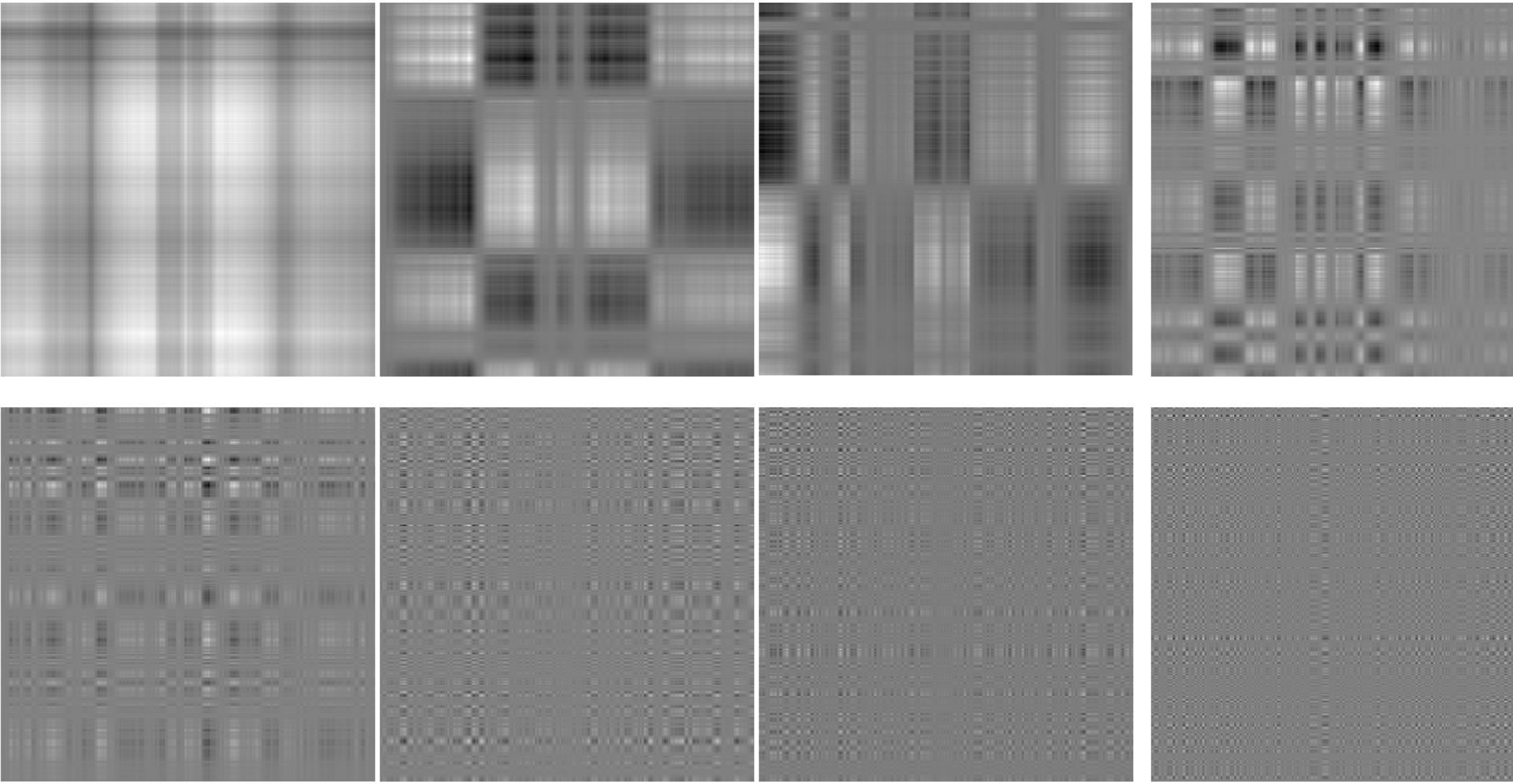
Singular values of the Mandrill Image: notice the rapid exponential decay of the values! This is characteristic of MOST natural images.

