# Numerical Analysis

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## Contents

# 1 Introduction

This course is an introduction to numerical analysis and is built on top of last term's linear algebra on which many concepts will reappear. This time however, we will mostly work in specific spaces rather than arbitrary inner product spaces. We will also consider issues of implementing algorithms and their ability to scale to large problems. This will be achieved by examining their efficiency, accuracy and stability. We will also consider typical numerical concepts such as iterations, conditioning, error analysis and operations count.

As a outline, we will first delve into numerical linear algebra, in which we will study orthogonalisation, least-squares problems, linear equations and factorisations. We will the move on to gradients and hessians, interpolations with orthogonal and non-orthogonal polynomials, Fourier series and lastly, numerical integration.

We will in this course mostly deal with the vector space $\mathbb{R}^n$ while unless mentioned otherwise, algorithms can easily extended to $\mathbb{C}^n$. We will use inner product and dot product interchangeably and define the outer product (tensor product) between two vectors $\mathbf{a}, \mathbf{b}$ to be the matrix $\mathbf{a} \otimes \mathbf{b} = \mathbf{a}\mathbf{b}^T = A \in M_n(\mathbb{R})$ where $A_{ij} = a_i b_j$. We also note that the dot product on the reals form a bilinear form, and so all associated properties apply.

Lastly, we define the $i$-th standard basis $e_i \in \mathbb{R}^n$ as the vector with the $j$-th entry equal to the $ij$-Kronecker delta. That is, $[e_i]_j = 1$ is $i = j$ and 0 otherwise. This is a nice set of basis as it is orthonormal and given some vector $\mathbf{v}$, the dot product $\langle e_i, \mathbf{v} \rangle$ is the $i$-th entry of $\mathbf{v}$.

# 2 Numerical Linear Algebra

## 2.1 Orthogonalisation

We would like to find an orthogonal basis from a set of linearly independent vectors. As, simply by normalising the resulting vectors, we also obtain an orthonormal basis. From first year, we know that this can be achieved through the Gram-Schmidt process while we will also take a look at another method which utilises the Householder transformation. In both cases, the methods are related to the QR-decomposition of a square matrix.

Suppose we have a set of $n$ linearly independent vectors $\{a_k\}_{k=1}^n$ in the $m$-dimensional space $\mathbb{R}^m$ where $n \leq m$. It is often advantageous to convert this set of vectors into an orthonormal basis such that the span of this basis is the same as the span of $\{a_k\}_{k=1}^n$.

To achieve this, we propose the first procedural method – the *classical Gram-Schmidt* (cGS) procedure.

**Algorithm 1** (Classical Gram-Schmidt Procedure)**.** Given a set of $n$ linearly independent vectors $\{\mathbf{a}_k\}_{k=1}^n$ in the $m$-dimensional space $\mathbb{R}^m$, we obtain an orthonormal basis of $\mathrm{sp}\{\mathbf{a}_k\}_{k=1}^n$.

1. Let $\mathbf{v}_1 := \mathbf{a}_1; \mathbf{q}_1 := \mathbf{v}_1/\|\mathbf{v}_1\|$. We call $\mathbf{v}_1$ the preliminary vector.
2. For $k = 2, \cdots, n$, let $\mathbf{v}_k := \mathbf{a}_k - \sum_{l=1}^{k-1} \langle \mathbf{a}_k, \mathbf{q}_l \rangle \mathbf{q}_l$; $\mathbf{q}_k := \mathbf{v}_k/\|\mathbf{v}_k\|$, that is, we define $\mathbf{v}_k$ such that it is orthogonal to all previous $\mathbf{q}_l$ while we normalise $\mathbf{v}_k$ resulting in $\mathbf{q}_k$.

Then, by the above procedure $\{\mathbf{q}_k\}_{k=1}^n$ is the required set of vectors.

Let us recall the proof for the correctness of the classical Gram-Schmidt procedure.

*Proof.* Normality and span (as $\mathbf{q}_k$ is a linear combination of $\mathbf{a}_i$ where $i \leq k$) is trivial so we shall show orthogonality.

