Singular Value Decomposition

An application to Big Data

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Outline

Singular Value Decomposition

Definition of SVD

Theorem

Given a matrix $A \in \mathbb{R}^{m \times n}$, it can always be found a decomposition such that

$$A = U \Sigma V^T \tag{1}$$

where $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ and $\Sigma \in \mathbb{R}^{m \times n}$.

U and V are two orthogonal matrices and Σ is a diagonal matrix, namely:

$$(\Sigma)_{ij} = \begin{cases} \sigma_i, & i = j \\ 0, & i \neq j \end{cases}$$

where $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_p \geq 0$, $p = \min\{m, n\}$.

Definition of SVD

The non-zero entries of Σ, denoted by σ_i, are called *singular values*.

They are arrenged in a nonincreasing order by convention.

The column vectors $\boldsymbol{u_i}$ of U are called *left singular vectors* and those $\boldsymbol{v_i}$ of V are called *right singular vectors*.

Since in general $m \neq n$, we have:

$$A = \sum_{i=1}^{p} \boldsymbol{u_i} \sigma_i \boldsymbol{v_i}^T$$

Definition of SVD

Theorem

If for some r such that $1 \leq r < p$ we have

$$\sigma_1 \geq \ldots \geq \sigma_r > \sigma_{r+1} = \ldots = \sigma_p = 0$$

then

- $\operatorname{rank}(A) = r$
- $A = \sum_{i=1}^{r} \boldsymbol{u_i} \sigma_i \boldsymbol{v_i}^T$

It means that all other $p - r$ dimensions of matrix A are linear combinations of the first r.

Definition of SVD

Lower rank approximation

Let $A \in \mathbb{R}^{m \times n}$ be a matrix whose rank is $\operatorname{rank}(A) = r$.

If for a fixed integer value $k < r$ we define

$$A_k = \sum_{i=1}^{k} \sigma_i \boldsymbol{u_i} \boldsymbol{v_i}^T \tag{2}$$

and

$$\mathcal{B} = \left\{ B \in \mathbb{R}^{m \times n} : \operatorname{rank}(B) = k \right\}$$

then

$$\min_{B \in \mathcal{B}} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$$

This result tell us that A_k represents the best approximation (considering the *spectral norm*) of rank k of matrix A.

Singular values computation

To compute the singular values, consider the transpose of A given its decomposition:

$$A^T = (U\Sigma V^T)^T = V\Sigma^T U^T$$

The symmetric matrix $A^T A$ is equal to:

$$A^T A = (V\Sigma^T U^T)(U\Sigma V^T) = V\Sigma^T \Sigma V^T$$

Furthermore, this equation can be written as:

$$A^T AV = V\Sigma^T \Sigma$$

It means that the diagonal entries of the square matrix $\Sigma^T \Sigma$, which are the square of the singular values, are the eigenvalues of matrix $A^T A$ and V is the matrix of eigenvectors.

Singular values computation

Similarly, consider the product of AA^T. It is equal to:

$$AA^T = (U\Sigma V^T)(V\Sigma^T U^T) = U\Sigma\Sigma^T U^T$$

Which means that:

$$AA^T U = U\Sigma\Sigma^T$$

Hence U is the matrix of eigenvectors of AA^T.

Since $\mathrm{rank}(A) = r$, only the first r eigenvalues of AA^T and $A^T A$ are non-zero.

Finding eigenvalues and eigenvectors

QR Method

A possible method to find eigenvalues and eigenvectors of a matrix is based on QR decompositions and this theorem:

Theorem

Suppose $A \in \mathbb{R}^{n\times n}$ is a matrix having eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_n$ satisfying

$$|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n| \tag{3}$$

then the following sequence for $A_1 = A$ and $k = 1, 2, \ldots$

$$\begin{cases} A_k = Q_k R_k \\ A_{k+1} = R_k Q_k \end{cases} \tag{4}$$

converges to an upper triangular matrix where $(A_k)_{ii} = \lambda_i,\ i = 1, 2, \ldots, n$.
In case (3) is not satisfied, this sequence converges to a triangular matrix with square blocks of order at most 2 along the diagonal.
If A is symmetric, then the sequence converges to a diagonal matrix.

