# Lecture Notes for Math 104: Fall 2010 (Week 5)

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CHAPTER 1

# Thirteenth Lecture

We discussed the Gram-Schmidt Orthogonalization and began discussing the $QR$ factorization of a matrix.

## 1. Gram-Schmidt Orthogonalization

We've mentioned a number of times already that given a basis $\mathbf{v}_1, \ldots, \mathbf{v}_k$ of $E \subset \mathbb{C}^n$ one can construct an orthonormal basis $\mathbf{q}_1, \ldots, \mathbf{q}_k$ of $E$. We will give you a simple algorithm for doing this. By doing so we give a proof of the existence of such a basis (since we already know every space has some basis).

There are a number of ways to do this, I'm going to start with the *classical Gram-Schmidt* procedure. This is the easiest orthogonalization procedure from a theoretical point of view, however computationally it has some problems (it is unstable, in other words the rounding errors on a computer can cause major problems).

The basic idea is to start with a given basis and to produce an orthonormal basis. The method to do so is iterative. Namely let $\mathbf{v}_1, \ldots, \mathbf{v}_k$ be a basis of $E \subset \mathbb{C}^n$. We proceed as follows: Start with $\mathbf{v}_1$ and let $E_1 = \mathit{span}\,\{\mathbf{v}_1\}$. We want to find an orthonormal basis of $E_1$. This is easy: set $\mathbf{q}_1 = \mathbf{v}_1/||\mathbf{v}_1||_2$. Notice that $\mathbf{v}_1 \neq 0$ (otherwise it couldn't be part of a basis. Now let $E_2 = \mathit{span}(\mathbf{v}_1, \mathbf{v}_2) = \mathit{span}(\mathbf{q}_1, \mathbf{v}_2)$. We want to find an orthonormal basis of $E_2$ this is a little bit harder as $\mathbf{q}_1$ and $\mathbf{v}_2$ need not be orthogonal. But notice that $P_{\mathbf{q}_1}\mathbf{v}_2 \neq \mathbf{v}_2$ and if we let $\hat{\mathbf{q}}_2 = \mathbf{v}_2 - P_{\mathbf{q}_1}\mathbf{v}_2 = P_{\perp\mathbf{q}_1}\mathbf{v}_2 = \mathbf{v}_2 - \langle \mathbf{q}_1, \mathbf{v}_2\rangle \mathbf{q}_1$ then $\hat{\mathbf{q}}_2 \in E_2$ is non-zero and $\langle \mathbf{q}_1, \hat{\mathbf{q}}_2\rangle = 0$. Hence we can set $\mathbf{q}_2 = \hat{\mathbf{q}}_2/||\mathbf{q}_2||_2$. The reason this works is if $P_{\mathbf{q}_1}\mathbf{v}_2 = \mathbf{v}_2$ then one would have that $\mathbf{v}_2 \in \mathit{span}(\mathbf{q}_1) = \mathit{span}(\mathbf{v}_1)$ i.e. $\mathbf{v}_2$ and $\mathbf{v}_1$ would be linearly dependent.

Inductively, we have a method that takes $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ and gives $\{\mathbf{q}_1, \ldots, \mathbf{q}_l, \mathbf{v}_{l+1}, \ldots, \mathbf{v}_k\}$ where $E_j = \mathit{span}\,\{\mathbf{q}_1, \ldots, \mathbf{q}_j\} = \mathit{span}\,\{\mathbf{v}_1, \ldots, \mathbf{v}_j\}$ and $\{\mathbf{q}_1, \ldots, \mathbf{q}_j\}$ is an orthonormal basis of $E_j$ here $1 \leq j \leq l$. We now wish to produce $\mathbf{q}_{l+1}$ from $\mathbf{v}_{l+1}$ so that now $\mathbf{q}_1, \ldots, \mathbf{q}_{l+1}$ is a orthonormal basis for $E_{l+1} = \mathit{span}\mathbf{v}_1, \ldots, \mathbf{v}_{l+1}$.

