II.2 Orthogonal and Unitary Matrices

A very important class of matrices are *orthogonal* and *unitary* matrices:

Definition 1 (orthogonal/unitary matrix) A square real matrix is *orthogonal* if its inverse is its transpose:

$$O(n) = \{Q \in \mathbb{R}^{n\times n} : Q^\top Q = I\}$$

A square complex matrix is *unitary* if its inverse is its adjoint:

$$U(n) = \{Q \in \mathbb{C}^{n\times n} : Q^\star Q = I\}.$$

Here the adjoint is the same as the conjugate-transpose: $Q^\star := \bar{Q}^\top$.

Note that $O(n) \subset U(n)$ as for real matrices $Q^\star = Q^\top$. Because in either case $Q^{-1} = Q^\star$ we also have $QQ^\star = I$ (which for real matrices is $QQ^\top = I$). These matrices are particularly important for numerical linear algebra for a number of reasons (we'll explore these properties in the problem sheets):

1. They are norm-preserving: for any vector $\mathbf{x} \in \mathbb{C}^n$ we have

$\|Q\mathbf{x}\| = \|\mathbf{x}\|$ where $\|\mathbf{x}\|^2 := \sum_{k=1}^n x_k^2$ (i.e. the 2-norm). 2. All eigenvalues have absolute value equal to 1 3. For $Q \in O(n)$, $\det Q = \pm 1$. 2. They are trivially invertible (just take the transpose). 3. They are generally "stable": errors are controlled. 4. They are *normal matrices*: they commute with their adjoint ($QQ^\star = QQ^\star$). See Chapter C for why this is important.

On a computer there are multiple ways of representing orthogonal/unitary matrices, and it is almost never to store a dense matrix storing the entries. We shall therefore investigate three classes:

1. *Permutation*: A permutation matrix permutes the rows of a vector and is a representation of the symmetric group.
2. *Rotations*: The simple rotations are also known as 2×2 special orthogonal matrices ($SO(2)$) and correspond to rotations in 2D.
3. *Reflections*: Reflections are $n \times n$ orthogonal matrices that have simple definitions in terms of a single vector.

We remark a very similar concept are rectangular matrices with orthogonal columns, e.g.

$$U = [\mathbf{u}_1 | \cdots | \mathbf{u}_n] \in \mathbb{R}^{m\times n}$$

where $m \geq n$ such that $U^\top U = I_n$ (the $n \times n$ identity matrix). In this case we must have $UU^\top \neq I_m$ as the rank of U is n. These will play an important role in the Singular Value Decomposition.

1. Permutation Matrices

Permutation matrices are matrices that represent the action of permuting the entries of a vector, that is, matrix representations of the symmetric group S_n, acting on $\mathbb{R}^n$. Recall every $\sigma \in S_n$ is a bijection between $\{1, 2, \ldots, n\}$ and itself. We can write a permutation σ in *Cauchy notation*:

$$\begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma_1 & \sigma_2 & \sigma_3 & \cdots & \sigma_n \end{pmatrix}$$

where $\{\sigma_1, \ldots, \sigma_n\} = \{1, 2, \ldots, n\}$ (that is, each integer appears precisely once). We denote the *inverse permutation* by σ^{-1}, which can be constructed by swapping the rows of the Cauchy notation and reordering.

We can encode a permutation in vector $\boldsymbol{\sigma} = [\sigma_1, \ldots, \sigma_n]$. This induces an action on a vector (using indexing notation)

$$\mathbf{v}[\boldsymbol{\sigma}] = \begin{bmatrix} v_{\sigma_1} \\ \vdots \\ v_{\sigma_n} \end{bmatrix}$$

Example 1 (permutation of a vector) Consider the permutation σ given by

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 4 & 2 & 5 & 3 \end{pmatrix}$$

We can apply it to a vector:

In [1]:
```julia
σ = [1, 4, 2, 5, 3]
v = [6, 7, 8, 9, 10]
v[σ] # we permutate entries of v
```

Out[1]:
```
5-element Vector{Int64}:
  6
  9
  7
 10
  8
```

Its inverse permutation σ^{-1} has Cauchy notation coming from swapping the rows of the Cauchy notation of σ and sorting:

$$\begin{pmatrix} 1 & 4 & 2 & 5 & 3 \\ 1 & 2 & 3 & 4 & 5 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 2 & 4 & 3 & 5 \\ 1 & 3 & 2 & 5 & 4 \end{pmatrix}$$

Julia has the function `invperm` for computing the vector that encodes the inverse permutation: And indeed:

In [2]:
```julia
σ⁻¹ = invperm(σ) # note that ⁻¹ are just unicode characters in the variable
```

Out[2]:
```
5-element Vector{Int64}:
 1
 3
 5
 2
 4
```

And indeed permuting the entries by `σ` and then by `σ⁻¹` returns us to our original vector:

