MATH96023/MATH97032/MATH97140 - Computational Linear Algebra

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CONTENTS

CHAPTER

ONE

PRELIMINARIES

In this preliminary section we revise a few key linear algebra concepts that will be used in the rest of the course, emphasising the column space of matrices. We will quote some standard results that should be found in an undergraduate linear algebra course.

1.1 Matrices, vectors and matrix-vector multiplication

We will consider the multiplication of a vector

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad x_i \in \mathbb{C},\ i = 1, 2, \ldots, n, \text{ i.e. } x \in \mathbb{C}^n,$$

by a matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \ldots & a_{mn} \end{pmatrix},$$

i.e. $A \in \mathbb{C}^{m\times n}$. A has m rows and n columns so that the product

$$b = Ax$$

produces $b \in \mathbb{C}^m$, defined by

$$b_i = \sum_{j=1}^{n} a_{ij}x_j,\ i = 1, 2, \ldots, m.$$

In this course it is important to consider the general case where $m \neq n$, which has many applications in data analysis, curve fitting etc. We will usually state generalities in this course for vectors over the field $\mathbb{C}$, noting where things specialise to $\mathbb{R}$.

We can quickly check that the map $x \to Ax$ given by matrix multiplication is a linear map from $\mathbb{C}^n \to \mathbb{C}^m$, since it is straightforward to check from the definition that

$$A(\alpha x + y) = \alpha A x + A y,$$

for all $x, y \in \mathbb{C}^n$ and $\alpha \in \mathbb{C}$. (Exercise: show this for yourself.)

It is very useful to interpret matrix-vector multiplication as a linear combination of the columns of A with coefficients taken from the entries of x. If we write A in terms of the columns,

$$A = \begin{pmatrix} a_1 & a_2 & \dots & a_n \end{pmatrix},$$

where

$$a_i \in \mathbb{C}^m,\ i = 1, 2, \dots, n,$$

then

$$b = \sum_{j=1}^{n} x_j a_j,$$

i.e. a linear combination of the columns of A as described above.

We can extend this idea to matrix-matrix multiplication. Taking $A \in \mathbb{C}^{l\times m}$, $C \in \mathbb{C}^{m\times n}$, $B \in \mathbb{C}^{l\times n}$, with $B = AC$, then the components of B are given by

$$b_{ij} = \sum_{k=1}^{m} a_{ik} c_{kj}, \quad 1 \leq i \leq l,\ 1 \leq j \leq n.$$

Writing $b_j \in \mathbb{C}^m$ as the jth column of B, for $1 \leq j \leq n$, and c_j as the jth column of C, we see that

$$b_j = A c_j.$$

This means that the jth column of B is the matrix-vector product of A with the jth column of C. This kind of "column thinking" is very useful in understanding computational linear algebra algorithms.

An important example is the outer product of two vectors, $u \in \mathbb{C}^m$ and $v \in \mathbb{C}^n$. Here it is useful to see these vectors as matrices with one column, i.e. $u \in \mathbb{C}^{m\times 1}$ and $v \in \mathbb{C}^{n\times 1}$. The outer product is $uv^T \in \mathbb{C}^{m\times n}$. The columns of v^T are just single numbers (i.e. vectors of length 1), so viewing this as a matrix multiplication we see

$$uv^T = \begin{pmatrix} uv_1 & uv_2 & \dots & uv_n \end{pmatrix},$$

which means that all the columns of uv^T are multiples of u. We will see in the next section that this matrix has rank 1.

1.2 Range, nullspace and rank

In this section we'll quickly rattle through some definitions and results.

Definition 1 (Range) *The range of A, range(A), is the set of vectors that can be expressed as Ax for some x.*

The next theorem follows as a result of the column space interpretation of matrix-vector multiplication.