To do this we again note that if we set $\hat{\mathbf{q}}_{l+1} = \mathbf{v}_{l+1} - P_{E_l}\mathbf{v}_{l+1} = \mathbf{v}_{l+1} - \sum_{j=1}^{l}\langle \mathbf{q}_j, \mathbf{v}_{l+1}\rangle \mathbf{q}_j$. Then $\hat{\mathbf{q}}_{l+1}$ is non-zero and orthogonal to each $\mathbf{q}_j$ $1 \leq j \leq l$. Setting $\mathbf{q}_{l+1} = \hat{\mathbf{q}}_{l+1}/||\hat{\mathbf{q}}_{l+1}||_2$. Then provides the iteative step. Again we have used the fact that the $\mathbf{v}_i$ are linearly independent to ensure that $\hat{\mathbf{q}}_{l+1} \neq 0$.

Iterating this $k$ times produces the desired $\mathbf{q}_1, \ldots, \mathbf{q}_k$.

We can write this algorithm in pseudo-code as:

For $j = 1$ to $k$ $\mathbf{a}_j = \mathbf{v}_j$
  For $i = 1$ to $j - 1$
    $r_{ij} = \mathbf{q}_i^*\mathbf{v}_j$
    $\mathbf{a}_j = \mathbf{a}_j - r_{ij}\mathbf{q}_i$
  $r_{jj} = ||\mathbf{a}_j||_2$ $\mathbf{q}_j = \mathbf{a}_j/r_{jj}$

Where this has numerical problems is when the $\mathbf{v}_i$ are close to parallel.

## 2. The QR factorization

We are now going to apply this idea of orthogonalization to a matrix. The idea is to look at a matrix $A \in \mathbb{C}^{m\times n}$ and try and get an orthonormal basis for the column space of $A$. But we are actually going to be more careful than that.

Consider the columns of $A$ so we have

$$A = \begin{bmatrix}\mathbf{a}_1 | & \cdots & | \mathbf{a}_n\end{bmatrix}$$

We get a whole sequence of spaces $E_1 = span(\mathbf{a}_1), E_2 = span(\mathbf{a}_1, \mathbf{a}_2), \ldots, E_n = span(\mathbf{a}_1, \ldots, \mathbf{a}_n)$. So $E_1 \subset E_2 \subset \ldots \subset E_n = R(A)$. What we want to do is in sense get an orthonormal basis for all of these subsets. That is find an orthonormal set $\mathbf{q}_1, \ldots, \mathbf{q}_k$ so that $E_1 = span(\mathbf{q}_1), E_2 = span(\mathbf{q}_1, \mathbf{q}_2), \ldots, E_n = span(\mathbf{q}_1, \ldots, \mathbf{q}_k)$. Being able to do this will be equivalent to given a good factorization of the matrix $A$. Notice that by a dimension count we are implicity assuming that the $\mathbf{a}_1, \ldots, \mathbf{a}_k$ are linearly independent.

Well starting from an arbitrary $A \in \mathbb{C}^{m\times n}$ and assume for this discussion that $m \geq n$ and that $A$ has full rank (i.e. $n$). This later condition implies that the columns are linearly independent. If we can find $\mathbf{q}_i \in \mathbb{C}^m$ as desired then we have

$$\mathbf{a}_1 = r_{11}\mathbf{q}_1, \mathbf{a}_2 = r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2, \ldots, \mathbf{a}_n = r_{1n}\mathbf{q}_1 + \ldots, r_{nn}\mathbf{q}_n$$

Notice this is equivalent to the matrix factorization

$$\begin{bmatrix}\mathbf{a}_1 | & \cdots & | \mathbf{a}_n\end{bmatrix} = \begin{bmatrix}\mathbf{q}_1 | & \cdots & | \mathbf{q}_n\end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & & & \\ & & & \\ \ddots & & \vdots & \\ 0 & \cdots & 0 & r_{nn} \end{bmatrix}$$

That is

$$A = \hat{Q}\hat{R}$$

where $\hat{Q} \in \mathbb{C}^{m\times n}$ has columns that are the orthonormal vectors $\mathbf{q}_i$ for $1 \leq i \leq n$ and $\hat{R} \in \mathbb{C}^{n\times n}$ is upper triangular. This is called the *reduced QR factorization*

