KTH Engineering Sciences

Computer Exercise 7

SVD-factorization for ill-posed least squares problems

Background: SVD-factorization and rank-deficient underdetermined systems

Singular Value Decomposition, SVD, of an $m \times n$ matrix A is defined as $A = U\Sigma V^T$, where U is an $m \times m$ orthogonal matrix, v is an $n \times n$ orthogonal matrix and Σ is an $m \times n$ matrix made up of a diagonal matrix and a matrix with zeroes. The diagonal elements of the diagonal matrix are called the *singular values* σ_i, $i = 1, 2, \ldots, k$. where $k = \min(m, n)$. They are non-negative satisfying $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_k \geq 0$. If $m > n$ the zero matrix is situated under the $n \times n$ diagonal matrix denoted by Σ_n (the last element is the singular value σ_n). If $m < n$ the zero matrix is situated to the right of the diagonal matrix Σ_m. If $m = n$ all matrices are $n \times n$. (Note: One can equivalently consider Σ to always be a $k \times k$ square matrix and let U or V be rectangular when $n \neq m$.)

In MATLAB the singular value decomposition of A is obtained from `[U,S,V]=svd(A)`.

For an underdetermined system $Ax = y$ where A is $m \times n$ with $m < n$ there is no unique solution x. If we add the condition that $||x||_2$ should be as small as possible, the solution $\hat{x}$ will be unique. To see how $\hat{x}$ is computed using the SVD, we look at the norm of the residual

$$||y - Ax||_2 = ||y - U\Sigma V^T x||_2 =: ||d - \Sigma z||_2,$$

where $d = U^T y$ is a known vector with m components and $z = V^T x$ has n components of unknowns. The residual is zero when $z_i = d_i/\sigma_i$, $i = 1, 2, \ldots, m$. But z has n components. How should the remaining $z_{m+1}, \ldots, z_n$ be chosen? Since

$$||x||_2^2 = ||Vz||_2^2 = \left(\frac{d_1}{\sigma_1}\right)^2 + \left(\frac{d_2}{\sigma_2}\right)^2 + \cdots \left(\frac{d_r}{\sigma_r}\right)^2 + z_{m+1}^2 + \cdots + z_n^2,$$

we get the smallest norm solution by putting $z_{m+1}, \ldots, z_n$ to zero and then let $x = Vz$.

When the SVD for an underdetermined system is truncated to a numerical rank r, where $r < m$, all singular values $\sigma_{r+1}, \ldots, \sigma_m$ are set to zero. To get the solution we proceed in the same way as above, i.e. the solution $z_i = d_i/\sigma_i$, $i = 1, 2, \ldots, r$ and the remaining $z_{r+1}, \ldots, z_n$ are set to zero. The minimum norm solution $\hat{x}$ will be smaller since

$$||x||_2^2 = ||Vz||_2^2 = \left(\frac{d_1}{\sigma_1}\right)^2 + \left(\frac{d_2}{\sigma_2}\right)^2 + \cdots \left(\frac{d_r}{\sigma_r}\right)^2,$$

is smaller the smaller the rank r is. The residual will however increase with smaller rank, since

$$||y - Ax||_2^2 = d_{r+1}^2 + \cdots + d_m^2.$$

Numerical solution of Fredholm's integral equation

Suppose $p(y)$ is a signal that we want to measure. For many measuring instruments the actual measured signal $f(y)$ can be modeled by a convolution

$$f(y) = \int_{\infty}^{\infty} K(x,y)p(x)dx,$$

where K is a known *apparatus function* (K as in kernel). In the ideal case $K(x,y) = \delta(x-y)$, the delta function, in which case the signal function p is identical to the observed function f. In general K is a smooth function that approximates a delta function. This means that f will be a local average of p. In practice there will also be some additional noise $n(y)$ added to the measured signal, which leads to the relationship

$$\int_{\infty}^{\infty} K(x,y)p(x)dx = \tilde{f}(y), \qquad \tilde{f} = f(y) + n(y).$$

If $\tilde{f}$ is given and we want to find p, this is an example of an *integral equation* named *Fredholm's integral equation of the first kind*. When K is smooth, it is an ill-posed problem which must be regularized to be solvable[1].