Theorem 2 *range(A) is the vector space spanned by the columns of A.*

Definition 3 (Nullspace) *The nullspace null(A) of A (or kernel) is the set of vectors x satisfying $Ax = 0$, i.e.*

$$\textit{null}(A) = \{x \in \mathbb{C}^n : Ax = 0\}.$$

Definition 4 (Rank) *The rank rank(A) of A is the dimension of the column space of A.*

If

$$A = \begin{pmatrix} a_1 & a_2 & \ldots & a_n \end{pmatrix},$$

the column space of A is span$(a_1, a_2, \ldots, a_n)$.

Definition 5 *An $m \times n$ matrix A is full rank if it has maximum possible rank i.e. rank equal to $\min(m, n)$.*

If $m \geq n$ then A must have n linearly independent columns to be full rank. The next theorem is then a consequence of the column space interpretation of matrix-vector multiplication.

Theorem 6 *An $m \times n$ matrix A is full rank if and only if it maps no two distinct vectors to the same vector.*

Definition 7 *A matrix A is called nonsingular, or invertible, if it is a square matrix ($m = n$) of full rank.*

1.3 Invertibility and inverses

This means that an invertible matrix has columns that form a basis for $\mathbb{C}^m$. Given the canonical basis vectors defined by

$$e_j = \begin{pmatrix} 0 \\ \ldots \\ 0 \\ 1 \\ 0 \\ \ldots \\ 0 \end{pmatrix},$$

i.e. e_j has all entries zero except for the jth entry which is 1, we can write

$$e_j = \sum_{k=1}^{m} z_{ik} a_k, \quad 1 \leq j \leq m.$$

In other words,

$$\begin{aligned} I = \begin{pmatrix} e_1 & e_2 & \ldots & e_m \end{pmatrix} \\ = ZA. \end{aligned}$$

We call Z a (left) inverse of A. (Exercises: show that Z is the unique left inverse of A, and show that Z is also the unique right inverse of A, satisfying $I = AZ$.) We write $Z = A^{-1}$.

The first four parts of the next theorem are a consequence of what we have so far, and we shall quote the rest (see a linear algebra course).

Theorem 8 *Let $A \in \mathbb{C}^{m\times m}$. Then the following are equivalent.*

1. *A has an inverse.*
2. *rank$(A) = m$.*
3. *range$(A) = \mathbb{C}^m$.*
4. *null$(A) = \{0\}$.*
5. *0 is not an eigenvalue of A.*
6. *0 is not a singular value of A.*
7. *The determinant $\det(A) \neq 0$.*

Finding the inverse of a matrix can be seen as a change of basis. Considering the equation $Ax = b$, we have $x = A^{-1}b$ for invertible A. We have seen already that b can be written as

$$b = \sum_{j=1}^{m} x_j a_j.$$

Since the columns of A span $\mathbb{C}^m$, the entries of x thus provide the unique expansion of b in the columns of A which form a basis. Hence, whilst the entries of b give basis coefficients for b in the canonical basis $(e_1, e_2, \ldots, e_m)$, the entries of x give basis coefficients for b in the basis given by the columns of A.

1.4 Orthogonal vectors and orthogonal matrices

Definition 9 (Adjoint) *The adjoint (or Hermitian conjugate) of $A \in \mathbb{C}^{m\times n}$ is a matrix $A^* \in \mathbb{C}^{n\times m}$ (sometimes written $A^\dagger$ or A'), with*

$$a^*_{ij} = \bar{a_{ji}},$$

where the bar denotes the complex conjugate of a complex number. If $A^* = A$ then we say that A is Hermitian.

For real matrices, $A^* = A^T$. If $A = A^T$, then we say that the matrix is symmetric.

The following identity is very important when dealing with adjoints.

Theorem 10 *For matrices A, B with compatible dimensions (so that they can be multiplied),*

$$(AB)^* = B^*A^*.$$

1.5 Inner products and orthogonality

The inner product is a critical tool in computational linear algebra.