For certain purposes it is convenient to have a different form of the factorization. That is we want to replace the $\hat{Q}$ term by a unitary term $Q$. As $m \geq n$, we can do this by adding extra elements to $Q$ that complete the columns fo $Q$ to an orthonormal basis of $\mathbb{C}^m$. Namely let $\mathbf{q}_{n+1}, \ldots, \mathbf{q}_m \in \mathbb{C}^m$ be an orthonormal basis of $R(A)^\perp = L - N(A)$. Then one has that $\mathbf{q}_1, \ldots, \mathbf{q}_m$ is an orthonormal basis of $\mathbb{C}^m$ so in particular

$$Q = \begin{bmatrix}\mathbf{q}_1 | & \cdots & | \mathbf{q}_m\end{bmatrix} \in \mathbb{C}^{m\times m}$$

Is unitary.

Then setting

$$R = \begin{bmatrix}\hat{R} \\ 0\end{bmatrix},$$

so $R \in C^{m\times n}$ is still upper triangular we obtain the full or unreduced $QR$ factorization as

$$A = QR.$$

Notice that the span of the "silent" columns in the full $QR$ factorization are precisely an orthonormal basis of $R(A)^{\perp} = L - Null(A)$.

One important geometric interpretation the full $QR$ factorization allows is the following: The range of the matrix $R$ is precisely the $n$-dimensional subspace of $\mathbb{C}^m$ where the last $m - n$ entries are zero. For instance if $m = 3$ and $n = 2$ then the range of $R$ is exactly the plane with third component zero. The matrix $Q$ then acts as a sort of "rotation" which allows us to obtain all other $n$-dimensional subspaces. One way to think of this is that the $Q$ tells us where $R(A)$ sits in $\mathbb{C}^m$ while $R$ tells us how vectors in $R(A)$ and in $\mathbb{C}^n$ are identified.

CHAPTER 2

# Fourteenth Lecture

We introduced the $QR$ factorization in the last lecture. We discuss it in a bit more depth.

## 1. The QR factorization

Recall, the $QR$ factorization worked by starting with a matrix $A \in \mathbb{C}^{m \times n}$ where $m \geq n$ and $A$ with full rank (i.e. $\dim R(A) = n$). We write

$$A = \begin{bmatrix} \mathbf{a}_1 | & \cdots & |\mathbf{a}_n \end{bmatrix}.$$

The *reduced $QR$ factorization* is a factorization:

$$A = \hat{Q}\hat{R}$$

where $\hat{Q} \in \mathbb{C}^{m \times n}$ has columns

$$\hat{Q} = \begin{bmatrix} \mathbf{q}_1 | & \cdots & |\mathbf{q}_n \end{bmatrix}$$

where $\{\mathbf{q}_i\} \in \mathbb{C}^m$ are an orthonormal set of vectors and $\hat{R} \in \mathbb{C}^{n \times n}$ is upper triangular. It is straight forward to verify that $span(\mathbf{a}_1, \cdots, \mathbf{a}_k) = span(\mathbf{q}_1, \cdots, \mathbf{q}_k)$ for $1 \leq k \leq n$.

For certain purposes it is convenient to have the so called *full $QR$ factorization* Here

$$A = QR$$

where

$$Q = \begin{bmatrix} \mathbf{q}_1 | & \cdots & |\mathbf{q}_n & \mathbf{q}_{n+1} | & \cdots & |\mathbf{q}_m \end{bmatrix}$$

is now in $\mathbb{C}^{m \times m}$ and is unitary. We then have $R \in \mathbb{C}^{m \times n}$ still upper triangular. Notice that then the bottom rows must be all zero then. The additional vectors $\mathbf{q}_{n+1}, \ldots, \mathbf{q}_m$ are "silent" and are arbitrary as long as they an orthonormal basis of $R(A)^{\perp} = L - Null(A)$.

We are also interested in the case where $A$ does not have full rank. In this case there is still a $QR$ factorization. We just have to modify our algorithm a bit.