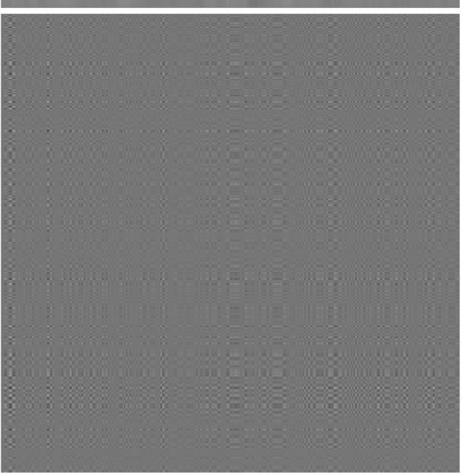






Left to right, top to bottom:
Reconstructed image using the first *i*= 1,2,3,5,10,25,50,100,150 singular values and singular vectors.
Last image: original





Left to right, top to bottom, we display:

$$\mathbf{u}_i \mathbf{v}_i^T$$

where $i$ = 1,2,3,5,10,25,50,100,150.
Note each image is independently re-scaled to the 0-1 range for display purpose.

Note: the spatial frequencies increase as the singular values decrease

# SVD: Use in Image Compression

- Instead of storing $mn$ intensity values, we store $(n+m+1)r$ intensity values where $r$ is the number of stored singular values (or singular vectors). The remaining $m-r$ singular values (and hence their singular vectors) are effectively set to 0.

- This is called as storing a low-rank (rank $r$) approximation for an image.

# Properties of SVD: Best low-rank reconstruction

- SVD gives us the **best possible** rank-*r* approximation to *any* matrix (it may or may not be a natural image matrix).
- In other words, the solution to the following optimization problem:

$$\min_{\hat{\mathbf{A}}} \left\| \hat{\mathbf{A}} - \mathbf{A} \right\|_F^2 \text{ where } \operatorname{rank}(\hat{\mathbf{A}}) = r, r \leq \min(m,n)$$

is given using the SVD of **A** as follows:

$$\hat{\mathbf{A}} = \sum_{i=1}^{r} \mathbf{S}_{ii} \mathbf{u}_i \mathbf{v}_i^t, \text{ where } \mathbf{A} = \mathbf{USV}^T$$

Note: We are using the singular vectors corresponding to the *r* **largest** singular values.

This property of the SVD is called the **Eckart Young Theorem**.

# Properties of SVD: Best low-rank reconstruction

$$\min_{\hat{\mathbf{A}}} \left\| \hat{\mathbf{A}} - \mathbf{A} \right\|_F^2 \text{ where } \operatorname{rank}(\hat{\mathbf{A}}) = r, r \leq \min(m, n)$$

$$\left\| \mathbf{A} \right\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} \mathbf{A}_{ij}^2}$$

Frobenius norm of the matrix (fancy way of saying you square all matrix values, add them up, and then take the square root!)

$$Note: \left\| \hat{\mathbf{A}} - \mathbf{A} \right\|_F^2 = \sigma_{\mathrm{r+1}}^2 + \sigma_{\mathrm{r+2}}^2 + \ldots + \sigma_n^2$$

Why?

# Geometric interpretation: Eckart-Young theorem

- The best linear approximation to an ellipse is its longest axis.
- The best 2D approximation to an ellipsoid in 3D is the ellipse spanned by the longest and second-longest axes.
- And so on!

# Properties of SVD: Singularity

- A square matrix **A** is non-singular (i.e. invertible or full-rank) if and only if all its singular values are non-zero.
- The ratio $\sigma_1/\sigma_n$ tells you how close **A** is to being singular. This ratio is called **condition number** of **A**. The larger the condition number, the closer the matrix is to being singular.