Definition 11 (Inner product) *Let $x, y \in \mathbb{C}^m$. Then the inner product of x and y is*

$$x^*y = \sum_{i=1}^{m} \bar{x}_i y_i.$$

(Exercise: check that the inner product is bilinear, i.e. linear in both of the arguments.)

We will frequently use the natural norm derived from the inner product to define size of vectors.

Definition 12 (2-Norm) *Let $x \in \mathbb{C}^m$. Then the 2-norm of x is*

$$\|x\| = \sqrt{\sum_{i=1}^{m} x_i^2} = \sqrt{x^* x}.$$

Orthogonality will emerge as an early key concept in this course.

> **Definition 13 (Orthogonal vectors)** *Let $x, y \in \mathbb{C}^m$. The two vectors are orthogonal if $x^* y = 0$.*
>
> *Similarly, let X, Y be two sets of vectors. The two sets are orthogonal if*
>
> $$x^* y = 0 \, \forall x \in X, \, y \in Y.$$
>
> *A set S of vectors is itself orthogonal if*
>
> $$x^* y = 0 \, \forall x, y \in S.$$
>
> *We say that S is orthonormal if we also have $\|x\| = 1$ for all $x \in S$.*

1.6 Orthogonal components of a vector

Let $S = \{q_1, q_2, \ldots, q_n\}$ be an orthonormal set of vectors in $\mathbb{C}^m$, and take another arbitrary vector $v \in \mathbb{C}^m$. Now take

$$r = v - (q_1^* v) q_1 - (q_2^* v) q_2 - \ldots (q_n^* v) q_n.$$

Then, we can check that r is orthogonal to S, by calculating for each $1 \leq i \leq n$,

$$q_i^* r = q_i^* v - (q_1^* v)(q_i^* q_1) - \ldots (q_n^* v)(q_i^* q_n)$$

= q_i^*v - q_i^*v = 0,

since $q_i^* q_j = 0$ if $i \neq j$, and 1 if $i = j$. Thus,

$$v = r + \sum_{i=1}^{n} (q_i^* v) q_i = r + \sum_{i=1}^{n} \underbrace{(q_i q_i^*)}_{\text{rank-1 matrix}} v.$$

If S is a basis for $\mathbb{C}^m$, then $n = m$ and $r = 0$, and we have

$$v = \sum_{i=1}^{m} (q_i q_i^*) v.$$

1.7 Unitary matrices

Definition 14 (Unitary matrices) *A matrix $Q \in \mathbb{C}^{m \times m}$ is unitary if $Q^* = Q^{-1}$.*

For real matrices, a matrix Q is orthogonal if $Q^T = Q^{-1}$.

Theorem 15 *The columns of a unitary matrix Q are orthonormal.*

Proof 16 *We have $I = Q^*Q$. Then using the column space interpretation of matrix-matrix multiplication,*

$$e_j = Q^* q_j,$$

where q_j is the jth column of Q. Taking row i of e_j, we have

$$\delta_{ij} = q_i^* q_j, \text{ where } \delta_{ij} = \left\{ \begin{array}{lll} 1 & \text{if} & i = j, \\ 0 & \text{otherwise} & \end{array} \right. .$$

Extending a theme from earlier, we can interpret $Q^* = Q^{-1}$ as representing a change of orthogonal basis. If $Qx = b$, then $x = Q^*b$ contains the coefficients of b expanded in the basis given by the orthonormal columns of Q.

1.8 Vector norms

Various vector norms are useful to measure the size of a vector. In computational linear algebra we need them for quantifying errors etc.

Definition 17 (Norms) *A norm is a function $\|\cdot\| : \mathbb{C}^m \to \mathbb{R}$, such that*

1. $\|x\| \geq 0$, *and* $\|x\| = 0 \implies x = 0$.
2. $\|x + y\| \leq \|x\| + \|y\|$ *(triangle inequality).*
3. $\|\alpha x\| = |\alpha| \|x\|$ *for all* $x \in \mathbb{C}^m$ *and* $\alpha \in \mathbb{C}$.