We assume p is known to be zero outside the interval (a,b). The integral equation then reduces to

$$\int_{a}^{b} K(x,y)p(x)dx = \tilde{f}(y).$$

We suppose furthermore that m measurements are made at different points y. We are thus given the observed values of $(y_i, \tilde{f}(y_i)) =: (y_i, \tilde{f}_i)$, for $i = 1, 2, \ldots, m$. The integral equation should then hold in each of these points, giving

$$\int_{a}^{b} K(x,y_i)p(x)dx = \tilde{f}_i, \qquad i = 1, 2, \ldots, m.$$

We now have m equations to determine the unknown function $p(x)$. The integral is approximated by the trapezoidal rule, where the interval $[a,b]$ is divided into $n+1$ subintervals of size h, with grid points x_i, i.e. $(n+1)h = b-a$ and $x_i = a + ih$. Letting $p_i \approx p(x_i)$ the discretized integral equation can be written as a linear system of equations

$$A\boldsymbol{p} = \tilde{\boldsymbol{f}}, \tag{1}$$

where A is an $m \times n$ matrix, $\boldsymbol{p}$ is an n-vector containing the inner p_i-values (recall that $p(a) = p(b) = 0$) and $\tilde{\boldsymbol{f}} \in \mathbb{R}^m$ contains the measured data $\tilde{f}_i$. The system can be over- or underdetermined. The more points n used in the trapezoidal rule, the better is the integral approximation. However, the system of equations will be larger and more underdetermined. In many applications the system of equations is ill-conditioned.

[1] In the main applications of this type of integral equations, K is however not smooth. It can for instance be the Green's function for the Laplace operator in 2D, $K(x,y) = \frac{1}{2\pi}\ln|x-y|$. Then the integral equation is well-posed and can be used to solve the Laplace equation.

Exercise: Solving the ill-posed integral equation with SVD

In this exercise your task is to solve (1) by making an SVD-factorization of A and truncate it to an appropriate numerical rank r.

Let the function K be given by the following expression

$$K(x,y) = \begin{cases} \frac{1}{2\beta}\left(1+\cos\frac{\pi(y-x)}{\beta}\right), & |y-x|<\beta, \\ 0, & \text{otherwise.} \end{cases}$$

Note: If the β-value is large the measuring instrument is not very good; the measured values are smeared out giving bad information about p. We assume $\beta = 1.5$. Use $m = 30$ measured points uniformly distributed in the interval $[0, 6]$ and $n+1 = 60$ intervals in the trapezoidal rule, giving a 30×60 matrix. Hence the number of singular values are 30, many of which are small. Simulate[2] the measured values $f(y_i)$ by generating yourself the $m = 30$ values using (1) and the function

$$p(x) = x(6-x)\left[0.8\cos(\pi x/6) - 0.4\cos(\pi x/2) + 1\right], \qquad 0 \le x \le 6.$$

Then add the noise $n(y)$ with the MATLAB command `ftilde=f+noise*randn(1,length(y))`, where `noise` is set to 0.01.

- Plot the singular values of A in a `semilogy` plot.
- Compute the solution candidates $\boldsymbol{p}_r$ obtained with SVD truncated to different numerical ranks r. Verify that for larger numerical rank r, the residual $||\tilde{\boldsymbol{f}} - A\boldsymbol{p}_r||_2$ decreases, while the solution $||\boldsymbol{p}_r||_2$ increases.
- Each $\boldsymbol{p}_r$ corresponds to a candidate solution function $p_r(x)$. Plot a representative number of those candidates $p_r(x)$ together with the exact solution $p(x)$. Inspect the graphs and try to find the best candidate. (Make sure you highlight the plot of this best one.) A balance must here be struck between small residual and small solution. If the graph contains many oscillations, the corresponding truncation takes too many singular values into account and should be rejected. On the other hand the choice of the "best" graph is a subjective choice. Report the numerical rank r that corresponds to your chosen candidate.
- Vary β and `noise`. Summarize how the results change and draw conclusions about the relationship between β, `noise` and your choice of best numerical rank r.
- Try a different set of measurement points $\{y_i\}$ which only covers a part of the interval $[0, 6]$. Explain how the results change.

[2]This is in fact "cheating" but it gives you full control of the solution p computed from the integral equation and the true solution.