STAT 309: MATHEMATICAL COMPUTATIONS I
FALL 2015
LECTURE 6

1. SOLVING LEAST SQUARES PROBLEMS

- given $A \in \mathbb{C}^{m\times n}$ and $\mathbf{b} \in \mathbb{C}^m$, the least squares problem ask to find $\mathbf{x} \in \mathbb{C}^n$ so that
$$\|\mathbf{b} - A\mathbf{x}\|_2^2$$
is minimized
- note that $\mathbf{x}$ minimizes $\|\mathbf{b} - A\mathbf{x}\|_2^2$ iff it minimizes $\|\mathbf{b} - A\mathbf{x}\|_2$, so whether we write the 'squared' or not doesn't really matter
- using SVD of A and the unitary invariance of the vector 2-norm in Homework 2, we can simplify this minimization problem as follows
$$\begin{aligned}\|\mathbf{b} - A\mathbf{x}\|_2^2 &= \|\mathbf{b} - U\Sigma V^*\mathbf{x}\|_2^2\\ &= \|U^*\mathbf{b} - \Sigma V^*\mathbf{x}\|_2^2\\ &= \|\mathbf{c} - \Sigma\mathbf{y}\|_2^2\\ &= (c_1 - \sigma_1 y_1)^2 + \cdots + (c_r - \sigma_r y_r)^2 + c_{r+1}^2 + \cdots + c_m^2\end{aligned}$$
where $\mathbf{c} = U^*\mathbf{b}$ and $\mathbf{y} = V^*\mathbf{x}$
- so we see that in order to minimize $\|A\mathbf{x} - \mathbf{b}\|_2$, we must set $y_i = c_i/\sigma_i$ for $i = 1, \dots, r$
- the unknowns y_i, for $i = r+1, \dots, m$, can have any value, since they do not affect the value of $\|\mathbf{c} - \Sigma\mathbf{y}\|_2$
- so all the least squares solution are of the form
$$\mathbf{x} = V\mathbf{y} = V\begin{bmatrix} c_1/\sigma_1\\ \vdots\\ c_r/\sigma_r\\ y_{r+1}\\ \vdots\\ y_n\end{bmatrix}$$
where $y_{r+1}, \dots, y_n \in \mathbb{C}$ are arbitrary
- our analysis above also shows that the minimum value of $\|\mathbf{b} - A\mathbf{x}\|_2^2$ is given by
$$\min_{\mathbf{x}\in\mathbb{C}^n} \|\mathbf{b} - A\mathbf{x}\|_2^2 = c_{r+1}^2 + \cdots + c_m^2$$

2. SOLVING MINIMUM LENGTH LEAST SQUARES PROBLEMS

- one of the best-known applications of the SVD is that it can be used to obtain the solution to the problem
$$\|\mathbf{b} - A\mathbf{x}\|_2 = \min, \quad \|\mathbf{x}\|_2 = \min.$$
- alternatively, we can write
$$\min\Big\{\|\mathbf{x}\|_2 : \mathbf{x} \in \operatorname*{argmin}_{\mathbf{x}\in\mathbb{C}^n}\|\mathbf{b} - A\mathbf{x}\|\Big\}$$

Date: November 7, 2015, version 1.1. Comments, bug reports: `lekheng@galton.uchicago.edu`.

- or using the normal equations

$$\min\{\|\mathbf{x}\|_2 : A^*A\mathbf{x} = A^*\mathbf{b}\}$$

- notation: $f : X \to \mathbb{R}$, for $S \subseteq X$, write

$$\operatorname*{argmin}_{x\in S} f(x) \quad \text{or} \quad \operatorname{argmin}\{f(x) : x \in S\}$$

for the *set* of minmizers, i.e.

