MATH 3795
Lecture 9. Linear Least Squares. Using SVD Decomposition.

Dmitriy Leykekhman

Fall 2008

Goals

- SVD-decomposition.
- Solving LLS with SVD-decomposition.

SVD Decomposition.

For any matrix $A \in \mathbb{R}^{m\times n}$ there exist orthogonal matrices $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ and a 'diagonal' matrix $\Sigma \in \mathbb{R}^{m\times n}$, i.e.,

$$\Sigma = \begin{pmatrix} \sigma_1 & & & & & 0 & \dots & 0 \\ & \ddots & & & & & & \\ & & \sigma_r & & & & & \\ & & & 0 & & & & \\ & & & & \ddots & & & \\ & & & & & 0 & \dots & 0 \end{pmatrix} \quad \text{for} \quad m \le n$$

with diagonal entries

$$\sigma_1 \ge \cdots \ge \sigma_r > \sigma_{r+1} = \cdots = \sigma_{\min\{m,n\}} = 0$$

such that $A = U\Sigma V^T$

SVD Decomposition.

For any matrix $A \in \mathbb{R}^{m\times n}$ there exist orthogonal matrices $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ and a 'diagonal' matrix $\Sigma \in \mathbb{R}^{m\times n}$, i.e.,

$$\Sigma = \begin{pmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ 0 & & & & & 0 \\ \vdots & & & & & \vdots \\ 0 & & & & & 0 \end{pmatrix} \quad \text{for} \quad m \geq n$$

with diagonal entries

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_{\min\{m,n\}} = 0$$

such that $A = U\Sigma V^T$

SVD Decomposition.

- The decomposition

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

is called **Singular Value Decomposition** (SVD). It is very important decomposition of a matrix and tells us a lot about its structure.

- It can be computed using the Matlab command svd.
- The diagonal entries σ_i of Σ are called the singular values of A. The columns of U are called *left singular vectors* and the columns of V are called *right singular vectors*.
- Using the orthogonality of V we can write it in the form

$$AV = U\Sigma$$

We can interpret it as follows: there exists a special orthonormal set of vectors (i.e. the columns of V), that is mapped by the matrix A into an orthonormal set of vectors (i.e. the columns of U).

Applications of SVD Decomposition.

Given the SVD-Decomposition of A,

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

with

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_{\min\{m,n\}} = 0$$

one may conclude the following:

- $rank(A) = r$,
- $R(A) = R([u_1, \ldots, u_r])$,
- $N(A) = R([v_{r+1}, \ldots, v_n])$,
- $R(A^T) = R([v_1, \ldots, v_r])$,
- $N(A^T) = R([u_{r+1}, \ldots, u_m])$.

Applications of SVD Decomposition.

Moreover if we denote

$$U_r = [u_1, \ldots, u_r], \quad \Sigma_r = diag(\sigma_1, \ldots, \sigma_r), \quad V_r = [v_1, \ldots, v_r],$$

then we have

$$A = U_r \Sigma_r V_r^T = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

This is called the *dyadic decomposition* of A, decomposes the matrix A of rank r into sum of r matrices of rank 1.

Applications of SVD Decomposition.

- The 2-norm and the Frobenius norm of A can be easily computed from the SVD decomposition

$$\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_1$$

$$\|A\|_F = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2 = \sqrt{\sigma_1^2 + \cdots + \sigma_p^2}, \quad p = \min\{m, n\}.$$

- From the SVD decomposition of A it also follows that

$$A^T A = V \Sigma^T \Sigma V^T \quad \text{and} \quad AA^T = U \Sigma \Sigma^T U^T.$$

Thus, σ_i^2, $i = 1, \ldots, p$ are the eigenvalues of symmetric matrices $A^T A$ and AA^T and v_i and u_i are the corresponding eigenvectors.

Applications of SVD Decomposition.

Theorem

Let the SVD of $A \in \mathbb{R}^{m\times n}$ be given by

$$A = U_r \Sigma_r V_r^T = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

with $r = rank(A)$. If $k < r$

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T,$$

then

$$\min_{rank(D)=k} \|A - D\|_2 = \|A - A_k\|_2 = \sigma_{k+1},$$

and

$$\min_{rank(D)=k} \|A - D\|_F = \|A - A_k\|_F = \sqrt{\sum_{k+1}^{p} \sigma_i^2}, \quad p = \min\{m, n\}.$$

Solving LLS with SVD Decomposition.

- Consider the LLS
$$\min_x \|Ax - b\|_2^2$$
- Let $A = U\Sigma V^T$ be the SVD of $A \in \mathbb{R}^{m\times n}$.
- Using the orthogonality of U and V we have

$$\|Ax - b\|_2^2 = \|U^T(AVV^Tx - b)\|_2^2 = \|\Sigma \underbrace{V^Tx}_{=z} - U^Tb)\|_2^2$$
$$= \sum_{i=1}^{r}(\sigma_i z_i - u_i^T b)^2 + \sum_{i=r+1}^{m}(u_i^T b)^2.$$

Solving LLS with SVD Decomposition.