QR Method

So a basic implementation would be like this:

```
while err > toll
    [Q, R] = qr(A);
    A = R * Q;

    err = max( max( abs( tril(A, -1) ) ) );
end
```

This method can be sped up by using a technique called *shifting*:

```
n = length( A );
while err > toll
    % A(n, n) is a usual choice, it can be any real number
    T = A(n, n) * eye(n);
    [Q, R] = qr( A - T );
    A = R * Q + T;

    err = max( max( abs( tril(A, -1) ) ) );
end
```

QR Method

In our case, this method must be applied to AA^T and A^TA, so if (4) converges then we have a diagonal matrix.
Now, consider the diagonalization of B, where $B = AA^T$ or $B = A^TA$:

$$B = P\Lambda P^{-1} = P\Lambda P^T$$

As B can be factored using (4), the matrix containing the eigenvectors must be equal to:

$$P = \prod_i Q_i = Q_1Q_2Q_3\cdots$$

Hence, for every iteration $B_k = Q_kR_k$ and $B_{k+1} = R_kQ_k$, requiring each step to have a computational cost equal to $O(\frac{2n^3}{3})$.

Hessemberg Reduction

To achieve a lower computational cost, one solution consists in transforming B in a similar tridiagonal matrix using Householder matrices.
A triangular matrix can be obtained because B is symmetric.

In general, the process of trasforming a matrix in a similar matrix using Householder matrices allows us to obtain a matrix in which $B_{ij} = 0$, for all $i > j + 1$. Such a matrix is called a *Hessemberg matrix*.

Consequently, after B has been transformed, each step of the previous code can be realized using *Givens rotation matrices*.

Givens rotation matrices

A *Givens rotation* can be represented with the following matrix:

$$G_{ij} = \begin{pmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & -s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{pmatrix} \begin{matrix} \\ \\ \longleftarrow \text{ i} \\ \\ \longleftarrow \text{ j} \\ \\ \\ \end{matrix}$$

$$\begin{matrix} & & \uparrow & & \uparrow & & \\ & & \text{i} & & \text{j} & & \end{matrix}$$

where $c = \cos\theta$ and $s = \sin\theta$, for a particular value of $\theta \in [0,\, 2\pi]$.

A rotation occurs in the plane spanned by the two coordinates axes i and j.

Givens rotation matrices

Using the following values:

$$\cos\theta = \frac{|b_{ii}|}{\sqrt{b_{ii}^2 + b_{ji}^2}}$$

$$\sin\theta = \operatorname{sign}\left(\frac{b_{ji}}{b_{ii}}\right) \frac{|b_{ji}|}{\sqrt{b_{ii}^2 + b_{ji}^2}}$$

when B gets left multiplied by G_{ij}, the final matrix will have the element in position $(j,\, i)$[1] equal to 0.
Therefore, instead of factoring B at each step by the QR method, if B is tridiagonal, we can simply iterate $n-1$ times by constructing $G_{k\,k+1}$ and eliminating the elements in position $(k+1,\, k)$ and $(k,\, k+1)$.

[1] Note that the indices are reversed

Pseudocode for finding eigenvalues and eigenvectors

A pseudocode of what to do should clarify what we have done so far (excluding shifting for brevity):

$B, P \leftarrow$ hessemberg(B)
while error > toll **do**
  for $k = 1, 2, \ldots, n$ **do**
    construct $G_{k\,k+1}$
    $B \leftarrow G_{k\,k+1} B$
  end for
  for $k = 1, 2, \ldots, n$ **do**
    $B \leftarrow B G^T_{k\,k+1}$
    $P \leftarrow P G^T_{k\,k+1}$
  end for
  update error
end while

The function implementing the Hessemberg reduction must also return the matrix used for the transformation, meaning that $B = PHP^T$.
Note that P is updated in this way because $Q_i = G^{(i)}_{12} G^{(i)}_{23} \cdots G^{(i)}_{n-1\,n}$, where i denotes the generic iteration for error minimization.

