Mathematical Toolkit **Autumn 2018**

Homework 2

Due: November 13, 2018

Note: *You may discuss these problems in groups. However, you must write up your own solutions and mention the names of the people in your group. Also, please do mention any books, papers or other sources you refer to. It is recommended that you typeset your solutions in LaTeX.*

1. **First things first**. **[3+2+4]**

   The following are some useful results we have sketched in class and also used some of them in proofs. Make sure you know how to prove them! For all the parts below, let V be a finite dimensional inner-product space with dimension n.

   (a) Let $\{w_1, \ldots, w_k\}$ be an orthonormal subset of V. Show that it can be completed to an orthonormal basis of V i.e., there exist vectors $\{w_{k+1}, \ldots, w_n\}$ such that the set $\{w_1, \ldots, w_n\}$ forms an orthonormal basis of V.

   (b) Let $\{w_1, \ldots, w_n\}$ and $\{u_1, \ldots, u_n\}$ be two different orthonormal bases of V. Prove that for all $v_1, v_2 \in V$

   $$\sum_{i=1}^{n} \overline{\langle w_i, v_1 \rangle} \cdot \langle w_i, v_2 \rangle = \sum_{i=1}^{n} \overline{\langle u_i, v_1 \rangle} \cdot \langle u_i, v_2 \rangle .$$

   Note that this implies that for all $v \in V$, $\sum_{i=1}^{n} |\langle w_i, v \rangle|^2 = \sum_{i=1}^{n} |\langle u_i, v \rangle|^2$.

   (c) We call $\varphi : V \to V$ a unitary operator if $\varphi\varphi^* = \varphi^*\varphi = \mathrm{id}$. Show that φ is a unitary operator *if and only if* for any orthonormal basis $\{w_1, \ldots, w_n\}$ of V, the set $\{\varphi(w_1), \ldots, \varphi(w_n)\}$ is also an orthonormal basis.

2. **Inner products from positive definite operators**. **[2+2]**

   Let V be an inner product space over $\mathbb{C}$ and let $\varphi : V \to V$ be a self-adjoint positive definite operator i.e., $\langle v, \varphi(v) \rangle > 0$ for all $v \in V \setminus \{0_V\}$. Let $\mu : V \times V \to \mathbb{C}$ be the function defined as $\mu(v, w) = \langle v, \varphi(w) \rangle$. Show that:

   (a) The function μ also defines an inner product on the vector space V.

   (b) The operator φ is also self-adjoint for the inner product defined by the function μ.

3. **Eigenvalue interlacing**. **[2+3+3+3]**

   Let α be a self-adjoint operator on an n-dimensional inner-product space V, and let $w_0 \in V \setminus 0$ be a non-zero vector with $\|w_0\| = 1$. Let $W \subseteq V$ denote the subspace defined as $W := \{v \in V \mid \langle w_0, v\rangle = 0\}$. Let $\beta : W \to V$ be defined as

   $$\beta(w) \;=\; \alpha(w) - \langle w_0, \alpha(w)\rangle \cdot w_0 \,.$$

   (a) Show that β is in fact an operator from W to W i.e., for all $w \in W$, we have $\beta(w) \in W$.

   (b) Show that $\beta : W \to W$ as defined above is self-adjoint.

   (c) Let $\lambda_1 \geq \cdots \geq \lambda_n$ denote the eigenvalues of α and let $\mu_1 \geq \cdots \geq \cdots \mu_{n-1}$ denote the eigenvalues of β (since $\dim(W) = n-1$). Show that $\lambda_1 \geq \mu_1$.

   (d) Show that the eigenvalues of α and β are *interlacing* i.e.,

   $$\lambda_i \;\geq\; \mu_i \;\geq\; \lambda_{i+1} \quad \forall i \in [n-1]\,.$$

4. **Low-rank approximation in Frobenius norm**. **[2+3+2+5]**

   In the lecture we showed that the singular value decomposition of a matrix A gives the best low-rank approximation to A in the spectral norm. Here, we will show that the SVD also gives the best approximation in the Frobenius norm defined as $\|M\|_F^2 = \sum_{ij} |M_{ij}|^2$. Let $A \in \mathbb{R}^{m\times n}$ be a matrix with the singular value decomposition

   $$A \;=\; \sum_{j=1}^{r} \sigma_j \cdot w_j v_j^T \,,$$

   with $\sigma_1 \geq \cdots \geq \sigma_r > 0$. For $k \leq r$, we will show that $A_k = \sum_{j=1}^{k} \sigma_j w_j v_j^T$ is also the best approximation of A in the Frobenius norm i.e., for any $B \in \mathbb{R}^{m\times n}$ of rank at most k we have

   $$\|A - B\|_F \;\geq\; \|A - A_k\|_F \,.$$

   (a) Given any $B \in \mathbb{R}^{m\times n}$ of rank $t \leq k$, let $b_i \in \mathbb{R}^n$ denote i^{th} row of B (written as a column vector). Let $S = \mathrm{Span}(\{b_1, \ldots, b_m\})$. What is the dimension of the space S?

   (b) Let $a_i \in \mathbb{R}^n$ denote the i^{th} row of A (written as a column vector). Show that

   $$\|A - B\|_F^2 \;=\; \sum_{i=1}^{m} \|a_i - b_i\|_2^2 \;\geq\; \sum_{i=1}^{m} \left(\mathrm{dist}(a_i, S)\right)^2 \,.$$

   (c) Let S_0 denote the subspace of dimension at most k which minimizes the quantity $\sum_{i=1}^{m} \left(\mathrm{dist}(a_i, V)\right)^2$ over all subspaces $V \subseteq \mathbb{R}^n$ with $\dim(V) \leq k$. Express S_0 in terms of the singular vectors of the matrix A.