- Thus,

$$\min_x \|Ax - b\|_2^2 = \sum_{i=1}^{r} (\sigma_i z_i - u_i^T b)^2 + \sum_{i=r+1}^{m} (u_i^T b)^2.$$

- The solution is given

$$z_i = \frac{u_i^T b}{\sigma_i}, \quad i = 1, \ldots, r,$$
$$z_i = \text{ arbitrary}, \quad i = r+1, \ldots, n.$$

- As a result

$$\min_x \|Ax - b\|_2^2 = \sum_{i=r+1}^{m} (u_i^T b)^2.$$

Solving LLS with SVD Decomposition.

Recall that $z = V^T x$. Since V is orthogonal, we find that

$$\|x\|_2 = \|VV^T x\|_2 = \|V^T x\|_2 = \|z\|_2.$$

All solutions of the linear least squares problem are given by $z = V^T x$ with

$$\begin{aligned} z_i &= \frac{u_i^T b}{\sigma_i}, \quad i = 1, \dots, r, \\ z_i &= \text{ arbitrary}, \quad i = r+1, \dots, n. \end{aligned}$$

Solving LLS with SVD Decomposition. Minimum norm solution

The minimum norm solution of the linear least squares problem is given by

$$x_\dagger = V z_\dagger,$$

where $z_\dagger \in \mathbb{R}^n$ is the vector with entries

$$z_i^\dagger = \frac{u_i^T b}{\sigma_i}, \quad i = 1, \dots, r,$$
$$z_i^\dagger = 0, \quad i = r+1, \dots, n.$$

The minimum norm solution is

$$x_\dagger = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i$$

Solving LLS with SVD Decomposition. MATLAB code.

```
% compute the SVD:
[U,S,V] = svd(A);
   s    = diag(S);
% determine the effective rank r of A using singular values
r = 1;
while( r < size(A,2) & s(r+1) >= max(size(A))*eps*s(1) )
    r = r+1;
end
d = U'*b;
x = V* ( [d(1:r)./s(1:r); zeros(n-r,1) ] );
```

Conditioning of a Linear Least Squares Problem.

- Suppose that the data b are

$$b = b_{ex} + \delta b,$$

where δb represents the measurement error.

- The minimum norm solution of min $\|Ax - (b_{ex} + \delta b)\|_2^2$ is

$$x_\dagger = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^{r} \left(\frac{u_i^T b}{\sigma_i} + \frac{u_i^T \delta b}{\sigma_i} \right) v_i.$$

- If a singular value σ_i is small, then $\frac{u_i^T(\delta b)}{\sigma_i}$ could be large, even if $u_i^T(\delta b)$ is small. This shows that errors δb in the data can be magnified by small singular values σ_i.

Conditioning of a Linear Least Squares Problem.

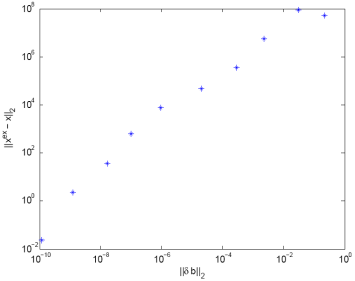
```
% Compute A
t = 10.^(0:-1:-10)';
A = [ ones(size(t)) t t.^2 t.^3 t.^4 t.^5];
% compute SVD of A
[U,S,V] = svd(A); sigma = diag(S);
% compute exact data
xex = ones(6,1); bex = A*xex;
for i = 1:10
    % data perturbation
    deltab = 10^(-i)*(0.5-rand(size(bex))).*bex;
    b = bex+deltab;
    % solution of perturbed linear least squares problem
    w = U'*b;
    x = V * (w(1:6) ./ sigma);
    errx(i+1) = norm(x - xex); errb(i+1) = norm(deltab);
end
loglog(errb,errx,'*');
ylabel('||x^{ex} - x||_2'); xlabel('||\delta b||_2')
```

Conditioning of a Linear Least Squares Problem.

- The singular values of A in the above Matlab example are:

$$\begin{array}{ll} \sigma_1 \approx 3.4 & \sigma_4 \approx 7.2 * 10^{-4} \\ \sigma_2 \approx 2.1 & \sigma_5 \approx 6.6 * 10^{-7} \\ \sigma_3 \approx 8.2 * 10^{-2} & \sigma_6 \approx 5.5 * 10^{-11} \end{array}$$

- The error $\|x_{ex} - x\|_2$ for different values of $\|\delta b\|_2$ (loglog-scale):



- We see that small perturbations δb in the measurements can lead to large errors in the solution x of the linear least squares problem if the singular values of A are small.