Week 6

Numerical methods for physicists, 2018/19 autumn semester

Gradient and conjugate gradient methods - `pcg, ichol`

PROBLEM. 1. Solve the system

$$4x + 2y = 7$$
$$2x + 3y = 10$$

manually with the gradient and the conjugate gradient methods. It is enough to calculate only two steps for each method. Compare the results. Check the calculations with the Matlab codes provided in the separate M-file.

Gradient method, $\mathbf{A} \in \mathbb{R}^{n\times n}$ SPD, $\overline{\mathbf{b}} \in \mathbb{R}^n$ given.

$k := 0$, $\overline{\mathbf{r}}_0 := \overline{\mathbf{b}}$, $\overline{\mathbf{x}}_0 := \mathbf{0}$
while $\overline{\mathbf{r}}_k \neq \mathbf{0}$ **do**
  $k := k + 1$
  $\alpha_k := \overline{\mathbf{r}}_{k-1}^T \overline{\mathbf{r}}_{k-1} / (\overline{\mathbf{r}}_{k-1}^T \mathbf{A} \overline{\mathbf{r}}_{k-1})$
  $\overline{\mathbf{x}}_k := \overline{\mathbf{x}}_{k-1} + \alpha_k \overline{\mathbf{r}}_{k-1}$
  $\overline{\mathbf{r}}_k := (\overline{\mathbf{b}} - \mathbf{A}\overline{\mathbf{x}}_k) = \overline{\mathbf{r}}_{k-1} - \mathbf{A}\alpha_k \overline{\mathbf{r}}_{k-1}$
end while

CGM, $\mathbf{A} \in \mathbb{R}^{n\times n}$ SPD, $\overline{\mathbf{b}} \in \mathbb{R}^n$ given.

$k := 0$, $\overline{\mathbf{r}}_0 := \overline{\mathbf{b}}$, $\overline{\mathbf{x}}_0 := \mathbf{0}$, $\overline{\mathbf{p}}_1 = \overline{\mathbf{r}}_0$
while $\overline{\mathbf{r}}_k \neq \mathbf{0}$ **do**
  $k := k + 1$
  $\alpha_k := \overline{\mathbf{r}}_{k-1}^T \overline{\mathbf{r}}_{k-1} / (\overline{\mathbf{p}}_k^T \mathbf{A} \overline{\mathbf{p}}_k)$
  $\overline{\mathbf{x}}_k := \overline{\mathbf{x}}_{k-1} + \alpha_k \overline{\mathbf{p}}_k$
  $\overline{\mathbf{r}}_k := \overline{\mathbf{r}}_{k-1} - \alpha_k \mathbf{A} \overline{\mathbf{p}}_k$
  $\beta_k' := \overline{\mathbf{r}}_k^T \overline{\mathbf{r}}_k / (\overline{\mathbf{r}}_{k-1}^T \overline{\mathbf{r}}_{k-1})$
  $\overline{\mathbf{p}}_{k+1} := \overline{\mathbf{r}}_k + \beta_k' \overline{\mathbf{p}}_k$
end while

PROBLEM. 2. For the multiplier α_k, we derived the formula $\alpha_k := \overline{\mathbf{p}}_k^T \overline{\mathbf{r}}_{k-1} / (\overline{\mathbf{p}}_k^T \mathbf{A} \overline{\mathbf{p}}_k)$. Show that we can replace the numerator $\overline{\mathbf{p}}_k^T \overline{\mathbf{r}}_{k-1}$ by $\overline{\mathbf{r}}_{k-1}^T \overline{\mathbf{r}}_{k-1}$ in the algorithm of the CGM (see the above algorithm).

PROBLEM. 3. What is the maximum number of the steps the CGM needs to compute the solution of the system $\mathbf{A}\overline{\mathbf{x}} = \overline{\mathbf{b}}$, where $\mathbf{A} = \text{tridiag}[-1, 2 - 1] \in \mathbb{R}^{20\times 20}$ and $\overline{\mathbf{b}} = [1, \ldots, 1]^T \in \mathbb{R}^{20}$? Check the result with the code provided in the separate m-file.

PROBLEM. 4. We solve the large sparse linear system Ax=b with Matlab, where the $9604 - \text{by} - 9604$ matrix A is defined as
`A = delsq(numgrid('S',100));` and `b = ones(size(A,1),1);` (solution of a discretized Laplace equation). Use Matlab's built-in solver `pcg` in the form

```
[x,flag,final_relative_residual,iter,vector_of_res_errors]=pcg(A,b,10^-8,100).
```

Interpret and improve the result. Solve the system again with preconditioning using the incomplete Cholesky factorization. Compare the change of the relative residual errors for the two methods.

Householder reflection, Givens rotation, QR decomposition - `qr`, `mldivide (\)`

PROBLEM. 5. Give a Householder reflection matrix to the vector $\overline{\mathbf{x}} = [2, 6, -3]^T$. Give a Givens rotation matrix to the 2:3 subvector of $\overline{\mathbf{x}}$.

PROBLEM. 6. Give the QR decomposition of the matrix

$$\mathbf{A} = \begin{bmatrix} 0 & 0 \\ 1 & 3 \\ 0 & 2 \end{bmatrix}$$

with Givens rotations. Compare the result with the result of the command `qr(A)`.

PROBLEM. 7. Show that if $\mathbf{A} = \mathbf{QR}$ is a QR decomposition of the non-singular matrix $\mathbf{A}$ such that all diagonal elements of $\mathbf{R}$ are positive, then the decomposition is unique.

PROBLEM. 8. Solve the over-determined system

$$\begin{aligned} 0x + 0y &= 3 \\ x + 3y &= 4 \\ 2y &= 1 \end{aligned}$$

with the `mldivide` command, with the solution of the normal equation, and with QR decomposition.

PROBLEM. 9. Give the second degree polynomial for which the graph of the polynomial is closest (in the sense of least squares: $\sum_i (ax_i^2 + bx_i + c_i - y_i)^2 \to \min$) to the points (1,1), (0,0), (1,3), (2,2).

HOMEWORK FOR WEEK 6 - to be submitted until the next computer lab (Thursday's group may submit the solutions together with the solutions of the problems of week 7) (The detailed solutions can be submitted either on A4 sheets of paper (printed or written) or in a pdf file (e.g. in an exported Matlab livescript) to rhorvath@math.bme.hu. Do not send Matlab files. Answer all questions with a sentence at the end of each problem.)

1. (2p) Show by giving an estimation for the spectral radius of the iteration matrix that the SOR method with $\omega = 1/2$ can be used to solve system

$$\begin{aligned} 9x_1 - 3x_2 &= 6 \\ -2x_1 + 8x_2 &= -4. \end{aligned}$$

Estimate the number of iteration steps we need to achieve an approximation of the exact solution with the error 10^{-8} (in 1-norm and starting from the zero vector). Perform the iteration in Matlab and give the corresponding approximation.

2. (1p) Solve the system

$$\begin{aligned} 2x_1 - x_2 &= 1 \\ -x_1 + 2x_2 &= 3 \end{aligned}$$

with the conjugate gradient method manually.

3. (2p) Give the QR decomposition of the matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 1 \\ 6 & 2 & 0 \\ -3 & -1 & -1 \end{bmatrix}$$

with Householder reflections. Give the two Householder matrices explicitly. Solve the system $\mathbf{A}\overline{\mathbf{x}} = [1, 2, 3]^T$ using the QR decomposition of the coefficient matrix.