Numerical Analysis FMN011

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Singular Value Decomposition

Singular values and singular vectors

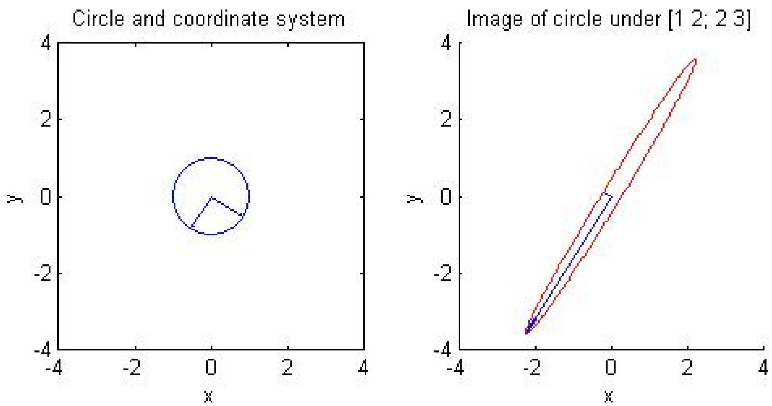
For every $m \times n$ matrix A there are orthonormal sets $\{u_1, \ldots, u_m\}$ and $\{v_1, \ldots, v_n\}$, and nonnegative numbers $s_1, \ldots, s_n$ such that $Av_i = s_i u_i$ for $1 \leq i \leq \min(m, n)$.

The s_i are called the singular values of A.

The v_i are called the right singular vectors of A.

The u_i are called the left singular vectors of A.

Image of the Unit Sphere Under A



(a) Unit sphere with orthogonal coordinate axes $\{v_1, v_2\}$.
(b) The image of the unit sphere in the orthogonal basis v_1, v_2 is an ellipsoid with axes s_1u_1, s_2u_2.

Orthogonal coordinate system $\{u_1, u_2\}$ for which $Av_i = s_iu_i$, $s_1 \geq s_2 \geq 0$.

Eigenvalues of $A^T A$

Let A be a real $m \times n$ matrix.

$A^T A$ is symmetric, so its eigenvalues are real.

Suppose λ is an eigenvalue of $A^T A$ with unit eigenvector v.

$$
\begin{aligned}
A^T A v &= \lambda v \\
v^T A^T A v &= \lambda v^T v \\
\lambda &= \|Av\|_2^2 \geq 0
\end{aligned}
$$

The eigenvalues of $A^T A$ are real and non-negative.

Eigenvectors of $A^T A$

Let A be a real $m \times n$ matrix.

Suppose $A^T A u = \lambda u$ and $A^T A v = \beta v$ with $\lambda \neq \beta$.

$$\begin{aligned} v^T A^T A u &= \lambda v^T u \Rightarrow (A^T A v)^T u = \lambda v^T u \\ \beta v^T u &= \lambda v^T u \Rightarrow v^T u = 0 \end{aligned}$$

The eigenvectors of $A^T A$ are orthogonal.

Singular Values and Singular Vectors

Eigenvalues of $A^T A$: $\lambda_1 = s_1^2 \geq \lambda_2 = s_2^2 \geq \cdots \geq \lambda_n = s_n^2 \geq 0$ with orthonormal eigenvectors $v_1, \ldots, v_n$.

Take $s_i \geq 0$.

Define $u_i,\ i = 1, \ldots, m$ such that

- If $s_i \neq 0$, $\boxed{Av_i = s_i u_i,}$ that is, $u_i = Av_i / s_i$.
- If $s_i = 0$, u_i is any unit vector orthogonal to $u_1, \ldots u_{i-1}$.

We now have

- $\{v_1, \ldots, v_n\}$ is an orthonormal basis of $\mathbb{R}^n$ (right singular vectors)
- $\{u_1, \ldots, u_m\}$ is an orthonormal basis of $\mathbb{R}^m$ (left singular vectors)
- $Av_i = s_i u_i$, with $s_1 \geq \cdots \geq s_n \geq 0$ (s_i are the singular values)

and

- $s_1, \ldots, s_n$ are the nonnegative square roots of the eigenvalues of $A^T A$
- $u_1, \ldots, u_m$ are orthonormal eigenvectors of AA^T
- $v_1, \ldots, v_n$ are orthonormal eigenvectors of $A^T A$

Singular Value Decomposition

U is the matrix whose columns are the left singular vectors

V is the matrix whose columns are the right singular vectors

S is the diagonal matrix whose elements are the singular values

$$\boxed{A = USV^T}$$

Example: a square diagonal matrix

$$A = \begin{pmatrix} 3 & 0 \\ 0 & 2/3 \end{pmatrix} \Rightarrow A^T A = \begin{pmatrix} 9 & 0 \\ 0 & 4/9 \end{pmatrix}$$