# Properties of SVD: Rank, Inverse, Determinant

- The rank of a rectangular matrix **A** is equal to the number of non-zero singular values. Note that rank(**A**) = rank(**S**).
- SVD can be used to compute inverse of a square matrix:

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \mathbf{A} \in R^{n\times n},$$
$$\mathbf{A}^{-1} = \mathbf{V}\mathbf{S}^{-1}\mathbf{U}^T$$

- Absolute value of the determinant of square matrix **A** is equal to the product of its singular values.

$$|\det(\mathbf{A})| = |\det(\mathbf{U}\mathbf{S}\mathbf{V}^T)| = |\det(\mathbf{U})\det(\mathbf{S})\det(\mathbf{V}^T)| = \det(\mathbf{S}) = \prod_{i=1}^{n} \sigma_i$$

# Properties of SVD: Pseudo-inverse

- SVD can be used to compute pseudo-inverse of a rectangular matrix:

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \mathbf{A} \in R^{m \times n},$$

$$\mathbf{A}^+ = \mathbf{V}\mathbf{S}_0^{-1}\mathbf{U}^T, \text{where } \mathbf{S}_0^{-1}(i,i) = \mathbf{S}^{-1}(i,i) = \frac{1}{\mathbf{S}(i,i)} \text{ for all}$$

$$\text{non-zero singular values and } \mathbf{S}_0^{-1}(i,i) = 0 \text{ otherwise.}$$

# Properties of SVD: Frobenius norm

- The Frobenius norm of a matrix is equal to the square-root of the sum of the squares of its singular values:

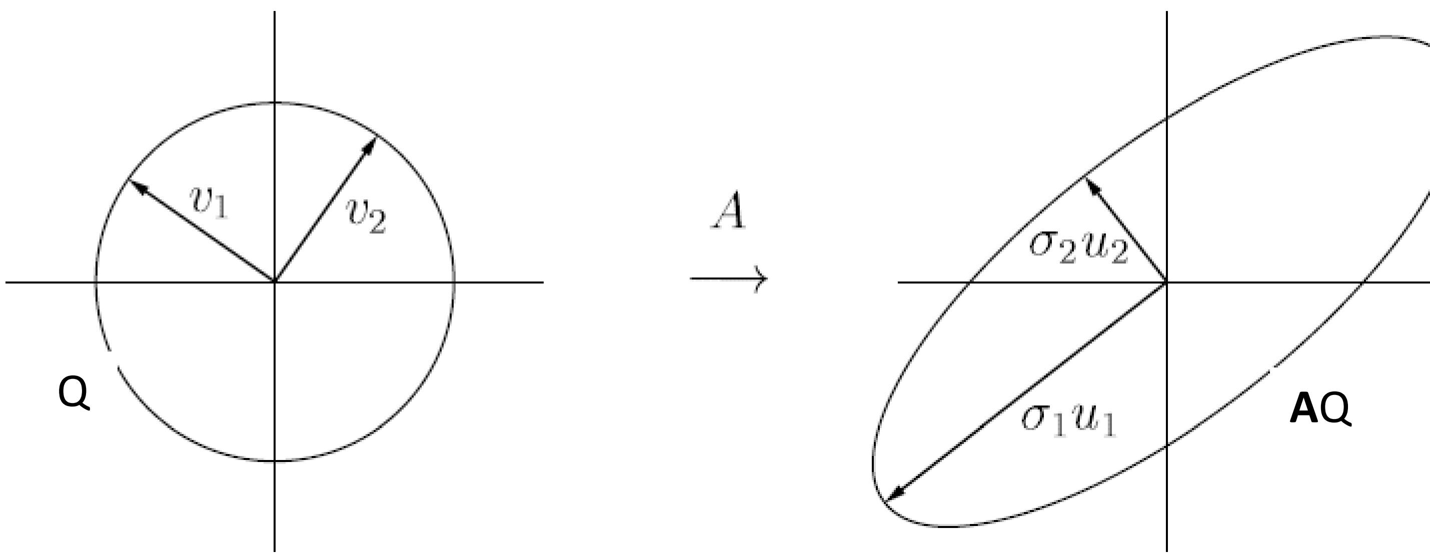
$$\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbf{A}_{ij}^2} = \sqrt{trace(\mathbf{A}^T\mathbf{A})} = \sqrt{trace((\mathbf{USV}^T)^T(\mathbf{USV}^T))}$$