The Algorithm

Calculation of left singular vectors

Suppose we start computing V by the method explained in the previous slides.
We apply the method to $A^T A$ and get $P = V$ and $B = \Sigma^2$.
Once we have take the square root of the singular values, by explicitly writing Σ, the matrix containing the left singular vectors can be calculated as:

$$A = U\Sigma V^T \Rightarrow U = AV\Sigma^{-1}$$

Unlike (1), U is a rectangular matrix, and Σ and V are square matrices.
The algorithm is now complete. The next slides will illustrate the code.

Function to calculate Givens rotation matrices

```
function [c, s] = givens(A, i, j)
%GIVENS Function to compute cos and sin of Gij
%   Given a matrix A, this function returns a vector containing the values
%   of givens rotation matrix Gij such that Gij * A is equal to A except
%   for the element (j, i), which will be zero.
     c = abs( A(i, i) ) / sqrt( A(i, i)^2 + A(j, i)^2 );
     s = - sign( A(j, i) / A(i, i) ) * abs( A(j, i) ) / sqrt( A(i, i)^2 + A
     (j, i)^2 );
end
```

Function to calculate the Hessemberg reduction i

```
function [A, P] = hessemberg(A)
%HESSEMBERG Fuction to compute the Hessember reduction of a matrix
%   Given a matrix A, this function trasform A in a similar hessemberg
%   matrix. It will be produced as output the hessember matrix and the
%   matrix P used for the transformation.
    n = size(A, 2);
    P = eye(n);
    for k=1:n-2
        sigma = sign(A(k+1, k)) * norm(A(k+1:n, k));
        v = [sigma + A(k+1, k); A(k+2:n, k)];
        beta = 1 / (sigma * (sigma + A(k+1, k)));
        % transform lower triangular matrix
        for j=k:n
            tau = beta * (v' * A(k+1:n, j));
            A(k+1:n, j) = A(k+1:n, j) - tau * v;
        end
        % transform upper triangular matrix
        for j=1:n
```

Function to calculate the Hessemberg reduction ii

```
19              tau = beta * (A(j, k+1:n) * v);
20              A(j, k+1:n) = A(j, k+1:n) - tau * v';
21              % modify P in a similar way
22              tau = beta * (P(j, k+1:n) * v);
23              P(j, k+1:n) = P(j, k+1:n) - tau * v';
24          end
25      end
26  end
```

Function to calculate singular values and singular vectors i

```
function [M, H] = singular_vectors(A, toll, left)
%SINGULAR_VECTORS Function to compute the left or right singular vectors
%   Given a matrix A and a tollerance for the stopping criterion, this
%   function computes the left or right singular vectors of A and its
%   corrisponding singular values. If left is true then U is calculated, V
%   otherwise.
    if left
        [H, P] = hessemberg(A * A.');
    else
        [H, P] = hessemberg(A.' * A);
    end

    n = length(H);

    % G will hold c and s for each step
    G = zeros(n - 1, 2);
    % G_aux will be equal to [c, -s; s, c] for each step
    G_aux = zeros(2);
```

Function to calculate singular values and singular vectors ii

```
19
20      % M will contain the eigenvectors
21      M = P;
22      err = toll + 1;
23
24      while err > toll
25          H1 = H;
26          T = H(n, n) * eye(n);
27
28          % shifting
29          H = H - T;
30
31          for k = 1:n-1
32              [G(k, 1), G(k, 2)] = givens(H, k, k+1);
33              G_aux(1, 1) = G(k, 1);
34              G_aux(1, 2) = - G(k, 2);
35              G_aux(2, 1) = G(k, 2);
36              G_aux(2, 2) = G(k, 1);
37
```

Function to calculate singular values and singular vectors iii

```
38          % nullify the elements below the diagonal
39          H(k:k+1, k:n) = G_aux * H(k:k+1, k:n);
40      end
41
42      for k = 1:n-1
43          G_aux(1, 1) = G(k, 1);
44          G_aux(1, 2) = G(k, 2);
45          G_aux(2, 1) = - G(k, 2);
46          G_aux(2, 2) = G(k, 1);
47
48          % reconstruct the Hessemberg form
49          H(1:k+1, k:k+1) = H(1:k+1, k:k+1) * G_aux;
50          % update M as M * Q = M * G12' * G23' * ...
51          M(1:n, k:k+1) = M(1:n, k:k+1) * G_aux;
52      end
53
54      % shifting
55      H = H + T;
56
```