Eigenvalues: 9 and 4/9, $\Rightarrow s_1 = 3, s_2 = 2/3$

Right singular vectors: $v_1 = (1, 0)$ and $v_2 = (0, 1)$

Left singular vectors: $u_1 = \frac{1}{3}\begin{pmatrix} 3 & 0 \\ 0 & 2/3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
$u_2 = \frac{3}{2} A v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\begin{pmatrix} 3 & 0 \\ 0 & 2/3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 3 & 0 \\ 0 & 2/3 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Example: a singular square matrix

$$A = \begin{pmatrix} 3 & 0 \\ 4 & 0 \end{pmatrix} \Rightarrow A^T A = \begin{pmatrix} 25 & 0 \\ 0 & 0 \end{pmatrix}$$

$s_1 = 5, s_2 = 0$; $v_1 = (1, 0), v_2 = (0, 1)$; $u_1 = (3/5, 4/5), u_2 = (-4/5, 3/5)$

$$\begin{pmatrix} 3 & 0 \\ 4 & 0 \end{pmatrix} = \begin{pmatrix} 3/5 & -4/5 \\ 4/5 & 3/5 \end{pmatrix} \begin{pmatrix} 5 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The unit circle is flattened to the line segment from (-3,-4) to (3,4)

Example: a rectangular matrix

$$A = \begin{pmatrix} 1 & -1 \\ 2 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow A^T A = \begin{pmatrix} 5 & -1 \\ -1 & 2 \end{pmatrix}$$

$s_1 = \sqrt{5.3028} = 2.3028, s_2 = \sqrt{1.6972} = 1.3028,$

$$v_1 = \begin{pmatrix} -0.9571 \\ 0.2898 \end{pmatrix}, v_2 = \begin{pmatrix} -0.2898 \\ -0.9571 \end{pmatrix}$$

$$u_1 = \begin{pmatrix} -0.5415 \\ -0.8313 \\ 0.1258 \end{pmatrix}, u_2 = \begin{pmatrix} 0.5122 \\ -0.4449 \\ -0.7347 \end{pmatrix}$$

To construct U we need to complete the basis for $\mathbb{R}^3$

Take $\hat{u}_3 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, orthogonalize, then normalize it:

$$\tilde{u}_3 = \hat{u}_3 - (\hat{u}_3^T\, u_1)\, u_1 - (\hat{u}_3^T\, u_2)\, u_2 = \begin{pmatrix} 0.4444 \\ -0.2222 \\ 0.4444 \end{pmatrix}$$

$$u_3 = \frac{u_3}{\|u_3\|_2} = \begin{pmatrix} 0.6667 \\ -0.3333 \\ 0.6667 \end{pmatrix}$$

$$A = USV^T$$

$$U = \begin{pmatrix} -0.5415 & 0.5122 & 0.6667 \\ -0.8313 & -0.4449 & -0.3333 \\ 0.1258 & -0.7347 & 0.6667 \end{pmatrix},$$

$$S = \begin{pmatrix} 2.3028 & 0 \\ 0 & 1.3028 \\ 0 & 0 \end{pmatrix},$$

$$V = \begin{pmatrix} -0.9571 & -0.2898 \\ 0.2898 & -0.9571 \end{pmatrix}$$

SVD of Symmetric Matrices

If A is symmetric, then $A^T A = A^2$.

$Au = \lambda u \Rightarrow A^T A u = \lambda^2 u$

$s_i = |\lambda_i|$, where $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_m|$

v_i are the corresponding unit eigenvectors of A

u_i are

- v_i if $\lambda_i \geq 0$
- $-v_i$ if $\lambda_i < 0$

Rank and SVD

The **rank** of an $m \times n$ matrix is the number of linearly independent rows (or columns)

$$A = USV^T$$

Because U and V are invertible,

rank(A)=rank(S)=number of nonzero elements of S

Determinant and SVD

$$A = USV^T$$

$U^T U = I$

$\det(U^T)\det(U) = 1 \Rightarrow \det(U)^2 = 1 \Rightarrow \det(U) = \pm 1$

$V^T V = I$

$\det(V^T)\det(V) = 1 \Rightarrow \det(V)^2 = 1 \Rightarrow \det(V) = \pm 1$

$\det(A) = \det(U)\det(S)\det(V^T) = \pm\det(S) = \pm s_1 \cdots s_n$

$$|\det(A)| = s_1 \cdots s_n$$

Inverse and SVD

Suppose A is an $m \times m$ invertible matrix

rank(A)=m, so S has m nonzero diagonal elements $\Rightarrow S$ is invertible

$$
\begin{aligned}
A &= USV^T \\
A^{-1} &= (USV^T)^{-1} = VS^{-1}U^T
\end{aligned}
$$