We have already seen the 2-norm, or Euclidean norm, which is part of a larger class of norms called p-norms, with

$$\|x\|_p = \left(\sum_{i=1}^m |x_i|^p \right)^{1/p},$$

for real 'p>0'. We will also consider weighted norms

$$\|x\|_{W,p} = \|Wx\|_p,$$

where W is a matrix.

1.9 Projectors and projections

Definition 18 (Projector) *A projector P is a square matrix that satisfies $P^2 = P$.*

If $v \in \text{range}(P)$, then there exists x such that $Pv = x$. Then,

$$Pv = P(Px) = P^2x = Px = v,$$

and hence multiplying by P does not change v.

Now suppose that $Pv \neq v$ (so that `vnotin mbox{range}(P)). Then,

$$P(Pv - v) = P^2v - Pv = Pv - Pv = 0,$$

which means that $Pv - v$ is the nullspace of P. We have

$$Pv - v = -(I - P)v.$$

Definition 19 (Complementary projector) *Let P be a projector. Then we call $I - P$ the complementary projector.*

To see that $I - P$ is also a projector, we just calculate,

$$(I - P)^2 = I^2 - 2P + P^2 = I - 2P + P = I - P.$$

If $Pu = 0$, then $(I - P)u = u$.

In other words, the nullspace of P is contained in the range of $I - P$.

On the other hand, if v is in the range of $I - P$, then

there exists some w such that

$$v = (I - P)w = w - Pw.$$

We have

$$Pv = P(w - Pw) = Pw - P^2 w = Pw - Pw = 0.$$

Hence, the range of $I - P$ is contained in the nullspace of P. Combining these two results we see that the range of $I - P$ is equal to the nullspace of P. Since P is the complementary projector to $I - P$, we can repeat the same argument to show that the range of P is equal to the nullspace of $I - P$.

We see that a projector P separates $\mathbb{C}^m$ into two subspaces, the nullspace of P and the range of P. In fact the converse is also true: given two subspaces S_1 and S_2 of $\mathbb{C}^m$ with $S_1 \cap S_2 = \{0\}$, then there exists a projector P whose range is S_1 and whose nullspace is S_2.

Now we introduce orthogonality into the concept of projectors.

Definition 20 (Orthogonal projector) *P is an orthogonal projector if*

$$(Pv)^*(Pv - v) = 0, \, \forall v \in \mathbb{C}^m.$$

In this case, P separates the space into two orthogonal subspaces.

1.10 Constructing orthogonal projectors from sets of orthonormal vectors

Let $\{q_1, \ldots, q_n\}$ be an orthonormal set of vectors in $\mathbb{C}^m$. We write

$$\hat{Q} = \begin{pmatrix} q_1 & q_2 & \ldots & q_n \end{pmatrix}.$$

Previously we showed that for any $v \in \mathbb{C}^m$, we have

$$v = \underbrace{r}_{\text{Orthogonal to column space of } \hat{Q}} + \underbrace{\sum_{i=1}^{n} (q_i q_i^*) v}_{\text{in the column space of } \hat{Q}}.$$

Hence, the map

$$v \mapsto Pv = \underbrace{\sum_{i=1}^{n} (q_i q_i^*)}_{=P} v,$$

is an orthogonal projector. In fact, P has very simple form.

Theorem 21 *The orthogonal projector P takes the form*

$$P = \hat{Q}\hat{Q}^*.$$

Proof 22 *From the change of basis interpretation of multiplication by $\hat{Q}^*$, the entries in $\hat{Q}^* v$ gives coefficients of the projection of v onto the column space of $\hat{Q}$ when expanded using the columns as a basis. Then, multiplication by $\hat{Q}$ gives the projection of v expanded again in the canonical basis. Hence, multiplication by $\hat{Q}\hat{Q}^*$ gives exactly the same result as multiplication by the formula for P above.*

This means that $\hat{Q}\hat{Q}^*$ is an orthogonal projection onto the range of $\hat{Q}$. The complementary projector is $P_\perp = I - \hat{Q}\hat{Q}^*$ is an orthogonal projection onto the nullspace of $\hat{Q}$.