Function to calculate singular values and singular vectors iv

```
57          err = norm(diag(H - H1), 1);
58      end
59
60      % calculate square root for singular values
61      H = sqrt( diag( diag( H ) ) );
62
63      % discard imaginary parts if too small
64      discard_imag = 10^-5;
65
66      if all( imag( diag(H) ) < discard_imag )
67          H = real(H);
68      end
69      if all( imag( diag(M) ) < discard_imag )
70          M = real(M);
71      end
72  end
```

Function to calculate SVD i

```
function [U, S, V] = custom_svd(A, toll)
%CUSTOM_SVD Function to compute the SVD decomposition of a matrix
%   Given a matrix A as input and a tollerance for the stopping criterion,
%   this function computes the SVD decomposition of A.
    [m, n] = size(A);
    [V, S1] = singular_vectors(A, toll, false);

    % sort singular values and right singular vectors if they are not
    % already
    if ~ issorted( diag(S1) )
        [New_Diag, s_order] = sort(diag(S1), 'descend');

        S = diag(New_Diag);

        new_order = 1:n;
        for h = 1:length(s_order)
            if h ~= s_order(h)
                new_order(h) = s_order(h);
```

Function to calculate SVD ii

```
19              end
20          end
21
22          V = V(:, new_order);
23      end
24
25      % take only non-zero diagonal entries
26      arr = New_Diag;
27      arr(arr > 0) = NaN;
28      [zero, index] = max(arr, [], 'omitnan');
29      if index ~= 1
30          arr = New_Diag(1 : index - 1);
31      else
32          arr = New_Diag;
33      end
34
35      % modify S1 = inv(S) to fit dimensions
36      S1 = diag( 1./ arr );
37      S1(n, 1) = 0;
```

Function to calculate SVD iii

```
38      S1(1, n) = 0;
39
40      % compute U
41      U = A*V*S1;
42  end
```

Application to Big Data

Dimensionality reduction

The SVD decomposition can be applied to Big Data in order to reduce the dimensionality of data sets.

As an example, consider the data set [5] containing 33 different attributes for 145 students, which includes student ID, personal information and data, and higher education performance ratings[2].
Dimensionality can be reduced as follows:

1. truncate the SVD retaining top-k singular values, $A \approx U_k \Sigma_k V_k^T$;
2. compute the modified data set as $D' = DV_k = U_k \Sigma_k$.

[2] https://archive.ics.uci.edu/ml/datasets/Higher+Education+Students+Performance+Evaluation+Dataset

Dimensionality reduction

D' represents a new data set that corresponds to the projection of the data set D on a k-dimensional basis system of right singular vectors.