We induction on $n$. For $n = 1$, orthogonality is trivial so let us assume the inductive hypothesis and suppose $n = i+1$. By the inductive hypothesis, the Gram-Schmidt procedure will result us with $\{\mathbf{q}_k\}_{k=1}^i$ – an orthonormal basis of $\mathrm{sp}\{\mathbf{a}_k\}_{k=1}^i$, and so, it suffices to show,

$$\langle \mathbf{q}_j, \mathbf{v}_{i+1} \rangle = \left\langle \mathbf{q}_j, \mathbf{a}_{i+1} - \sum_{l=1}^{i} \langle \mathbf{a}_{i+1}, \mathbf{q}_l \rangle \mathbf{q}_l \right\rangle = 0,$$

for all $j = 1, \cdots, i$. But, this is true as,

$$\left\langle \mathbf{q}_j, \mathbf{a}_{i+1} - \sum_{l=1}^{i} \langle \mathbf{a}_{i+1}, \mathbf{q}_l \rangle \mathbf{q}_l \right\rangle = \langle \mathbf{q}_j, \mathbf{a}_{i+1} \rangle - \sum_{l=1}^{i} \langle \mathbf{a}_{i+1}, \mathbf{q}_l \rangle \langle \mathbf{q}_j, \mathbf{q}_l \rangle = \langle \mathbf{q}_j, \mathbf{a}_{i+1} \rangle - \langle \mathbf{q}_j, \mathbf{a}_{i+1} \rangle = 0,$$

where the second equality holds since by the inductive hypothesis $\langle q_j, q_l \rangle = \delta_{jl}$. □

While we have proved the correctness of the algorithm, the question remains on whether or not we can always perform such an procedure. We see that, by induction, to see that the algorithm can always be performed, it suffices to show that there does not exists a case where $\mathbf{v}_2 \neq 0$ (we can then apply induction).

Suppose $\mathbf{v}_2 = 0$, then $\mathbf{a}_2 - \langle \mathbf{a}_2, \mathbf{q}_1 \rangle \mathbf{q_1} = 0$. But this would mean $\mathbf{a}_2$ is a multiple of $\mathbf{q}_1$ which is in turn a multiple of $\mathbf{a}_1$, contradicting the linearly independent assumption. So, this cannot occur and so cGS can always be performed.

While the cGS is mathematically correct, when implementing the algorithm on computers, it is possible to find special cases where the cGS suffers from accuracy and stability. As we shall see on in an exercise, it is possible to construct a slightly different version of the Gram-Schmidt procedure – *modified Gram-Schmdit* (mGS) such that this is no longer a problem.

## 2.2 QR-Decomposition I

The QR-decomposition is a very important decomposition in numerical analysis and we shall, in fact, look at two methods of achieving the QR-decomposition, and hence the name of this section. The QR-decomposition decomposes a matrix into the product of two matrices $Q$ and $R$ where $Q$ is orthogonal and $R$ is upper triangular.

Suppose we have the linearly independent sequence of vectors $\{\mathbf{a}_k\}_{k=1}^n$ and the orthonormal basis of this resulted from Gram-Schmidt $\{\mathbf{q}_k\}_{k=1}^n$ in $\mathbb{R}^m$. Then by defining

$$A := (\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n) \in \mathbb{R}^{m\times n},$$

and similarly,

$$Q := (\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n) \in \mathbb{R}^{m\times n},$$

we seek to establish the relation $R \in \mathbb{R}^{n\times n}$ such that $A = QR$. Indeed, by considering the classical Gram-Schmidt procedure, where

$$\mathbf{v}_k := \mathbf{a}_k - \sum_{l=1}^{k-1} \langle \mathbf{a}_k, \mathbf{q}_l\rangle \mathbf{q}_l,$$

we see that $\mathbf{a}_j$ is a linear combination of $\mathbf{q}_i$ where $j \leq i$, and so it follows that $R$ is upper triangular.