$$= \sqrt{trace(\mathbf{V}^T\mathbf{S}^2\mathbf{V})} = \sqrt{trace(\mathbf{VV}^T\mathbf{S}^2)} = \sqrt{trace(\mathbf{S}^2)}$$

$$= \sqrt{\sum_i \sigma_i^2}$$

# Geometric interpretation of the SVD

- Any *m* x *n* matrix **A** transforms a hypersphere $\mathrm{Q}$ of unit radius (called as unit sphere) in $\mathcal{R}^n$ into a hyperellipsoid in $\mathcal{R}^m$ (assume *m* >= *n*).



# Geometric interpretation of the SVD

- But why does **A** transform the hypersphere into a *hyperellipsoid*?
- This is because **A = USV**$^T$.
- **V**$^T$ transforms the hypersphere into another (rotated/reflected) hypersphere.
- **S** stretches the sphere into a hyperellipsoid whose semi-axes coincide with the coordinate axes as per **V**.
- **U** rotates/reflects the hyperellipsoid without affecting its shape.
- As any matrix **A** has an SVD decomposition, it will always transform the hypersphere into a hyperellipsoid.
- If **A** does not have full rank, then some of the semi-axes of the hyperellipsoid will have length 0!

# Geometric interpretation of the SVD

- Assume **A** has full rank for now.
- The singular values of **A** are the lengths of the *n* principal semi-axes of the hyperellipsoid. The lengths are thus $\sigma_1, \sigma_2, \ldots, \sigma_n$.
- The *n* left singular vectors of **A** are the directions $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$ (all unit-vectors) aligned with the *n* semi-axes of the hyperellipsoid.
- The *n* right singular vectors of **A** are the directions $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ (all unit-vectors) in hypersphere Q, which the matrix **A** transforms into the semi-axes of the hyperellipsoid, i.e.

$$\forall i, \mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i$$

# Geometric interpretation of the SVD

- Expanding on the previous equations, we get the reduced form of the SVD

$$\begin{bmatrix} \\ \\ & A & \\ \\ \\ \end{bmatrix} \left[\begin{array}{c|c|c|c} \\ v_1 & v_2 & \cdots & v_n \\ \\ \end{array}\right] = \left[\begin{array}{c|c|c|c} \\ \\ u_1 & u_2 & \cdots & u_n \\ \\ \\ \end{array}\right] \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}$$

*n* x *n* orthonormal matrix **V**

*m* x *n* matrix (*m* >> *n*) with orthonormal columns - **U**

*n* x *n* diagonal matrix - **S**

# Computation of the SVD

- We will not explore algorithms to compute the SVD of a matrix, in this course.
- SVD routines exist in the LAPACK library and are interfaced through the following MATLAB functions:

s = svd(X) returns a vector of singular values.

[U,S,V] = svd(X) produces a diagonal matrix S of the same dimension as X, with nonnegative diagonal elements in decreasing order, and unitary matrices U and V so that X = U*S*V'.

[U,S,V] = svd(X,0) produces the "economy size" decomposition. If X is m-by-n with m > n, then svd computes only the first n columns of U and S is n-by-n.

[U,S,V] = svd(X,'econ') also produces the "economy size" decomposition. If X is m-by-n with m >= n, it is equivalent to svd(X,0) . For m < n, only the first m columns of V are computed and S is m-by-m.

s = svds(A,k) computes the k largest singular values and associated singular vectors of matrix A.