THEOREM 1.1. *Every $A \in \mathbb{C}^{m \times n}$ with ($m \geq n$) has a full $QR$ factorization.*

PROOF. We will actually construct a reduced $QR$ factorization of $A$ and then complete it to a full $QR$ factorization as needed. The proof is just the Gram-Schmidt algorithm. However, we can no longer ensure that the columns of $A$ are linearly independent. In particular it may happen that $span(\mathbf{a}_1, \ldots, \mathbf{a}_j) = span(\mathbf{a}_1, \ldots, \mathbf{a}_{j+1})$.

More precisely. Start with $\mathbf{a}_1$ if $\mathbf{a}_1 = 0$ choose $\mathbf{q}_1$ an arbitrary unit vector and in this case take $r_{11} = 0$. If $\mathbf{a} \neq 0$ set $\mathbf{q}_1 = \mathbf{a}_1 / ||\mathbf{a}_1||_2$ take $r_{11} = ||\mathbf{a}_1||_2$. Notice in both cases:

$$\mathbf{a}_1 = r_{11}\mathbf{q}_1.$$

Now proceed inductively: That is suppose we've gotten $\mathbf{q}_1, \ldots, \mathbf{q}_k$ from $\mathbf{a}_1, \ldots, \mathbf{a}_k$. Notice that in this case $span(\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}) \supset span(\mathbf{a}_1, \ldots, \mathbf{a}_{j-1})$ We want to find $\mathbf{q}_j$. To do so, we (as before) set $r_{ij} = \langle \mathbf{a}_j, \mathbf{q}_j \rangle$ and $\hat{\mathbf{q}}_j = \mathbf{a}_j - \sum_i = 1^{j-1} r_{ij}\mathbf{q}_j$. By the bilinearity of the inner product $\langle \hat{\mathbf{q}}_j, \mathbf{a}_j \rangle = 0$. If $\hat{\mathbf{q}}_j = 0$ we take $r_{jj} = 0$ and pick $\mathbf{q}_j$ to be any unit vector orthogonal to $\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}$ otherwise set $r_{jj} = ||\hat{\mathbf{q}}_j||_2$ and $\mathbf{q}_j = r_{jj}^{-1}\hat{\mathbf{q}}_j$. Then

$$\mathbf{a}_j = \sum_{i=1}^{j} r_{ij}\mathbf{q}_j$$

Hence, if we set

$$\hat{Q} = \begin{bmatrix} \mathbf{q}_1 | & \ldots & \mathbf{q}_n \end{bmatrix}$$

and

$$\hat{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & r_{nn} \end{bmatrix}$$

we obtain a reduced $QR$ factorization of $A$. To get the full $QR$ factorization we can add the silent columns as before. That is we find $\mathbf{q}_{n+1}, \ldots, \mathbf{q}_m$ forming an orthonormal basis of $span(\mathbf{q}_1, \ldots, \mathbf{q}_m)$. □

Remark 1.2. Notice that $R(A) \subset span(\mathbf{q}_1, \ldots, \mathbf{q}_m)$ with equality only when $A$ has full rank. One consequence is that the silent columns $\mathbf{q}_{n+1}, \ldots, \mathbf{q}_m$ while lying in $L - Null(A)$ no longer need to form a basis. Another consequence is that $A$ has full rank when and only when $r_{ii} \neq 0$ for all $i = 1, \cdots, n$.

Remark 1.3. One may wonder how to find $\mathbf{q}_j$ when $r_{jj} = 0$. Notice that we want $\mathbf{q}_j$ to be orthogonal to each $\mathbf{q}_i$ for $1 \leq i \leq j-1$. That is if we set

$$\hat{Q}_{j-1} = \begin{bmatrix} \mathbf{q}_1 | & \cdots & \mathbf{q}_{j-1} \end{bmatrix} \in \mathbb{C}^{m \times (j-1)}$$

we need $\hat{Q}_{j-1}\mathbf{q}_j = 0$ and $||\mathbf{q}_j||_2 = 1$. Another way to think about this that $\mathbf{q}_j \in \hat{Q}^*_{j-1})$ so $\mathbf{q}_j$ can be found by Gaussian elimination (though there is likely a more efficient algorithm).