Suppose we denote the $ij$-th entry of $R$ as $r_{ij}$, then $\mathbf{a}_k = \sum_{l=1}^{k} r_{lk}\mathbf{q}_l$, by the definition of matrix multiplication. Since $\mathbf{q}_1 = \mathbf{a}_1/\|\mathbf{a}_1\|$, we have $\mathbf{a}_1 = \|\mathbf{a}_1\|\mathbf{q}_1$, and so, $r_{11} = \|\mathbf{a}_1\|$. Similarly, for $\mathbf{a}_k$, we have

$$\mathbf{a}_k := \mathbf{v}_k + \sum_{l=1}^{k-1} \langle \mathbf{a}_k, \mathbf{q}_l\rangle \mathbf{q}_l,$$

where $\mathbf{v}_k = \|\mathbf{v}_k\|\mathbf{q}_k$, so,

$$\mathbf{a}_k := \|\mathbf{v}_k\|\mathbf{q}_k + \sum_{l=1}^{k-1} \langle \mathbf{a}_k, \mathbf{q}_l\rangle \mathbf{q}_l.$$

Thus, by comparing coefficients, we find $\|\mathbf{v}_k\| = r_{kk}$ and $\langle \mathbf{a}_k, \mathbf{q}_l\rangle = r_{lk}$ for $1 \leq l < k$. With this, using Gram-Schmdit, we have found a method to decompose a matrix as a product of an orthogonal and an upper triangular matrix.

However, the question of why this decomposition is importan remains. Suppose we would like to solve the linear system $A\mathbf{x} = \mathbf{b}$ (where $A$ has full rank). If we have a QR-decomposition on $A$, say $A = QR$, then the problem becomes $QR\mathbf{x} = \mathbf{b}$. As $Q$ is orthogonal, $Q^TQ = I$ and so,

$$\mathbf{d} := Q^T\mathbf{b} = Q^TQR\mathbf{x} = R\mathbf{x}.$$

Now, as $R$ is upper triangular, the linear system $R\mathbf{x} = \mathbf{d}$ becomes easy to solve by **backwards substitution**; that is, since $R$ is upper triangular, we have

$$x_n = d_n / r_{nn},$$

and

$$x_k = \frac{1}{r_{kk}} \left( d_k - \sum_{i=k+1}^{n} r_{ki} x_i \right).$$

We note that we claimed $Q$ is orthogonal throughout the argument. This is true as the column vectors are orthonormal, and hence, by the definition of matrix multiplication, we have

$$[Q^T Q]_{ij} = \langle \mathbf{q}_i, \mathbf{q}_j \rangle = \delta_{ij},$$

and so $Q^T Q = I$.

Indeed, the orthogonal matrices are a nice set of matrices and and the dot product and hence the norm is invariant under transformations by orthogonal matrices. Indeed,

$$\langle Q\mathbf{x}, Q\mathbf{y} \rangle = \mathbf{x}^T Q^T Q \mathbf{y} = \mathbf{x}^T \mathbf{y} = \langle \mathbf{x}, \mathbf{y} \rangle.$$

By thinking in Euclidean spaces, we see that these types of transformations are rotations and so, the transformations induced by an orthogonal matrix is often refereed as a rotation.

## 2.3 Projectors and QR-decomposition II

Having established one algorithm for computing the QR-decomposition, we will now design a second and complementary method to accomplish the same task. The second method will depend on *projectors* and *reflectors* so we will discuss them first.

**Definition 2.1** (Projector)**.** A matrix $P \in M_n(\mathbb{R})$ is a projector if

$$P^2 = P.$$

A projector matrix is refereed to as being idempotent.

Given a projector $P$, the matrix $I - P$ is also a projector. Indeed,

$$(I - P)^2 = I^2 - 2P + P^2 = 1 - P.$$

The matrix $I - P$ is refereed to as the *complementary projector* to $P$.

Straight away, we see that if a projector has full rank, than $P^2 = P \implies P^{-1}P^2 = P^{-1}P \implies P = I$, resulting in the trivial projector with the complementary projector the zero map $\mathbf{0}$. So, assuming a projector is non-trivial, then as $P$ maps the vector space onto $\mathrm{Im}P$, we may interpret geometrically that $P$ *projects* vectors onto its image.