$$\operatorname*{argmin}_{x\in S} f(x) = \left\{x_* \in S : f(x_*) = \min_{x\in S} f(x)\right\}$$

we often write (sloppily) $x_* = \operatorname{argmin} f(x)$ or $\operatorname{argmin} f(x) = x_*$ to mean that x_* is a minimizer of f over S even though the proper notation ought to have been $x_* \in \operatorname{argmin} f(x)$
- note that from the last part of the last lecture that if A does not have full rank, then there are infinitely many solutions to the least squares problem because the residual in does not depend on $y_{r+1}, \dots, y_m$ and these are thus free parameters that we may freely choose:

$$\mathbf{x} = V\mathbf{y} = V\begin{bmatrix} c_1/\sigma_1 \\ \vdots \\ c_r/\sigma_r \\ y_{r+1} \\ \vdots \\ y_n \end{bmatrix} \tag{2.1}$$

where $\mathbf{c} = U^*\mathbf{b}$
- we can claim that the unique solution with minimum 2-norm is given by setting $y_{r+1} = \cdots = y_m = 0$, i.e.

$$\mathbf{x}_+ = V\begin{bmatrix} c_1/\sigma_1 \\ \vdots \\ c_r/\sigma_r \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{2.2}$$

where $\mathbf{c} = U^*\mathbf{b}$
- this follows because

$$\|\mathbf{x}_+\|_2^2 = \left|\frac{c_1}{\sigma_1}\right|^2 + \cdots + \left|\frac{c_r}{\sigma_r}\right|^2 \le \left|\frac{c_1}{\sigma_1}\right|^2 + \cdots + \left|\frac{c_r}{\sigma_r}\right|^2 + |y_{r+1}|^2 + \cdots + |y_n|^2 = \|\mathbf{x}\|_2^2$$

whatever our choice of $y_{r+1}, \dots, y_n$ in (2.1)
- we may also write (2.2) in terms of the Moore–Penrose pseudo inverse

$$\mathbf{x}_+ = V\Sigma^\dagger\mathbf{c} = V\Sigma^\dagger U^*\mathbf{b} = A^\dagger\mathbf{b}$$

since $\Sigma^\dagger$ has precisely the right form

$$\Sigma^\dagger = \begin{bmatrix} \sigma_1^{-1} & & & & & \\ & \ddots & & & & \\ & & \sigma_r^{-1} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix}$$

3. FINDING BASES FOR FOUR FUNDAMENTAL SUBSPACES

- given $A \in \mathbb{C}^{m\times n}$ we may regard it as a linear operator $A : \mathbb{C}^n \to \mathbb{C}^m$, $\mathbf{x} \mapsto A\mathbf{x}$
- there are four subspaces associated with A that we call the fundamental subspaces
  - $\ker(A) = \{\mathbf{x} \in \mathbb{C}^n : A\mathbf{x} = \mathbf{0}\}$
  - $\operatorname{im}(A) = \{\mathbf{y} \in \mathbb{C}^m : \mathbf{y} = A\mathbf{x} \text{ for some } \mathbf{x} \in \mathbb{C}^n\}$
  - $\ker(A^*) = \{\mathbf{y} \in \mathbb{C}^m : A^*\mathbf{x} = \mathbf{0}\}$
  - $\operatorname{im}(A^*) = \{\mathbf{x} \in \mathbb{C}^n : A^*\mathbf{y} = \mathbf{x} \text{ for some } \mathbf{y} \in \mathbb{C}^m\}$
- they are called the kernel, image, cokernel, and coimage respectively
  - the word null space is often used in place of kernel
  - the word range space is often used in place of image
- as we see from Homework 2, they are related by

$$\ker(A^*) = \operatorname{im}(A)^\perp \quad \text{and} \quad \operatorname{im}(A^*) = \ker(A)^\perp$$

- furthermore they decompose the domain and codomain of A into orthogonal subspaces

$$\mathbb{C}^n = \operatorname{im}(A^*) \oplus \ker(A) \quad \text{and} \quad \mathbb{C}^m = \ker(A^*) \oplus \operatorname{im}(A)$$