The full $QR$ factorization tends not to be unique. This is because silent columns are not specified by the algorithm. While this is not an issue with the reduced $QR$ factorization. There is still non-uniqueness in this case. To see this, note one can multiply the $i$th column of $\hat{Q}$ by some $\lambda \in \mathbb{C}$ so that $|\lambda| = 1$ and get a new matrix $\hat{Q}'$ which still has orthonormal columns, if one multiplies the $i$th row of $\hat{R}$ by $\lambda^{-1}$ to get $\hat{R}'$ then this is still upper triangular and $\hat{Q}\hat{R} = \hat{Q}'\hat{R}'$. This corresponds to the arbitrary choice that one makes in the Gram-Schmidt algorithm.

However, there is uniqueness if $A$ is full rank and one demands $\hat{R}$ have a special form.

Theorem 1.4. *For each $A \in Cx^{m \times n}$ with $m \geq n$ and so that $A$ has full rank there is a unique reduced QR factorization*

$$A = \hat{Q}\hat{R}$$

*So that the diagonal entries of $\hat{R}$ are positive real numbers (i.e. $r_{ii} > 0$).*

PROOF. If we look at the proof of the preceeding theorem we see that everything is determined except the"sign" of $r_{ii}$. If we insist that $r_{ii} > 0$ then we are done. $\square$

## 2. Solving a System via $QR$ factoriation.

One thing the $QR$ factorization allows us to do is to solve systems. Let $A \in \mathbb{C}^{m\times m}$ be non-singular matrix (i.e. of full rank). And fix $\mathbf{b} \in \mathbb{C}^m$. We want to solve

$$A\mathbf{x} = \mathbf{b}$$

The usual way is to use Gaussian elimination, which in a sense is a better approach to this specific problem. First theroem of this lecture there is a $QR$ factorization of $A$ and as $m = n$ the reduced is the same as the full so we write

$$A = QR$$

Here $Q$ is unitary and $R$ is upper triangular with no non-zero entries on the diagonal. This latter fact follows as $A$ is non-singular.

Hence, one has

$$R\mathbf{x} = Q^*\mathbf{b}$$

Now we are solving a system of equations where the system consists of an upper triangular matrix. This can easily be solved by back-substitution.

An example: Let

$$A = \begin{bmatrix} 0 & -3 & 0 \\ 0 & 4 & 1 \\ 4 & 0 & 1 \end{bmatrix}$$

And lets solve

$$A\mathbf{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

To start

$$\mathbf{a}_1 = \begin{bmatrix} 0 \\ 0 \\ 4 \end{bmatrix} \Rightarrow \mathbf{q}_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

and so $r_{11} = 4$. Now $\langle \mathbf{a}_2, \mathbf{q}_1 \rangle = 0$ and so $r_{12} = 0$ and

$$\mathbf{q}_2 = \begin{bmatrix} -3/5 \\ 4/5 \\ 0 \end{bmatrix}$$

and $r_{22} = 5$. Finally, $\langle \mathbf{a}_3, \mathbf{q}_1 \rangle = 1$ and $\langle \mathbf{a}_3, \mathbf{q}_2 \rangle = 4/5$ so $r_{13} = 1$ and $r_{23} = 4/5$ thus

$$\hat{\mathbf{q}}_3 = \begin{bmatrix} 12/25 \\ 9/25 \\ 0 \end{bmatrix}$$

so $r_{33} = 3/5$ and

$$\mathbf{q}_3 = \begin{bmatrix} 4/5 \\ 3/5 \\ 0 \end{bmatrix}$$

Hence

$$A = \begin{bmatrix} 0 & -3/5 & 4/5 \\ 0 & 4/5 & 3/5 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 & 0 & 1 \\ 0 & 5 & 4/5 \\ 0 & 0 & 3/5 \end{bmatrix}$$

And so

$$R\mathbf{x} = A^*\mathbf{b} = \begin{bmatrix} 0 & 0 & 1 \\ -3/5 & 4/5 & 0 \\ 4/5 & 3/5 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -3/5 \\ 4/5 \end{bmatrix}$$