**Definition 2.2** (Orthogonal Projector)**.** A projector $P$ is called an orthogonal projector if $P^T = P$.

As the name might suggest, if $P$ is an orthogonal projector, then $P$ projects vectors onto its image orthogonally. Indeed, if $\langle \cdot, \cdot \rangle$ is the dot product, then

$$\langle P\mathbf{v}, P\mathbf{v} - \mathbf{v} \rangle = \langle P\mathbf{v}, P\mathbf{v} \rangle - \langle P\mathbf{v}, \mathbf{v} \rangle = \mathbf{v}^T P^T P\mathbf{v} - \mathbf{v}^T P^T \mathbf{v} = \mathbf{v}^T P^2 \mathbf{v} - \mathbf{v}^T P\mathbf{v} = 0.$$

Furthermore, for an orthogonal projector $P$, its image and the image of its complementary projector are perpendicular. Say, if $\mathbf{x}, \mathbf{y}$ are vectors, then

$$\langle P\mathbf{x}, (I - P)\mathbf{y} \rangle = \mathbf{x}^T P^T (I - P)\mathbf{y} = \mathbf{x}^T (P - P^2)\mathbf{y} = 0.$$

There are many methods to construct orthogonal projectors. One simple method is to realise that, for all normalised vector $\mathbf{q}$, the outer product of $\mathbf{q}$ with itself is in fact an orthogonal projector. To see this, we have, for all $\mathbf{v}$, if $P = \mathbf{q} \otimes \mathbf{q}$,

$$P^2 = \mathbf{q}\mathbf{q}^T \mathbf{q}\mathbf{q}^T = \mathbf{q}\langle \mathbf{q}, \mathbf{q} \rangle \mathbf{q}^T = \mathbf{q}\mathbf{q}^T = P,$$

and

$$P\mathbf{v} = \mathbf{q}\mathbf{q}^T \mathbf{v} = \langle \mathbf{v}, \mathbf{q} \rangle \mathbf{q}.$$

Using this concept of projectors, we can find an different method for computing the QR-decomposition of an arbitrary matrix. Specifically, the method uses the *Householder reflectors*. As a general outline, this second method achieves the QR-decomposition by sequentially applying orthogonal matrices onto $A$, eventually resulting in a upper triangular matrix.

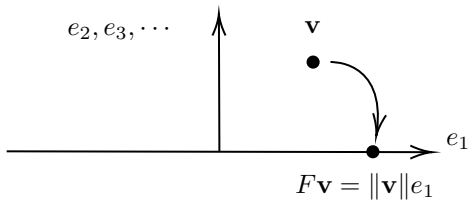
$$A = \begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix} \xrightarrow{Q_1} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{pmatrix} \xrightarrow{Q_2} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{pmatrix} \xrightarrow{Q_3} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{pmatrix} = R$$

With this in mind, we see that the orthogonal matrices $Q_k$ does not change the first $k-1$ rows, and so $Q_k = I_{k-1} \oplus F_{n-k+1}$ where $F_{n-k+1}$ introduces zeros in the lower $n-k$ rows and are refereed to as the *Householder reflectors*.

Since the Householder reflectors are constrained by the fact that they are orthogonal, they must preserve the lengths of the vectors it acts on. So, as we require the Householder reflectors to introduce zeros, the vectors it acted on is therefore in the form

$$F\mathbf{x} = F(\times, \times, \times, \cdots)^T = (\|\mathbf{x}\|, 0, 0, \cdots)^T.$$

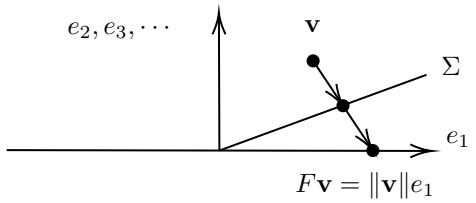
Geometrically consider the following diagram where we have labelled the first basis on one axis and the remaining bases on the other. We would like to find a mapping $F$ such that $\mathbf{v}$ is mapped onto the horizontal axis. Since $F$ needs to be orthogonal, the natural candidate for $F$ is a rotation. To achieve this, we may construct a hyperplane $\Sigma$, between $\mathbf{v}$ and $F\mathbf{v}$, and by reflecting $\mathbf{v}$ by $\Sigma$, the transformation is equivalent to a single rotation.



