Numerical Linear Algebra TMA265/MMA600 Computer exercise 1: Solution of least squares problem

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Computer exercise 1 (1 B.P.)

Solution of least squares problem

Consider the nonlinear model equation

 $y(T) = A \cdot \exp^{\frac{E}{T - T_0}}$

presenting one of the models of the viscosity of glasses (see paper [3] G. S. Fulcher, "ANALY-SIS OF RECENT MEASUREMENTS OF THE VISCOSITY OF GLASSES" on the course homepage). Here, T is the known temperature, y(T) is the known output data. Determine parameters A, E, T_0 which are positive constants by knowing T and output data y(T).

Hints:

- 1. Transform first the nonlinear function y(T) to the linear one and formulate then the linear least squares problem. Discretize T by N points and compute discrete values of y(T) as $y_i = y(T_i)$ for the known values of parameters A, E, T_0 . Then forget about these parameters (we will call them exact parameters A^*, E^*, T_0^*) and solve the linear least squares problem to recover these exact parameters.
- 2. You can choose exact parameters A^*, E^*, T_0^* as well as the interval for the temperature T as some positive constants accordingly to the Table II of the paper G. S. Fulcher, "ANALYSIS OF RECENT MEASUREMENTS OF THE VISCOSITY OF GLASSES".

For example, take $E^* = 6 \cdot 10^3$, $A^* = exp^{-2.64}$, $T_0^* = 400$, T = 750 + 10 * i, i = 1, ..., N, where N is the number of discretization points. Interval for T can be, for example, T = [750, 2000].

3. Investigate effect of random initialization noise δ in data Y(T) obtained after transformation procedure, on the reconstruction of parameters A, E, T_0 .

Random noise δ to data Y(T) can be added using the formula

$$Y_{\delta}(T) = Y(T)(1 + \delta\alpha), \qquad (0.1)$$

where $\alpha \in (-1, 1)$ is randomly distributed number and $\delta \in [0, 1]$ is the noise level. For example, if noise in data is 5%, then $\delta = 0.05$. You can use several Matlab's functions to test adding of the noise. Below is an example of the Matlab code which shows how to add noise for solution of Poisson's equation (example of section 8.4.4 of the course book [1]) (see Figure 0.1):

```
r = randi([-1 1],size(u),1)
for j=1:n
    for i=1:n
        udelta(n*(i-1)+j) = u(n*(i-1)+j)*(1 + 0.1*r(n*(i-1)+j));
    end
end
```

Try also add normally distributed Gaussian noise

$$N(y|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}}e^{\frac{-(y-\mu)^2}{2\sigma^2}}.$$

Here, μ is mean, σ^2 is variance, σ is standard deviation.

Below is example how to add Gaussian noise $N(y|\mu, \sigma^2)$ with mean $\mu = 0$ and variance $\sigma^2 = 0.01$ to matrix A in MATLAB:

```
Anoise = A + 0.01*randn(size(A)) + 0;
```

4. Solve the linear least squares problem using the method of normal equations, QR and then SVD decompositions. Analyze obtained results by computing the relative errors e_A, e_E, e_{T_0} in the computed parameters depending on the different noise level $\delta \in [0, 1]$ in data $Y_{\sigma}(T)$ for every method.

The relative errors e_A, e_E, e_{T_0} in the computed parameters A, E, T_0 compute as:

$$e_{A} = \frac{|A - A^{*}|}{|A^{*}|},$$

$$e_{E} = \frac{|E - E^{*}|}{|E^{*}|},$$

$$e_{T_{0}} = \frac{|T_{0} - T_{0}^{*}|}{|T_{0}^{*}|}.$$
(0.2)

Here, A^*, E^*, T_0^* are exact values and A, E, T_0 are computed one. Present results how relative errors (0.2) depend on the random noise $\delta \in [0, 1]$ in graphical form and in the corresponding table.

- 5. Choose different number of discretization points N in the interval for temperature T and present results of computations in graphical form and in the corresponding table. More precisely, present how relative errors (0.2) depend on the number of measurements N if you solve the linear least squares problem using 3 methods: the method of normal equations, QR and then SVD decomposition.
- 6. Using results obtained in items 4 and 5, analyze, what is the minimal number of observations N to get reasonable reconstruction of parameters A, E, T_0 within the noise level σ ?

REFERENCES

- L. Beilina, E. Karchevskii, M. Karchevskii, Numerical Linear Algebra: Theory and Applications, Springer, 2017.
- [2] Christopher M. Bishop, Pattern recognition and machine learning, Springer, 2009.
- G. S. Fulcher, Analysis of recent measurements of the viscosity of glasses, Journal of American Ceramic Society, https://doi.org/10.1111/j.1151-2916.1925. tb16731.x, 1925



Figure 0.1: Top figures: Solution of Poisson's equation (example of section 8.4.4 of the course book [1]). Middle figures: Noisy solution obtained via (0.1). Bottom figures: noisy solution obtained via adding normally distributed Gaussian noise N(y|0, 0.01).

- [4] Ian Goodfellow, Yoshua Bengio and Aaron Courville, Deep Learning, MIT Press, 2016, http://www.deeplearningbook.org
- [5] Miroslav Kurbat, An Introduction to Machine Learning, Springer, 2017.