Then

$$\begin{bmatrix} 4 & 0 & 1 \\ 0 & 5 & 4/5 \\ 0 & 0 & 3/5 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 0 \\ -3/5 \\ 4/5 \end{bmatrix}$$

So $x_3 = 4/3$, $5x_2 = -3/5 - 16/15 = -5/3$ so $x_2 = -1/3$. Then $4x_1 = -4/3$ so

$$\mathbf{x} = \begin{bmatrix} -1/3 \\ -1/3 \\ 4/3 \end{bmatrix}$$

CHAPTER 3

# Fifteenth Lecture

We use the $QR$ factorization to study a problem about solve overdetermined systems of linear equations "approximately"..

## 1. Least Squares Method

Recall we say that a system of linear equations is overdetermined if there are more equations then unknowns. That is one has $A \in \mathbb{C}^{m \times n}$ with $m > n$ and look at

$$A\mathbf{x} = \mathbf{b}$$

for a fixed $\mathbf{b} \in \mathbb{C}^m$. By the rank-nullity theorem $dim R(A) \leq n < m$ so for "most" $\mathbf{b}$ this equation has no solution.

In this case what we do is study the so called *residual*

$$\mathbf{r} = \mathbf{b} - A\mathbf{x} \in \mathbb{C}^m$$

The idea is to try and find the $\mathbf{x}$ that makes the residual as small as possible.

In order to do this we need to have a notion of "size" for vectors. We will discuss this more later but for now we take the 2-norm, that is we try and minimize:

$$||\mathbf{b} - A\mathbf{x}||_2.$$

That is we try and find $\mathbf{x}$ so that $\mathbf{r}$ has least length, in other words so$A\mathbf{x}$ is the closest vector in $R(A)$ to $\mathbf{b}$. This turns out to be natural from both geometric point of view and from more experience. It also has the advantage of being mathematically and algorithmically very tractable.

So how do we find the $\mathbf{x}$ that minimizes the residual? It turns out that there is a nice characterization in terms of linear algebra that we have already developed:

Theorem 1.1. *Let $A \in \mathbb{C}^{m \times n}$ $(m \geq n)$ and $\mathbf{b} \in \mathbb{C}^m$. A vector $\mathbf{x} \in \mathbb{C}^n$ minimizes the residual $||\mathbf{r}||_2 = ||\mathbf{b} - A\mathbf{x}||_2$ if and only if $\mathbf{r}$ is orthogonal to $R(A)$ that is $\mathbf{r} \in L - Null(A)$ (i.e. $A^*\mathbf{r} = 0$).*

Proof. $\Rightarrow$ By our hypothesis for any $\mathbf{y} \in R(A)$, and $t \in \mathbb{R}$ for $t \neq 0$ then $||\mathbf{b} - (A\mathbf{x} + t\mathbf{y})||_2 \geq ||\mathbf{r}||_2$. We can square both sides so obtain:

$$\begin{aligned} ||\mathbf{b} - A\mathbf{x} - t\mathbf{y}||_2^2 &\geq ||\mathbf{r}||_2^2 \\ ||\mathbf{r} - t\mathbf{y}||_2^2 &\geq ||\mathbf{r}||_2^2 \\ ||\mathbf{r}||_2^2 - t(\langle \mathbf{r}, \mathbf{y}\rangle + \langle \mathbf{y}, \mathbf{r}\rangle + t^2||\mathbf{y}||_2^2 &\geq ||\mathbf{r}||_2^2 \end{aligned}$$

Here the last line follows by expanding out the inner product. Thus, after dividing by $t$ (since it is not 0)

$$-(\langle \mathbf{r}, \mathbf{y}\rangle + \langle \mathbf{y}, \mathbf{r}\rangle) + t||\mathbf{y}||_2^2 \geq 0.$$

By letting $t \to 0$ get

$$-(\langle \mathbf{r}, \mathbf{y}\rangle + \langle \mathbf{y}, \mathbf{r}\rangle) \geq 0$$

