MTMM.00.005 Numerical Methods
Practical lesson 11: Least squares method

April 23, 2019

To get a positive result, student has to solve all of the exercises given in practical lessons, explain the programming code and answer the questions.

The deadline for the 11th set of exercises is April 30.

NB! In order to use the nonstandard packages as *numpy* and *matplotlib* one could use Command Prompt and type

```
H:\nm> "C:\Program Files\Anaconda3\python" <filename>.py
```

Here `H:\nm` is the folder for `<filename>.py`.

Least squares method

Consider the system

$$\begin{cases} a_{11}x_1 + \ldots + a_{1n}x_n = f_1, \\ \ldots \\ a_{m1}x_1 + \ldots + a_{mn}x_n = f_m, \end{cases} \quad \Leftrightarrow \quad Ax = f, \tag{1}$$

where $m \geq n$, A is $m \times n$ matrix, $x \in \mathbb{R}^n$, $f \in \mathbb{R}^m$. If $m > n$ it may happen that the system is not solvable. Then we consider the least squares solution.

Define the error term $R(x) = f - Ax$ and consider the square of Euclidean norm (or 2-norm)

$$\|R(x)\|^2 = \|f - Ax\|^2 = \sum_{i=1}^{m} \left(f_i - \sum_{j=1}^{n} a_{ij}x_j \right)^2.$$

A vector $x \in \mathbb{R}^n$ is called the least squares solution of system (1) if

$$\|R(x)\|^2 = \min_{y \in \mathbb{R}^n} \|R(y)\|^2.$$

For system (1) we define the **normal system of equations** as

$$A^T Ax = A^T f \quad \Leftrightarrow \quad \sum_{j=1}^{n} \left(\sum_{i=1}^{m} a_{ik}a_{ij} \right) x_j = \sum_{i=1}^{m} a_{ik}f_i, \; k = 1, \ldots, n. \tag{2}$$

Here $A^T A$ is $n \times n$ matrix and $A^T f \in \mathbb{R}^n$, i.e., the number of equations and the number of unknowns coincide.

Theorem. A vector x is the least squares solution of the system (1) if and only if x is the solution of system (2).

Theoreem. System (2) is uniquely solvable if and only if the columns of matrix A are linearly independent.

Function approximation by least squares method

Let us have given knots $x_0, \ldots, x_m$ and corresponding numbers $f_0 = f(x_0), \ldots, f_m = f(x_m)$. Choose some linearly independent coordinate functions φ_j, $j = 0, \ldots, n$, $n \le m$, and consider the approximation

$$\varphi(x) = \sum_{j=0}^{n} c_j \varphi_j(x),$$

where $c_j \in \mathbb{R}$, $j = 0, \ldots, n$. The coefficients c_j are found from the system $\varphi(x_i) = f_i$, $i = 0, \ldots, m$. If $n = m$, we have an interpolation problem, if $n < m$, we must find the least squares solution.

If we approximate by polynomials the coordinate functions are

$$\varphi_0(x) = 1, \varphi_1(x) = x, \ldots, \varphi_n(x) = x^n.$$

The coefficients of the corresponding system $\varphi(x_i) = f_i$, $i = 0, \ldots, m$, are $a_{ij} = \varphi_j(x_i) = x_i^j$, the normal system of equations is

$$\sum_{j=0}^{n} \left(\sum_{i=0}^{m} x_i^{k+j} \right) c_j = \sum_{i=0}^{m} x_i^k f_i, \quad k = 0, \ldots, n. \tag{3}$$

Theorem. System (3) is uniquely solvable if and only if there are at least $n+1$ pairwise distinct knots among $x_0, \ldots, x_m$.

Exercise. Approximate the function $f(x) = |x|$, $x \in [-1, 1]$, by polynomials $P_n(x) = c_0 + c_1 x + \ldots + c_n x^n$ using the least squares method and the knots $x_i = -1 + \frac{2}{m} i$, $i = 0, \ldots, m$, $m > n$.
Estimate the error $\varepsilon_n = \max\limits_{-1 \le x \le 1} |P_n(x) - f(x)|$ by finding the error on a ten times denser grid, i.e.,

$$\bar{\varepsilon}_n = \max_{0 \le i \le 10m} |P_n(z_i) - f(z_i)|, \ z_i = -1 + \frac{2}{10m} i.$$

Draw the graphs of functions $P_n(x)$, add the initial data $(x_i, f(x_i))$, $i = 0, \ldots, m$ to the graph. Choose the parameters m and n according to the value of α:

- If $\alpha \vdots 3$, then $n = 5$ and $m = 6, 7, 8, \ldots$ Consider the odd and even values of m separately. What happens to the error $\bar{\varepsilon}$ if m increases?
- If $(\alpha - 1) \vdots 3$, then $m = 20$, $n = 1, \ldots, 19$. Which polynomial gives the best approximation?
- If $(\alpha - 2) \vdots 3$, then $m = 21$, $n = 1, \ldots, 20$. Which polynomial gives the best approximation?