(d) Using the characterization for S_0 derived above, show that

$$\sum_{i=1}^{m} (\mathrm{dist}(a_i, S_0))^2 \; = \; \|A - A_k\|_F^2 \, .$$

This completes the proof since then

$$\|A - B\|_F^2 \; \geq \; \sum_{i=1}^{m} (\mathrm{dist}(a_i, S))^2 \; \geq \; \sum_{i=1}^{m} (\mathrm{dist}(a_i, S_0))^2 \; = \; \|A - A_k\|_F^2 \, .$$

5. **Perturbation of eigenvalues.** **[2+2+4+4]**

In this problem, we will apply the Gershgorin disc theorem to derive a bound on the change in the eigenvalues of a matrix due to perturbation.

(a) Two matrices $A, B \in \mathbb{C}^{n \times n}$ are called similar if there exists a non-singular matrix S such that $B = S^{-1}AS$. Show that if A and B are similar, then they have the same eigenvalues.

(b) A matrix A is called diagonalizable if it is similar to a diagonal matrix. If A is similar to a diagonal matrix Λ, find the eigenvalues of A in terms of the entries of Λ.

(c) Let $A \in \mathbb{C}^{n \times n}$ be a diagonalizable matrix such that $S^{-1}AS = \Lambda$ for a diagonal matrix Λ. Let $E \in \mathbb{C}^{n \times n}$ be an arbitrary matrix, which we think of as a "perturbation" of A. Let μ be an eigenvalue of $A + E$. Show that there exists an eigenvalue λ of A such that

$$|\lambda - \mu| \; \leq \; \max_i \sum_{j=1}^{n} \left| (S^{-1}ES)_{ij} \right| \, .$$

(d) Show that when A and E are both Hermitian (self-adjoint) the estimate can be improved. Note that in this case S is unitary ($S^*S = \mathrm{id}$). Prove that If $\lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of A, while $\mu_1 \leq \cdots \leq \cdots \mu_n$ are the eigenvalues of $A + E$, then one can get for all $i \in [n]$:

$$|\lambda_i - \mu_i| \; \leq \; \|E\|_2 \, .$$

(Recall that $\|E\|_2 = \max_{x \neq 0} \|Ex\|_2 \,/\, \|x\|_2$. Also think about why is this estimate better than the previous one.)

6. **Orthonormal bases for Krylov subspaces**. **[2+3+7]**

Let V be a vector space and let $\varphi : V \to V$ be a linear operator. Let $v \in V$ be any vector. Then the subspace

$$\mathcal{K}_t(\varphi, v) \;:=\; \text{Span}\left(\left\{v, \varphi(v), \varphi^2(v), \ldots, \varphi^{t-1}(v)\right\}\right) ,$$

is known as the Krylov subspace of order t defined by φ and v. In the conjugate gradient algorithm and the Lanczos method, we need to compute an orthonormal basis for the space $\mathcal{K}_t(\varphi, v)$ when V is an inner product space and φ is a self-adjoint operator with respect to this inner product. Here we will show that one can improve on the complexity of the Gram-Schmidt orthogonalization procedure when φ is a self-adjoint operator.

(a) Show that $\dim(\mathcal{K}_t(\varphi, v)) \leq t$ for all $\varphi : V \to V$ and all $v \in V$.

(b) For all $v, w \in V$, let the number of operations (arithmetic operations over $\mathbb{C}$) required to compute $\langle v, w \rangle$ and $\varphi(v)$ be at most N. Then show that one can apply the Gram-Schmidt process to the set $\left\{v, \varphi(v), \varphi^2(v), \ldots, \varphi^{t-1}(v)\right\}$ to find an orthonormal basis for $\mathcal{K}_t(\varphi, v)$ using $O(t^2 \cdot N)$ operations.

(c) When using the conjugate gradient algorithm, a complexity of $O(t^2 \cdot N)$ turns out to be too large for computing an orthonormal basis. We have $t = O(\sqrt{\kappa})$ and hence spending time $O(t^2 \cdot N)$ in computing the basis would not give us any advantage over steepest descent.

However, when φ is self-adjoint, an orthonormal basis can be computed using $O(t \cdot N)$ operations. Assume $\dim(\mathcal{K}_t(\varphi, v)) = t$ (and hence $v \neq 0$). Use induction (on i) to show that there exists a set of orthonormal vectors $\{u_0, \ldots, u_{t-1}\}$ such:

i. $\text{Span}\left(\{u_0, \ldots, u_{i-1}\}\right) \;=\; \mathcal{K}_i(\varphi, v)$ for all $i \leq t$.

ii. $\text{Span}\left(\{u_0, \ldots, u_{i-1}, \varphi(u_{i-1})\}\right) \;=\; \mathcal{K}_{i+1}(\varphi, v)$ for all $i \leq t - 1$.

iii. $\left\langle \varphi(u_i), u_j \right\rangle = 0$ for all $1 \leq i \leq t-1$ and all $j \leq i - 2$.

Note that to construct an orthonormal basis with the properties above, one only needs to compute $\langle u_i, \varphi(u_i) \rangle$ and $\langle u_{i-1}, \varphi(u_i) \rangle$ at every step. Thus, the basis can be constructed using $O(t \cdot N)$ operations.