Notice that by replacing $\mathbf{y}$ by $-\mathbf{y}$ be get

$$\begin{aligned} -(\langle \mathbf{r}, -\mathbf{y}\rangle + \langle -\mathbf{y}, \mathbf{r}\rangle) &\geq 0 \\ \langle \mathbf{r}, \mathbf{y}\rangle + \langle \mathbf{y}, \mathbf{r}\rangle &\geq 0 \end{aligned}$$

So $\langle \mathbf{r}, \mathbf{y}\rangle + \langle \mathbf{y}, \mathbf{r}\rangle = (\langle \mathbf{r}, \mathbf{y}\rangle + \overline{\langle \mathbf{r}, \mathbf{y}\rangle} = 0$ this means $\langle \mathbf{r}, \mathbf{y}\rangle$ is purely imaginary. By replacing $\mathbf{y}$ by $\pm\mathbf{y}$ be get

$$\begin{aligned} -(\langle \mathbf{r}, \pm I\mathbf{y}\rangle + \langle \pm I\mathbf{y}, \mathbf{r}\rangle) &\geq 0 \\ -(\pm I\langle \mathbf{r}, \mathbf{y}\rangle \mp I\langle \mathbf{y}, \mathbf{r}\rangle) &\geq 0 \\ \mp I(\langle \mathbf{r}, I\mathbf{y}\rangle - \langle I\mathbf{y}, \mathbf{r}\rangle) &\geq 0 \end{aligned}$$

This implies $\langle \mathbf{r}, \mathbf{y}\rangle$ is purely real and hence combining with the above is 0.

$\Leftarrow$. We need to show that if $\mathbf{r}$ is orthogonal to $R(A)$ then for any point $\mathbf{y} \in R(A)$ one has $||\mathbf{b} - \mathbf{y}||_2 \geq ||\mathbf{r}||_2$. To do so we note that $A\mathbf{x} - \mathbf{y} \in R(A)$ and $\mathbf{b} - A\mathbf{x} = \mathbf{r}$ is orthogonal to this so

$$||\mathbf{b} - \mathbf{y}||_2^2 = ||\mathbf{b} - A\mathbf{x} + A\mathbf{x} - \mathbf{y}||_2^2 = ||\mathbf{b} - A\mathbf{x}||_2^2 + ||A\mathbf{x} - \mathbf{y}||_2^2 \geq ||\mathbf{r}||_2^2$$

Here we used the Pythagorean theorem. □

A useful consequence of this theorem is then: Let $P \in \mathbb{C}^{m\times m}$ be a orthogonal projection onto $R(A)$. Then $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ minimizes the residual norm if and only if $\mathbf{x}$ solves

$$A\mathbf{x} = P\mathbf{b}.$$

which we know has at least one solution (since $P\mathbf{b} \in R(A)$). Notice that $\mathbf{x}$ is unique when only when $N(A) = \{0\}$ i.e. if $A$ has full rank. We will usually assume this.

One other way to think about this is as a *right approximate inverse* Idea is let $A \in \mathbb{C}^{m\times n}$ with $m \geq n$ and $A$ of full rank. For each $\mathbf{e}_i$ a standard basis vector of $\mathbb{C}^m$ let $\mathbf{b}_i$ be the unique vector in $\mathbb{C}^n$ so that

$$A\mathbf{b}_i = P\mathbf{e}_i$$

and set

$$B = \begin{bmatrix}\mathbf{b}_1 | & cdots & |\mathbf{b}_m\end{bmatrix} \in \mathbb{C}^{n\times m}$$

Now $AB = P$. In other words, if we let $Q$ be the compelementary projector to $P$ (so $Q$ projects orthogonally onto $R(A)^\perp = L - Null(A)$ then

$$AB = I - Q$$

So for instance if the left null space is zero we have an actual inverse.

## 2. Least Squares from $QR$ factorization

So how do we use this in practice? We need to find the the projection onto $R(A)$. The key is getting an orthonormal basis. We've used this before (but maybe not said it so clearly). Basically, let $\mathbf{v}_1, \ldots, \mathbf{v}_k$ be an orthonormal basis of $R(A)$. Then one checks that

$$P = \sum_{i=1}^{k} \mathbf{v}_i\mathbf{v}_i^* = VV^* \in \mathbb{C}^{m\times m}$$

gives orthogonal projection onto $R(A)$. It suffices to verify that $P^2 = P$, $P^* = P$ and that $R(P) = R(A)$. I leave this as an excersize.