# SVD Uniqueness

- If the singular values of a matrix are all distinct, the SVD is unique – up to a multiplication of the corresponding columns of **U** and **V** by a sign factor.
- Why?

$$\mathbf{A} = \sum_{i=1}^{r} \mathbf{S}_{ii}\mathbf{u}_i\mathbf{v}_i^t = \mathbf{S}_{11}\mathbf{u}_1\mathbf{v}_1^t + \mathbf{S}_{22}\mathbf{u}_2\mathbf{v}_2^t + \ldots + \mathbf{S}_{rr}\mathbf{u}_r\mathbf{v}_r^t$$

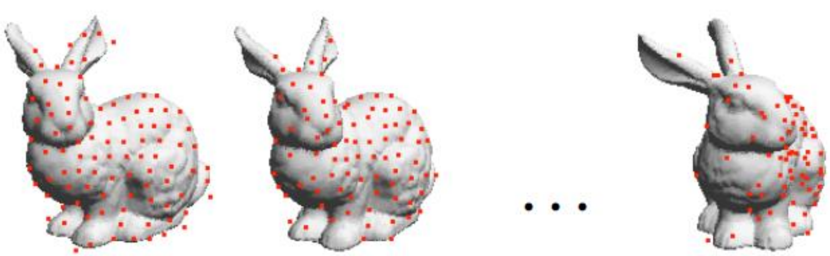
$$= \mathbf{S}_{11}(\mathbf{-u}_1)(\mathbf{-v}_1^t) + \mathbf{S}_{22}\mathbf{u}_2\mathbf{v}_2^t + \ldots + \mathbf{S}_{rr}(\mathbf{-u}_r)(\mathbf{-v}_r^t)$$

# SVD Uniqueness

- A matrix is said to have *degenerate* singular values, if it has the same singular value for 2 or more pairs of left and right singular vectors.
- In such a case any normalized linear combination of the left (right) singular vectors is a valid left (right) singular vector for that singular value.

# Any other applications of SVD?

- **Face recognition** – the popular eigenfaces algorithm can be implemented using SVD too!
- **Point matching:** Consider two sets of points, such that one point set is obtained by an unknown rotation of the other. Determine the rotation!
- **Structure from motion:** Given a sequence of images of a object undergoing rotational motion, determine the 3D shape of the object as well as the 3D rotation at every time instant!



# PCA Algorithm using SVD

1. Compute the mean of the given points:

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i, \mathbf{x}_i \in R^d, \bar{\mathbf{x}} \in R^d$$

2. Deduct the mean from each point:

$$\bar{\mathbf{x}}_\mathbf{i} = \mathbf{x}_\mathbf{i} - \bar{\mathbf{x}}$$

3. Compute the covariance matrix of these mean-deducted points:

$$\mathbf{C} = \frac{1}{N-1}\sum_{i=1}^{N}\bar{\mathbf{x}}_i\bar{\mathbf{x}}_i^T = \frac{1}{N-1}\mathbf{X}\mathbf{X}^T, Note: \mathbf{C} \in R^{d\times d}$$

$$\mathbf{X} = [\bar{\mathbf{x}}_\mathbf{1} \,|\, \bar{\mathbf{x}}_\mathbf{2} \,|\, \ldots \,|\, \bar{\mathbf{x}}_\mathbf{N}] \in R^{d\times N}$$

# PCA Algorithm using SVD

4. Instead of finding the eigenvectors of **C**, we find the left singular vectors of **X** and its singular values

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \mathbf{U} \in R^{d \times d}$$

$$\mathbf{U} \text{ contains the eigenvectors of } \mathbf{X}\mathbf{X}^T.$$

**U**,**S**,**V** are obtained by computing the SVD of **X**.

5. Extract the *k* eigenvectors in **U** corresponding to the *k* largest singular values to form the extracted **eigenspace:**

$$\hat{\mathbf{U}}_{\mathbf{k}} = \mathbf{U}(:,1:k)$$

There is an implicit assumption here that the first *k* indices indeed correspond to the *k* largest eigenvalues. If that is not true, you would need to pick the appropriate indices.

# References


- Scientific Computing, Michael Heath
- Numerical Linear Algebra, Treftehen and Bau
- http://en.wikipedia.org/wiki/Singular_value_decomposition