An important special case is when $\hat{Q}$ has just one column, and then

$$P = q_1 q_1^*,\ P_\perp = I - q_1 q_1^*.$$

We notice that $P^* = (\hat{Q}\hat{Q}^*) = \hat{Q}\hat{Q}^* = P$. In fact the following is true.

Theorem 23 *$P = P^*$ if and only if Q is an orthogonal projector.*

CHAPTER TWO

QR FACTORISATION

A common theme in computational linear algebra is transformations of matrices and algorithms to implement them. A transformation is only useful if it can be computed efficiently and sufficiently free of pollution from truncation errors (either due to finishing an iterative algorithm early, or due to round-off errors). A particularly powerful and insightful transformation is the QR factorisation. In this section we will introduce the QR factorisation and some good and bad algorithms to compute it.

2.1 What is the QR factorisation?

We start with another definition.

Definition 24 (Upper triangular matrix) *An $m \times n$ upper triangular matrix R has coefficients satisfying $r_{ij} = 0$ when $i \geq j$.*

It is called upper triangular because the nonzero rows form a triangle on and above the main diagonal of R.

Now we can describe the QR factorisation.

Definition 25 (QR factorisation) *A QR factorisation of an $m \times n$ matrix A consists of an $m \times m$ unitary matrix Q and an $m \times n$ upper triangular matrix R such that $A = QR$.*

The QR factorisation is a key tool in analysis of datasets, and polynomial fitting. It is also at the core of one of the most widely used algorithms for finding eigenvalues of matrices. We shall discuss all of this later during this course.

When $m > n$, R must have all zero rows after the n block of R consisting of the first n rows, which we call $\hat{R}$. Similarly, in the matrix vector product QR, all columns of Q beyond the n, so it makes sense to only work with the first n columns of Q, which we call $\hat{Q}$. We then have the reduced QR factorisation, $\hat{Q}\hat{R}$.

In the rest of this section we will examine some algorithms for computing the QR factorisation, before discussing the application to least squares problems. We will start with a bad algorithm, before moving on to some better ones.

2.2 QR factorisation by classical Gram-Schmidt algorithm

The classical Gram-Schmidt algorithm for QR factorisation is motivated by the column space interpretation of the matrix-matrix multiplication $A = QR$, namely that the jth column a_j of A is a linear combination of the orthonormal columns of Q, with the coefficients given by the jth column r_j of R.

The first column of R only has a non-zero entry in the first row, so the first column of Q must be proportional to A, but normalised (i.e. rescaled to have length 1). The scaling factor is this first row of the first column of R. The second column of R has only non-zero entries in the first two rows, so the second column of A must be writeable as a linear combination of the first two columns of Q. Hence, the second column of Q must by the second column of A with the first column of Q projected out, and then normalised. The first row of the second column of R is then the coefficient for this projection, and the second row is the normalisation scaling factor. The third row of Q is then the third row of A with the first two columns of Q projected out, and so on.

Hence, finding a QR factorisation is equivalent to finding an orthonormal spanning set for the columns of A, where the span of the first 'j' elements of the spanning set and of the first `j' columns of 'A' is the same, for 'j=1,ldots, n'.

Hence we have to find R coefficients such that

$$
\begin{aligned}
q_1 &= \frac{a_1}{r_1 1}, \\
q_2 &= \frac{a_2 - r_{12}q_1}{r_{22}} \\
&\vdots \\
q_n &= \frac{q_n - \sum_{i=1}^{n-1} r_{in}q_i}{r_{nn}},
\end{aligned}
$$

with $(q_1, q_2, \ldots, q_n)$ an orthonormal set. The non-diagonal entries of R are found by inner products, i.e.,

$$r_{ij} = q_i^* a_j, \; i > j,$$

and the diagonal entries are chosen so that $\|q_i\| = 1$, for $i = 1, 2, \ldots, n$, i.e.

$$|r_{jj}| = \left\| a_j - \sum_{i=1}^{j-1} r_{ij} q_i \right\|.$$

Note that this absolute value does leave a degree of nonuniqueness in the definition of R. It is standard to choose the diagonal entries to be real and non-negative.