Number of singular values

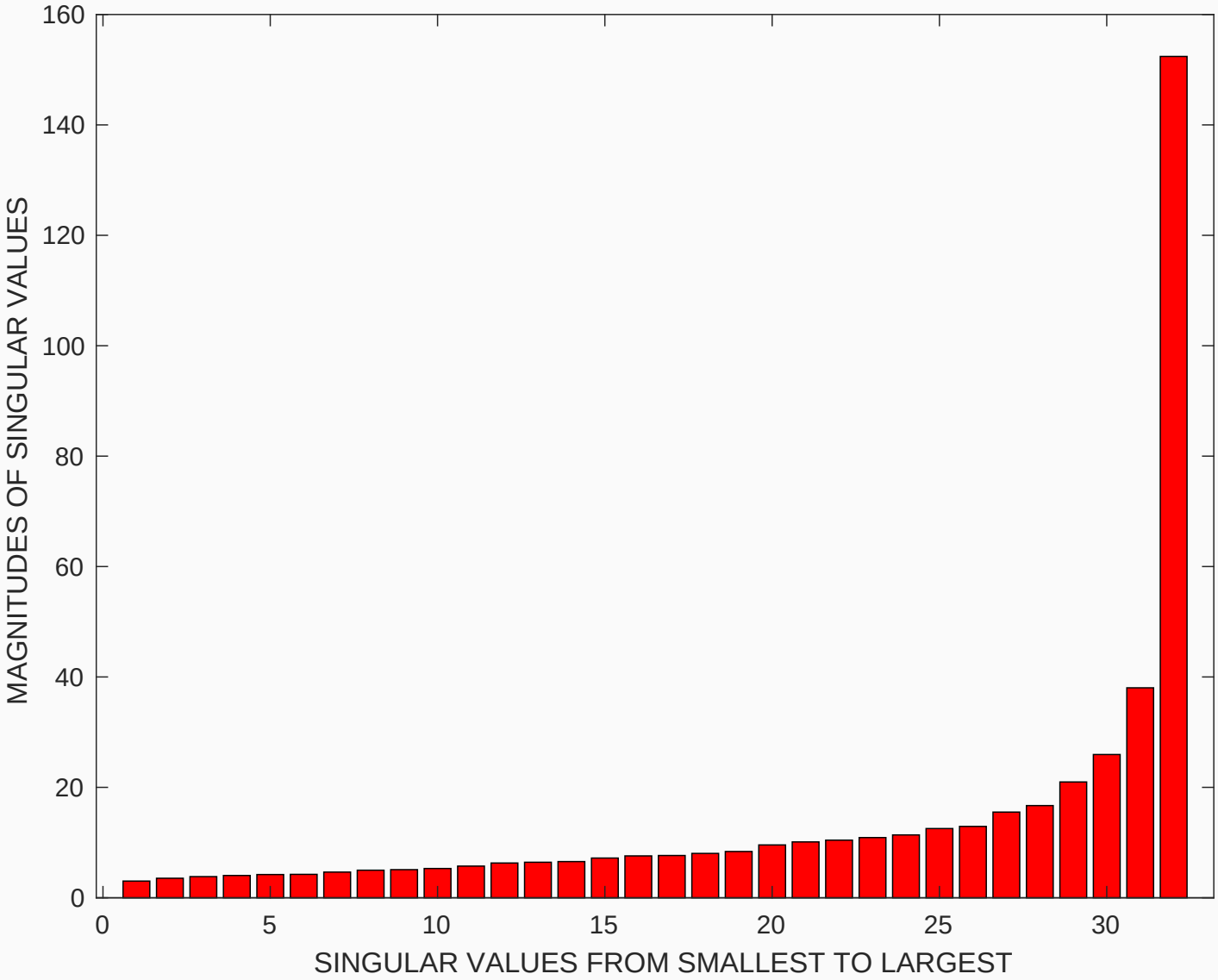
As indicated in [3], a usual choice of k is dictated by maintaining enough singular values to make up 90% of the energy in Σ.
The total energy of a data set is:

$$\mathrm{E}(\Sigma) = \sum_{i=1}^{r} \sigma_i^2$$

where $r = \mathrm{rank}(D)$.