Low Rank Approximation

A can be written as the sum of rank-1 matrices

$$\boxed{A = \sum_{i=1}^{r} s_i u_i v_i^T}$$

where r is the rank of A, u_i and v_i are the columns of U and V respectively

The best least squares approximation to A of rank $p \leq r$ is provided by retaining the first p terms of the sum

Example: best rank-1 approximation

$$\begin{bmatrix} 7 & -1 \\ 2 & -1 \\ -2 & 1 \end{bmatrix} =$$

$$\begin{bmatrix} -0.92 & 0.40 & 0.00 \\ -0.28 & -0.65 & 0.70 \\ 0.28 & 0.65 & 0.70 \end{bmatrix} \begin{bmatrix} 7.69 & 0 \\ 0 & 0.92 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -0.98 & 0.19 \\ -0.19 & 0.98 \end{bmatrix} =$$

$$7.69 \begin{bmatrix} -0.92 \\ -0.28 \\ 0.28 \end{bmatrix} \begin{bmatrix} -0.98 & 0.19 \end{bmatrix} + 0.92 \begin{bmatrix} 0.40 \\ -0.65 \\ 0.65 \end{bmatrix} \begin{bmatrix} -0.19 & 0.98 \end{bmatrix}$$

$$A = \begin{bmatrix} 6.93 & -1.36 \\ 2.11 & -0.41 \\ -2.11 & 0.41 \end{bmatrix} + \begin{bmatrix} 0.07 & 0.36 \\ -0.11 & -0.59 \\ 0.11 & 0.59 \end{bmatrix}$$

$\begin{bmatrix} 6.93 & -1.36 \\ 2.11 & -0.41 \\ -2.11 & 0.41 \end{bmatrix}$ is the best rank-1 approximation to A

Compression

If A is an $n \times n$ matrix, each term in

$$A = \sum_{i=1}^{r} s_i u_i v_i^T$$

requires $2n + 1$ numbers

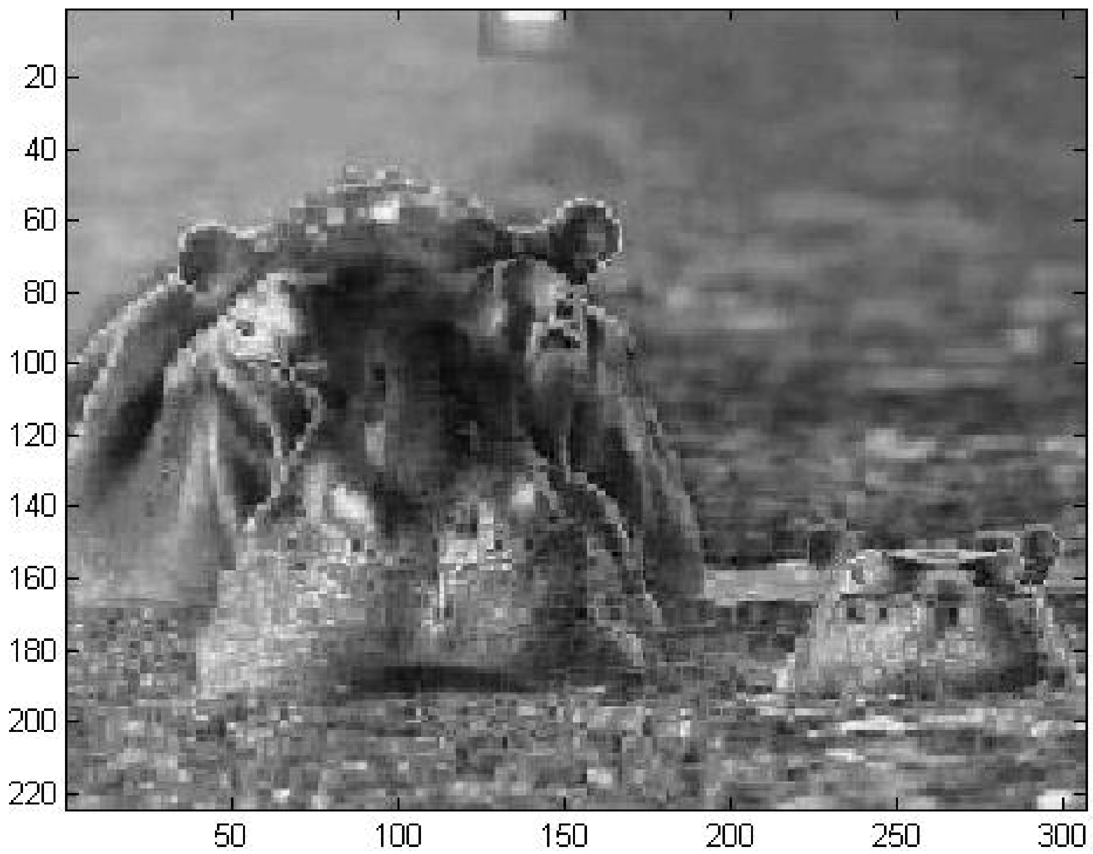
If the first singular value is much larger than the rest, most of the information is captured by the first term.

