Norwegian University of Science and Technology
Department of Mathematical Sciences

TMA4205 Numerical Linear Algebra
Fall 2014

Solutions to exercise set 5

1 After applying m steps of Arnoldi process to a matrix A we obtain the matrix V_m containing the orthonormal basis for $\mathcal{K}_m(A, v_1)$ and an upper Hessenberg matrix H_m satisfying the equality $H_m = V_m^{\mathrm{T}} A V_m$. Assuming that $A^{\mathrm{T}} = -A$, the matrix on the right hand side of the equality sign is anti-symmetric. Therefore H_m is also antisymmetric and thus has only two non-zero diagonals:

$$H_m = \begin{pmatrix} 0 & -h_{2,1} & \dots & 0 \\ h_{2,1} & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & -h_{m,m-1} \\ 0 & \dots & h_{m,m-1} & 0 \end{pmatrix} \tag{1}$$

As a result, Arnoldi process simplifies to

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v_1 := v/||v||_2, v_0 := 0, h_{1,0} := 0
for j=1,...,m do
    w_j := A v_j + h_{j,j-1} v_{j-1}
    h_{j+1,j} := ||w_j||_2
    if h_{j+1,j} = 0 then stop
    end if
    v_{j+1} := w_j / h_{j+1,j}
end for
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a) Since A is SPD, it follows from Exercise 2, Problem **1c)**, that A^{-1} is also SPD. Thus, it can be used to define the A^{-1}-norm in the same way as the SPD matrix A defines the A-norm.

b) We are given the system $Ax = b$, where A is SPD. Then, for all $\tilde{x} \in \mathbb{R}^n$,

$$\begin{aligned} \|x - \tilde{x}\|_A^2 &= (x - \tilde{x})^{\mathrm{T}} A (x - \tilde{x}) \\ &= (x - \tilde{x})^{\mathrm{T}} A A^{-1} A (x - \tilde{x}) \\ &= (Ax - A\tilde{x})^{\mathrm{T}} A^{-1} (Ax - A\tilde{x}) \\ &= (b - A\tilde{x})^{\mathrm{T}} A^{-1} (b - A\tilde{x}) \\ &= \tilde{r}^{\mathrm{T}} A^{-1} \tilde{r} \\ &= \|\tilde{r}\|_{A^{-1}}^2. \end{aligned}$$

Hence,

$$x_m = \operatorname*{argmin}_{\tilde{x} \in \mathcal{K}_m} \|x - \tilde{x}\|_A^2 = \operatorname*{argmin}_{\tilde{x} \in \mathcal{K}_m} \|\tilde{r}\|_{A^{-1}}^2.$$

c) The functional $f : \mathbb{R}^n \to \mathbb{R}$ is given by $f(w) = \frac{1}{2} w^{\mathrm{T}} A w - w^{\mathrm{T}} b$. This functional attains a minimum since A is SPD. Starting at x_j and minimizing f along the search direction p_j gives

$$\begin{aligned} f(x_j + \alpha p_j) &= \tfrac{1}{2}(x_j + \alpha p_j)^{\mathrm{T}} A (x_j + \alpha p_j) - (x_j + \alpha p_j)^{\mathrm{T}} b, \\ &= \tfrac{1}{2} x_j^{\mathrm{T}} A x_j + \alpha x_j^{\mathrm{T}} A p_j + \tfrac{1}{2}\alpha^2 p_j^{\mathrm{T}} A p_j - x_j^{\mathrm{T}} b - \alpha p_j^{\mathrm{T}} b. \end{aligned}$$

At the minimum,

$$\begin{aligned} 0 = \frac{\mathrm{d}f}{\mathrm{d}\alpha} &= x_j^{\mathrm{T}} A p_j + \alpha p_j^{\mathrm{T}} A p_j - p_j^{\mathrm{T}} b \\ &= -p_j^{\mathrm{T}} r_j + \alpha p_j^{\mathrm{T}} A p_j \\ &\Downarrow \\ \alpha &= \frac{(p_j, r_j)}{(A p_j, p_j)}. \end{aligned}$$

But

$$\begin{aligned} p_j &= r_j + \beta_{j-1} p_{j-1} \\ &= r_j + \beta_{j-1}(r_{j-1} + \beta_{j-2} p_{j-2}) \\ &\vdots \\ &= r_j + \sum_{i=0}^{j-1} c_i r_i, \end{aligned}$$

where c_i are constants. Hence, due to the orthogonality of the residuals r_i, we get that $(p_j, r_j) = (r_j, r_j)$, which in turn gives us the result

$$\alpha = \frac{(r_j, r_j)}{(A p_j, p_j)}.$$

$\boxed{3}$ Let H_{m-1}, $\bar{H}_{m-1}$, $V_{m-1} = [v_1, \dots, v_{m-1}]$, $V_m = [v_1, \dots, v_m]$ be the usual matrices obtained after $m-1$ steps of Arnoldi process starting from $v_1 = A v_0 / \|A v_0\|_2$, where $v_0 = r_0$. We will also write $\bar{V}_m = [v_0, V_{m-1}]$.

Since V_{m-1} contains the orthonormal basis for $\mathcal{K}_{m-1}(A, A r_0)$, the columns of $\bar{V}_m$ form a basis for $\mathcal{K}_m(A, r_0)$.

As in any residual-projection algorithm, in GMRES we are looking for an approximate solution in the form $x_m = x_0 + \bar{V}_m y_m$, where the unknowns $y_m \in \mathbb{R}^m$ are chosen in such a way as to minimize the 2-norm of the residual

$$\begin{aligned} r_m = r_0 - A\bar{V}_m y_m &= r_0 - [A v_0, A V_{m-1}] y_m = r_0 - [\|A v_0\|_2 v_1, V_m \bar{H}_{m-1}] y_m \\ &= r_0 - V_m [\|A v_0\|_2 e_1, \bar{H}_{m-1}] y_m. \end{aligned}$$

Let $P_m = V_m V_m^{\mathrm{T}}$ be the orthogonal projector onto $\operatorname{span}(v_1, \dots, v_m)$.

$$\begin{aligned} \|r_m\|_2 &= \|(I - P_m)\{r_0 - V_m[\|A v_0\|_2 e_1, \bar{H}_{m-1}] y_m\}\|_2 + \|P_m\{r_0 - V_m[\|A v_0\|_2 e_1, \bar{H}_{m-1}] y_m\}\|_2 \\ &= \|r_0 - V_m V_m^{\mathrm{T}} r_0\|_2 + \|V_m\{V_m^{\mathrm{T}} r_0 - [\|A v_0\|_2 e_1, \bar{H}_{m-1}] y_m\}\|_2. \end{aligned}$$

The first term is independent from the selection of y_m, whereas the second term can be made zero by chosing y_m to be a solution of a *triangular* (recall: $\bar{H}_{m-1}$ is $m \times m-1$ upper Hessenberg with $h_{j+1,j} > 0$) $m \times m$ system

$$[\|Av_0\|_2 e_1, \bar{H}_{m-1}]\, y_m = V_m^{\mathrm{T}} r_0.$$

Thus $r_m = (I - P_m) r_0$ and is therefore orthogonal to $\operatorname{ran} P_m = \operatorname{span}(v_1, \ldots, v_m)$. Its norm $\|r_0 - V_m V_m^{\mathrm{T}} r_0\|_2$ is computable without the need to know y_m or x_m.