We now present the classical Gram-Schmidt algorithm as pseudo-code.

- FOR $j = 1$ TO n
  - $v_j \leftarrow a_j$
  - FOR $i = 1$ TO $j - 1$
    * $r_{ij} \leftarrow q_i^* a_j$
    * $v_j \leftarrow v_j - r_{ij} q_i$
  - END FOR
  - $r_{jj} \leftarrow \|v_j\|_2$
  - $q_j \leftarrow v_j / r_{jj}$
- END FOR

(Remember that Python doesn't have END FOR statements, but instead uses indentation to terminate code blocks. We'll write END statements for code blocks in pseudo-code in these notes.)

2.3 Projector interpretation of Gram-Schmidt

At each step of the Gram-Schmidt algorithm, a projector is applied to a column of A. We have

$$
\begin{aligned}
q_1 &= \frac{P_1 a_1}{\|P_1 a_1\|}, \\
q_2 &= \frac{P_2 a_2}{\|P_2 a_2\|}, \\
&\vdots \\
q_n &= \frac{P_n a_n}{\|P_n a_n\|},
\end{aligned}
$$

where P_j are orthogonal projectors that project out the first $j-1$ columns $(q_1, \ldots, q_{j-1})$ (P_1 is the identity as this set is empty when $j=1$). The orthogonal projector onto the first $j-1$ columns is $\hat{Q}_{j-1}\hat{Q}^*_{j-1}$, where

$$\hat{Q}_{j-1} = \begin{pmatrix} q_1 & q_2 & \ldots & q_{j-1} \end{pmatrix}.$$

Hence, P_j is the complementary projector, $P_j = I - \hat{Q}_{j-1}\hat{Q}^*_{j-1}$.

2.4 Modified Gram-Schmidt

There is a big problem with the classical Gram-Schmidt algorithm. It is unstable, which means that when it is implemented in inexact arithmetic on a computer, round-off error unacceptably pollutes the entries of Q and R, and the algorithm is not useable in practice. What happens is that the columns of Q are not quite orthogonal, and this loss of orthogonality spoils everything. We will discuss stability later in the course, but right now we will just discuss the fix for the classical Gram-Schmidt algorithm, which is based upon the projector interpretation which we just discussed.

To reorganise Gram-Schmidt to avoid instability, we decompose P_j into a sequence of $j-1$ projectors of rank $m-1$, that each project out one column of Q, i.e.

$$P_j = P_{\perp q_{j-1}} \ldots P_{\perp q_2} P_{\perp q_1},$$

where

$$P_{\perp q_j} = I - q_j q_j^*.$$

Then,

$$v_j = P_j a_j = P_{\perp q_{j-1}} \ldots P_{\perp q_2} P_{\perp q_1} a_j.$$

Here we notice that we must apply $P_{\perp q_1}$ to all but one columns of A, and $P_{\perp q_2}$ to all but two columns of A, $P_{\perp q_3}$ to all but three columns of A, and so on. In fact, the applying $P_{\perp q_j}$ to the first $j-1$ columns does nothing, because q_j is already orthogonal to all of those columns. Even further, it is actually a good thing, because it helps to keep all of the columns as orthonormal as possible under inexact arithmetic.

Hence, we can equivalently apply $P_{\perp q_1}$ to all columns of A, then obtain q_2 by normalising the second column, then apply $P_{\perp q_2}$ to all the columns of A, and obtain q_3 by normalising the second column and so on.

sequential transformations of A