E.g., if $n = 256$, the matrix has 65 536 numbers, but the first term requires only 513 numbers: this saves 99% in space. Keeping the first 8 terms saves 94% (compression ratio 16:1), and keeping the first 32 terms saves 75% (compression ratio 4:1).

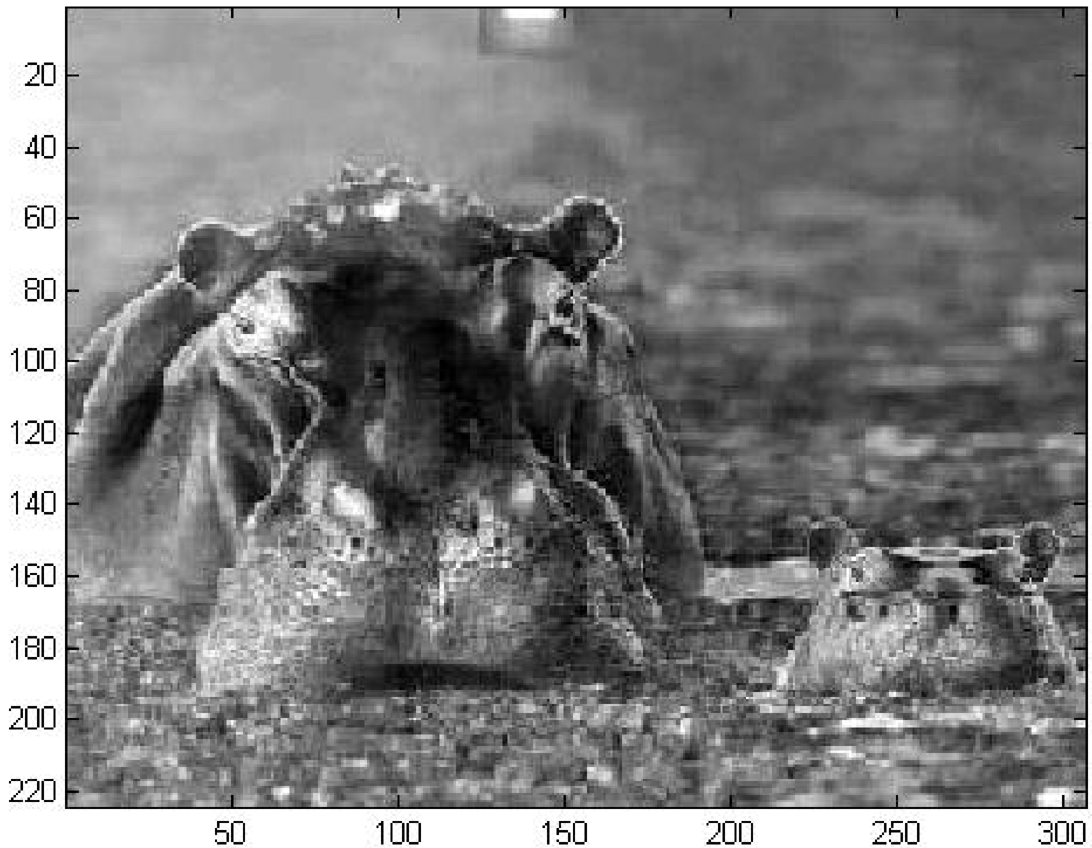
Rank 1 compression

```
xin = imread('hippo1.jpg'); x = double(xin); xc=x-128;
for i=1:56
    for j=1:102
        A=xc(4*(i-1)+1:4*i,3*(j-1)+1:3*j);
        [U,S,V]=svd(A);
        Ac=round(U(:,1)*S(1,1)*V(:,1)');
        xc(4*(i-1)+1:4*i,3*(j-1)+1:3*j)=Ac;
    end
end
xc=xc+128; xc=uint8(xc); imwrite(xc,'hippo5.jpg','jpg')
```

Grayscale picture in a 306×224 grid.



Grayscale picture compressed by rank 1 SVD.



Grayscale picture compressed by rank 3 SVD.