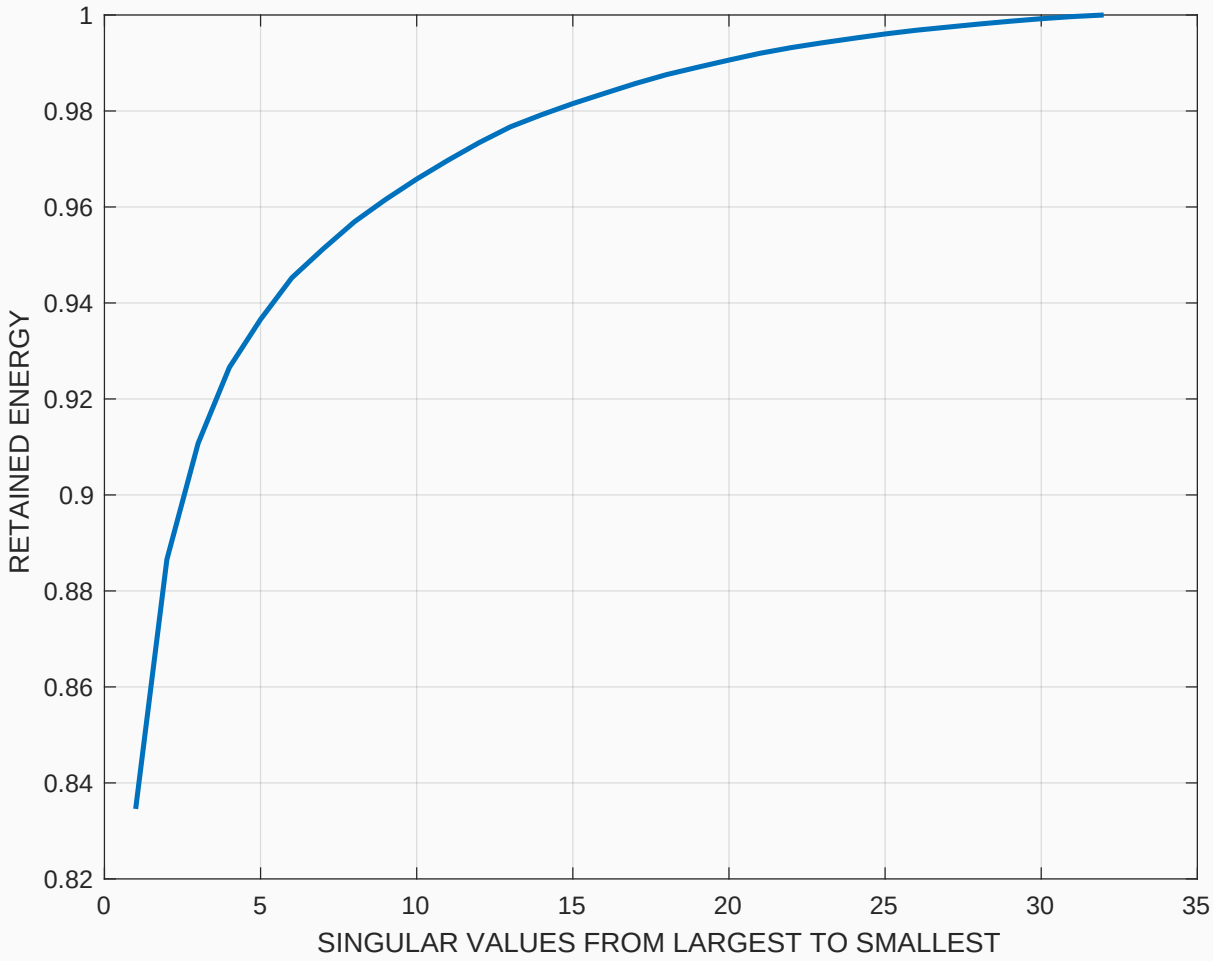
By plotting the singular values we can get an insight of how they are distributed and how many of them we can retain.