Thus we need to find an orthonormal basis of $R(A)$. The $QR$ factorization provides a good way to do this. To make this work we need to work with full rank $A$ in $\mathbb{C}^{m\times n}$ $(m \geq n)$. If we take the reduced $QR$ factorization ie.

$$A = \hat{Q}\hat{R}$$

then if we set

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

then $P \in \mathbb{C}^{m\times m}$ is orthogonal projection onto $R(A)$. (Recall the columns of $\hat{Q}$ are an orthonormal basis of $R(A)$). Notice if $A$ is not full rank, then we can't ensure that the columns of $\hat{Q}$ are not necessarily inside of $R(A)$. This is one reason to start with $A$ of full rank. So we are solving

$$\hat{Q}\hat{R}\mathbf{x} = P\mathbf{b} = \hat{Q}\hat{Q}^*\mathbf{b}.$$

That is

$$\hat{Q}\hat{R}\mathbf{x} - P\mathbf{b} = \hat{Q}\hat{Q}^*\mathbf{b} = \hat{Q}\left(\hat{R}\mathbf{x} - \hat{Q}^*\mathbf{b}\right) = 0.$$

As $\hat{Q}$ has columns which are orthonormal, the columns are all linearly independent so $N(\hat{Q}) = 0$. Thus the equation we want to solve is:

$$\hat{R}\mathbf{x} = \hat{Q}^*\mathbf{b}.$$

This yields the following algorithm for solving the problem (at least for full rank $A \in \mathbb{C}^{m\times n}$):

(1) Compute the (reduced) QR factorization $A = \hat{Q}\hat{R}$.
(2) Compute the vector $\mathbf{b}' = \hat{Q}^*\mathbf{b}$
(3) Solve the upper-triangular system $\hat{R}\mathbf{x} = \mathbf{b}'$.

Notice that (1) is the most computationally intensive step. We can do it by either the Gram-Schmidt algorithm already discussed or some other approachs we discuss in the next lecture. For the last step one uses back substitution.

## 3. Application:NIC

Least-Squares is used in many different contexts. I'll present one important instance, namely fitting a polynomial to data. The basic set is to start with $m$ points $(x_1, y_1), \ldots, (x_m, y_m)$ in $\mathbb{R}^2$ (or $\mathbb{C}^2$). We assume $x_i \neq x_j$ for $i \neq j$. With out this hypthoesesis the points wouldn't lie on any graph of any function of $x$. We look for a polynomial $P$ of degree $n-1$ so that $P(x_i) = y_i$.

If we write

$$P(x) = c_0 + c_1 x + \ldots + c_{n-1}x^{n-1}$$

then we are looking for $c_0, \ldots, c_{n-1}$ so that $P(x_i) = y_y$. Finding such $c_i$ is a linear problem (even though polynomials tend to be very non-linear). Indeed, if we write:

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & & & & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^{n-1} \end{bmatrix} \begin{bmatrix} c_0 \\ \vdots \\ c_{n-1} \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

We see we are really solving a system of linear equations. We shorten this to

$$X\mathbf{c} = \mathbf{y}$$

Here $X \in \mathbb{C}^{m \times n}$ is the called the Vandermonde matrix.

It turns out that the condition that $x_i \neq x_j$ implies that $X$ is full rank (Excercise!). In particular, if $m = n$ we can always find the desired $P$ so taht $P(x_i) = y_i$.

It turns out choosing such a polynomial is less than ideal. The problem is that the graph doesn't interpolate the points well. That is, in between adjacent values $x_1, x_2$ the graph might become very far from $y_1$ and $y_2$. A related issue is that if the $x_i$ and $y_i$ are changed slightly, the approximating polynomial might change radically. Since data is noisy this is not desirable. It turns out that this issue is lessened if one uses a lower degree polynomial. That is take $m < n$. In this case one has an overdetermined system of equations so one has to look at "approximate" solutions as above.