Suppose we define $\mathbf{w} = \|\mathbf{v}\|e_1 - \mathbf{v}$, then, we have $\mathbf{w}$ is orthogonal to the hyperplane $\Sigma$. With that in mind, we see that the image of the projector defined by

$$P' = \frac{\mathbf{w}\mathbf{w}^T}{\mathbf{w}^T\mathbf{w}}$$

is the plane orthogonal to $\Sigma$. Hence, the projector to $\Sigma$ is simply the complementary projector to $P'$, $P = I - P'$.

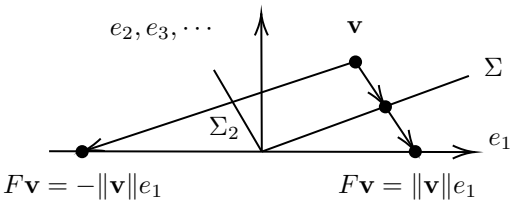



However, we do not wish to project into $\Sigma$ but to reflect around it. Thus, to reflect around $\Sigma$ we projecting twice as the distance in the same direction. This results in the desired Householder reflector,

$$F = I - 2\frac{\mathbf{w}\mathbf{w}^T}{\mathbf{w}^T\mathbf{w}},$$

where $\mathbf{w} = \|\mathbf{v}\|e_1 - \mathbf{v}$.

We note that this is not the only possible reflection as we may reflect around the hyperplane $\Sigma_2$ as demonstrated in the figure below.




Mathematically, the choice does not matter as both transformations results in the vector with only components in $e_1$, however, as often times in numerical analysis, we need to consider the computers in computing these values. Indeed, by considering that if we reflect by a plane which is almost parallel to the $e_1$-axis, the computer is required to work with large numbers and so, could possible encounter cancellation errors. Thus, it is usually better to choose the shallow plane to reflect around.

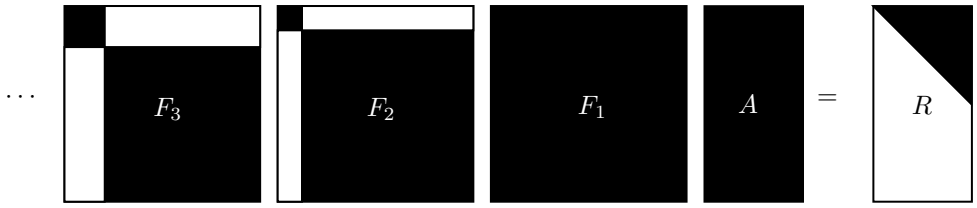
With that, we arrive at the Householder-based QR-decomposition.

**Algorithm 2** (Householder-based QR-decomposition)**.** If $A \in M_{m\times n}(\mathbb{R})$ be the matrix we are decomposing, then, for $k = 1, \cdots n$, we define

- $\mathbf{x} := A_{k:m,k}$ that is, the $k$ to $m$-th entry of the $k$-th row of $A$;
- $\mathbf{v}_k := \text{sign}(x_1)\|\mathbf{x}\|e_1 + \mathbf{x}$;
- $\mathbf{v}_k := \mathbf{v}_k/\|\mathbf{v}_k\|$;

- $A_{k:m,k:n} := A_{k:m,k:n} - 2\mathbf{v}_k(\mathbf{v}_k^T A_{k:m,k:n})$.

Thus, by successively applying the Householder reflection, we achieve the QR-decomposition.




By recalling the Gram-Schmdit QR-decomposition where we can consider the algorithm as sequentially applying upper triangular matrices to $A$ until it becomes orthogonal, so,

$$AR_1R_2\cdots R_n = Q,$$

and thus, $\prod R_i = R^{-1}$. With that, we can describe the Gram-Schmidt process as a *triangular orthogonalisation* while, on the other hand, the Householder algorithm is a *orthogonal triangularisation*. Indeed, the two process are not equivalent and consequentially, the resulting QR-decompositions are different. We notice that the Gram-Schmidt procedure results in $R$ being square while $Q$ rectangular, that is, it yields the *reduced form* of the QR-decomposition. The Householder decomposition, on the other hand, results in $Q$ being square while $R$ being rectangular. This is refereed as the *full form* of the QR-decomposition and by noticing that the additional parts of $Q$ are multiplied by 0, we have that the full form provides us with information about the null-space of $A$.