- this decomposition is sometimes called *Fredholm alternative* and is very useful for studying linear systems $A\mathbf{x} = \mathbf{b}$ and least squares problems (cf. Homework 2)
- there is a variant called Farkas Lemma that applies to linear inequalities $A\mathbf{x} \le \mathbf{b}$
- the full SVD of A allows us to simply read off orthonormal bases for the four fundamental subspaces, which will be useful if we want to compute projections
- let $\operatorname{rank}(A) = r$ and let $\mathbf{u}_1, \dots, \mathbf{u}_m$ and $\mathbf{v}_1, \dots, \mathbf{v}_n$ be the left and right singular vectors of A, indexed in the usual way in desceding magnitude of their corresponding singular values
  - $\ker(A) = \operatorname{span}\{\mathbf{v}_{r+1}, \dots, \mathbf{v}_n\}$
  - $\operatorname{im}(A) = \operatorname{span}\{\mathbf{u}_1, \dots, \mathbf{u}_r\}$
  - $\ker(A^*) = \operatorname{span}\{\mathbf{u}_{r+1}, \dots, \mathbf{u}_m\}$
  - $\operatorname{im}(A^*) = \operatorname{span}\{\mathbf{v}_1, \dots, \mathbf{v}_r\}$
- this is easy to see, let us do $\operatorname{im}(A)$ for example
  - first observe that an orthonormal basis for $\operatorname{im}(\Sigma)$ is the first r standard basis vectors $\mathbf{e}_1, \dots, \mathbf{e}_r \in \mathbb{C}^m$ since

$$\Sigma\mathbf{x} = \sigma_1 x_1 \mathbf{e}_1 + \cdots + \sigma_r x_r \mathbf{e}_r$$

  - now just observe that

$$\operatorname{im}(A) = \operatorname{im}(U\Sigma V^*) = \operatorname{im}(U\Sigma) = \operatorname{span}\{U\mathbf{e}_1, \dots, U\mathbf{e}_r\} = \operatorname{span}\{\mathbf{u}_1, \dots, \mathbf{u}_r\}$$

  - there is a useful fact worth noting: for nonsingular matrices $S \in \mathrm{GL}(m)$ and $T \in \mathrm{GL}(n)$,

$$\operatorname{im}(AT) = \operatorname{im}(A) \quad \text{and} \quad \ker(SA) = \ker(A)$$

4. ASIDE: PROJECTION

- the solution $\mathbf{x}$ of the least-squares problem minimizes $\|A\mathbf{x} - \mathbf{b}\|_2$, and therefore is the vector that solves the system $A\mathbf{x} = \mathbf{b}$ as closely as possible
- we can use the SVD to show that $\mathbf{x}$ is the exact solution to a related system of equations
- write $\mathbf{b} = \mathbf{b}_0 + \mathbf{b}_1$, where

$$\mathbf{b}_1 = AA^\dagger\mathbf{b}, \quad \mathbf{b}_0 = (I - AA^\dagger)\mathbf{b}$$

- the matrix $AA^\dagger$ has the form

$$AA^\dagger = U\Sigma V^* V\Sigma^\dagger U^* = U\Sigma\Sigma^\dagger U^* = U \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} U^*$$

- it follows that $\mathbf{b}_1$ is a linear combination of $\mathbf{u}_1, \dots, \mathbf{u}_r$, the columns of U that form an orthogonal basis for the range of A
- from $\mathbf{x} = A^\dagger \mathbf{b}$ we obtain
$$A\mathbf{x} = AA^\dagger \mathbf{b} = P_1 \mathbf{b} = \mathbf{b}_1$$
where $P_1 = AA^\dagger \in \mathbb{C}^{m\times m}$
- therefore, the solution to the least squares problem, is also the exact solution to the system
$$A\mathbf{x} = P_1 \mathbf{b}$$
- it can be shown that the matrix P_1 is an *orthogonal projection*
- in general a matrix $P \in \mathbb{C}^{m\times m}$ is called a *projection* if $P^2 = P$ (this condition is also called idempotent in ring theory)
- a projection is called an orthogonal projection if it is also Hermitian, i.e. an orthogonal projection is a matrix $P \in \mathbb{C}^{m\times m}$ satisfying
  (i) $P = P^*$
  (ii) $P^2 = P$
- caveat: an orthogonal projection is in general *not* an orthogonal/unitary matrix (i.e., $P^* \neq P^{-1}$) in fact, projections are usually non-invertible
- example: $\left[\begin{smallmatrix} 1 & \alpha \\ 0 & 0 \end{smallmatrix}\right]$ is a projection for any $\alpha \in \mathbb{C}$, it is an orthogonal projection if and only if $\alpha = 0$
- if $P \in \mathbb{C}^{m\times m}$ is a projection and $\operatorname{im}(P) = W$, we say that P is a projection onto the subspace W
- if $P \in \mathbb{C}^{m\times m}$ is a projection matrix, then $I - P$ is also a projection
- furthermore if $\operatorname{im}(P) = W$ and $\operatorname{im}(I - P) = W'$, then
$$\mathbb{C}^m = W \oplus W'$$
- if P is an orthogonal projection and $\operatorname{im}(P) = W$, then $\operatorname{im}(I - P) = W^\perp$
- we sometimes write P_W if we know the subspace P that projects onto
- in particular, $P_1 = AA^\dagger$ is a projection onto the space spanned by the columns of A, i.e., $\operatorname{im}(A)$, so $P_1 = P_{\operatorname{im}(A)}$