Magnitudes of singular values



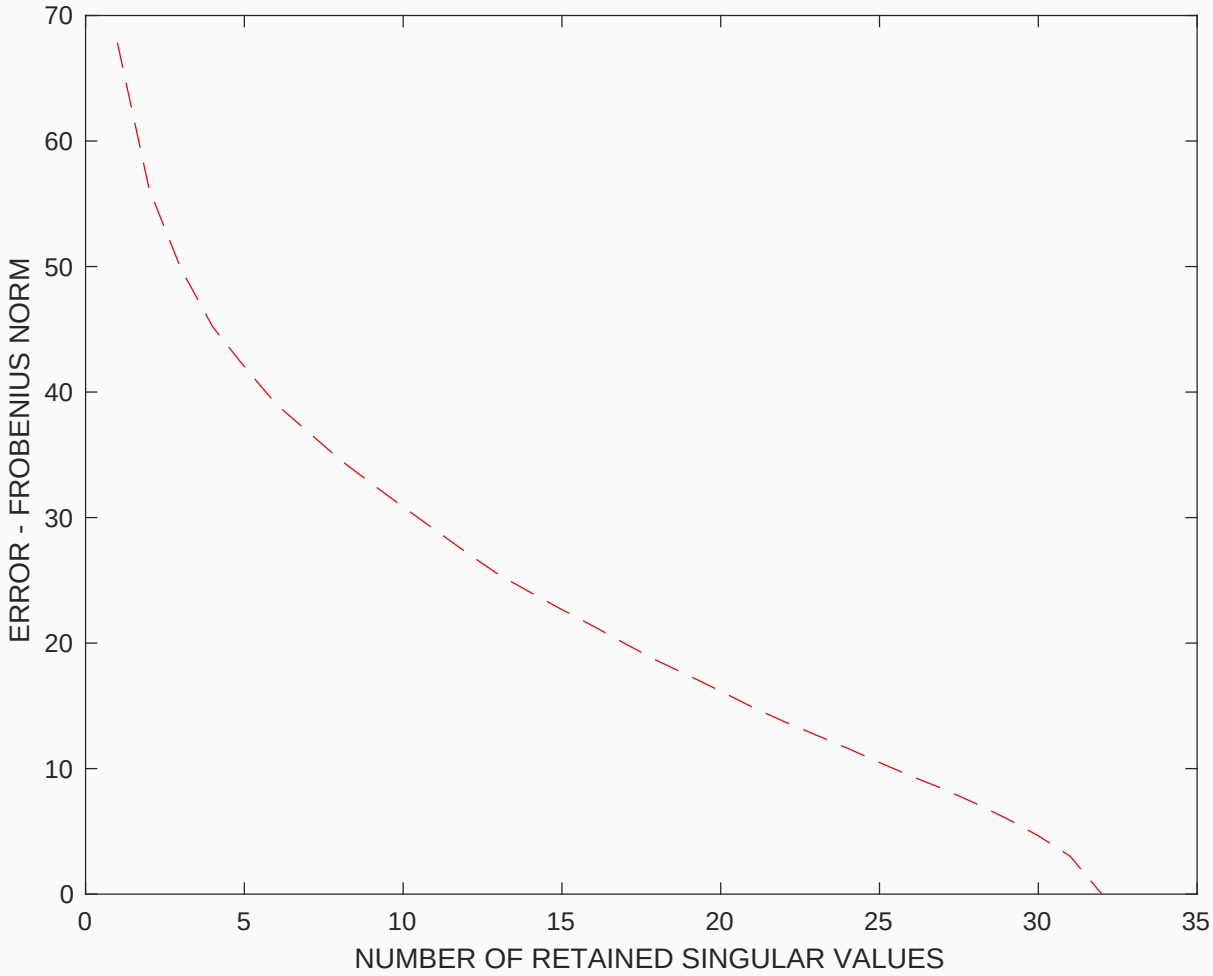
Retained energy

From what we can see, with 3 singular values we can get about $25,346$ of energy, which is enough to exceed 90% of $\mathrm{E}(\Sigma) = 27,830$.



Decreasing error as singular values increase

By increasing the number of retained singular values, the following graph is obtained:



References

References

[1] G. Monegato, *Metodi e algoritmi per il calcolo numerico*. Clut, 2008.

[2] C. C. Aggarwal *et al.*, *Data mining: the textbook*. Springer, 2015, vol. 1.

[3] J. Leskovec, A. Rajaraman, and J. D. Ullman, *Mining of massive data sets*. Cambridge university press, 2020.

[4] C. F. Van Loan and G. Golub, "Matrix computations (johns hopkins studies in mathematical sciences)," *Matrix Computations*, 1996.

References ii

[5] N. Yılmaz and B. Sekeroglu, "Student performance classification using artificial intelligence techniques," in *10th International Conference on Theory and Application of Soft Computing, Computing with Words and Perceptions - ICSCCW-2019*, R. A. Aliev, J. Kacprzyk, W. Pedrycz, M. Jamshidi, M. B. Babanli, and F. M. Sadikoglu, Eds., Cham: Springer International Publishing, 2020, pp. 596–603, ISBN: 978-3-030-35249-3.

[6] D. Dua and C. Graff, *UCI machine learning repository*, 2017. [Online]. Available: `http://archive.ics.uci.edu/ml`.

Quote

"No problem can withstand the assault of sustained thinking."

– Voltaire