5. Computing projections onto fundamental subspaces

- we can write down the orthogonal projections onto all four fundamental subspaces in terms of the pseudoinverse
$$P_{\operatorname{im}(A)} = AA^\dagger, \quad P_{\ker(A^*)} = I - AA^\dagger, \quad P_{\operatorname{im}(A^*)} = A^\dagger A, \quad P_{\ker(A)} = I - A^\dagger A$$
- note that $P_{\operatorname{im}(A)}, P_{\ker(A^*)} \in \mathbb{C}^{m\times m}$ and $P_{\operatorname{im}(A^*)}, P_{\ker(A)} \in \mathbb{C}^{n\times n}$
- with the SVD, we can write down the projections in terms of unitary matrices
$$P_{\operatorname{im}(A)} = U \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} U^* = U_r U_r^*, \quad P_{\ker(A^*)} = U \begin{bmatrix} 0 & 0 \\ 0 & I_{m-r} \end{bmatrix} U^* = U_{m-r} U_{m-r}^*,$$
$$P_{\operatorname{im}(A^*)} = V \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} V^* = V_r V_r^*, \quad P_{\ker(A)} = V \begin{bmatrix} 0 & 0 \\ 0 & I_{n-r} \end{bmatrix} V^* = V_{n-r} V_{n-r}^*$$
where $U = [U_r, U_{m-r}]$ and $V = [V_r, V_{m-r}]$

6. Finding rank and numerical rank

- matrix rank is a discrete notion that is sometimes too imprecise, for example both
$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 \\ 0 & 10^{-14} \end{bmatrix}$$
have rank 2

- another example: take a randomly generated vector $\mathbf{x} \sim N(\mathbf{0}, I_n)$ and consider the $n \times n$ matrices

$$X = [\mathbf{x}, 2\mathbf{x}, \dots, n\mathbf{x}] \quad \text{and} \quad \mathrm{fl}(X) = [\mathrm{fl}(\mathbf{x}), \mathrm{fl}(2\mathbf{x}), \dots, \mathrm{fl}(n\mathbf{x})]$$

- in the presence of rounding error, we will get

$$\operatorname{rank}(X) = 1 \quad \text{and} \quad \operatorname{rank}(\mathrm{fl}(X)) = n$$

- the singular values are much more informative

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

- the profile or decay rate of these can often tell us the 'true rank' of a matrix
- exercise: plot the singular value profile of $\mathrm{fl}(X)$ in MATLAB
- this is the notion of what is often called *numerical rank*
- SVD tells us about numerical rank
- but some folks insist that numerical rank of a matrix must be a number like rank, not a decomposition
- there are several proposals on how it could be defined, three of the most common ones are defined as follows
- let $\tau > 0$ be some predetermined tolerance level (in practice a small number ≈ 0.1) and $A \in \mathbb{C}^{m \times n}$ be a non-zero matrix
- the term *numerical rank* of A have variously been given to
  - the positive integer

$$\rho \operatorname{rank}(A) := \min \left\{ r \in \mathbb{N} : \frac{\sigma_{r+1}(A)}{\sigma_r(A)} \leq \tau \right\}$$

  - or the positive integer

$$\mu \operatorname{rank}(A) := \min \left\{ r \in \mathbb{N} : \frac{\sum_{i \geq r+1} \sigma_i(A)^2}{\sum_{i \geq 1} \sigma_i(A)^2} \leq \tau \right\}$$

  - or the positive real number

$$\nu \operatorname{rank}(A) = \frac{\|A\|_F^2}{\|A\|_2^2} = \frac{\sum_{i=1}^{\min(m,n)} \sigma_i(A)^2}{\sigma_1(A)^2}$$