In [3]:
```julia
v[σ][σ⁻¹] # permuting by σ and then σⁱ gets us back
```

Out[3]:
```
5-element Vector{Int64}:
  6
  7
  8
  9
 10
```

Note that the operator

$$P_\sigma(\mathbf{v}) = \mathbf{v}[\boldsymbol{\sigma}]$$

is linear in $\mathbf{v}$, therefore, we can identify it with a matrix whose action is:

$$P_\sigma \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} v_{\sigma_1} \\ \vdots \\ v_{\sigma_n} \end{bmatrix}.$$

The entries of this matrix are

$$P_\sigma[k, j] = \mathbf{e}_k^\top P_\sigma \mathbf{e}_j = \mathbf{e}_k^\top \mathbf{e}_{\sigma_j^{-1}} = \delta_{k,\sigma_j^{-1}} = \delta_{\sigma_k, j}$$

where $\delta_{k,j}$ is the *Kronecker delta*:

$$\delta_{k,j} := \begin{cases} 1 & k = j \\ 0 & \text{otherwise} \end{cases}.$$

This construction motivates the following definition:

Definition 2 (permutation matrix) $P \in \mathbb{R}^{n \times n}$ is a permutation matrix if it is equal to the identity matrix with its rows permuted.

Example 2 (5×5 permutation matrix) We can construct the permutation representation for σ as above as follows:

In [4]:
```julia
P = I(5)[σ,:]
```

Out[4]:
```
5×5 Matrix{Bool}:
 1  0  0  0  0
 0  0  0  1  0
 0  1  0  0  0
 0  0  0  0  1
 0  0  1  0  0
```

And indeed, we see its action is as expected:

In [5]:
```julia
P * v
```

Out[5]:
```
5-element Vector{Int64}:
  6
  9
  7
 10
  8
```

Remark (advanced) Note that `P` is a special type `SparseMatrixCSC`. This is used to represent a matrix by storing only the non-zero entries as well as their location. This is an important data type in high-performance scientific computing, but we will not be using general sparse matrices in this module.

Proposition 1 (permutation matrix inverse) Let P_σ be a permutation matrix corresponding to the permutation σ. Then

$$P_\sigma^\top = P_{\sigma^{-1}} = P_\sigma^{-1}$$

That is, P_σ is *orthogonal*:

$$P_\sigma^\top P_\sigma = P_\sigma P_\sigma^\top = I.$$

Proof

We prove orthogonality via:

$$\mathbf{e}_k^\top P_\sigma^\top P_\sigma \mathbf{e}_j = (P_\sigma \mathbf{e}_k)^\top P_\sigma \mathbf{e}_j = \mathbf{e}_{\sigma_k^{-1}}^\top \mathbf{e}_{\sigma_j^{-1}} = \delta_{k,j}$$

This shows $P_\sigma^\top P_\sigma = I$ and hence $P_\sigma^{-1} = P_\sigma^\top$.

∎

2. Rotations

We begin with a general definition:

Definition 3 (Special Orthogonal and Rotations) *Special Orthogonal Matrices* are

$$SO(n) := \{Q \in O(n) | \det Q = 1\}$$

And (simple) *rotations* are $SO(2)$.

In what follows we use the following for writing the angle of a vector:

Definition 4 (two-arg arctan) The two-argument arctan function gives the angle `θ` through the point $[a, b]^\top$, i.e.,

$$\sqrt{a^2+b^2}\begin{bmatrix}\cos\theta \\ \sin\theta\end{bmatrix} = \begin{bmatrix} a \\ b\end{bmatrix}$$

It can be defined in terms of the standard arctan as follows:

$$\mathrm{atan}(b,a) := \begin{cases} \mathrm{atan}\frac{b}{a} & a > 0 \\ \mathrm{atan}\frac{b}{a} + \pi & a < 0 \text{ and } b > 0 \\ \mathrm{atan}\frac{b}{a} - \pi & a < 0 \text{ and } b < 0 \\ \pi/2 & a = 0 \text{ and } b > 0 \\ -\pi/2 & a = 0 \text{ and } b < 0 \end{cases}$$

This is available in Julia via the function `atan(y,x)`.

We show $SO(2)$ are exactly equivalent to standard rotations:

Proposition 2 (simple rotation) A 2×2 *rotation matrix* through angle θ is

$$Q_\theta := \begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}$$

We have $Q \in SO(2)$ iff $Q = Q_\theta$ for some $\theta \in \mathbb{R}$.

Proof

We will write $c = \cos\theta$ and $s = \sin\theta$. Then we have

$$Q_\theta^\top Q_\theta = \begin{pmatrix} c & s \\ -s & c\end{pmatrix}\begin{pmatrix} c & -s \\ s & c\end{pmatrix} = \begin{pmatrix} c^2+s^2 & 0 \\ 0 & c^2+s^2\end{pmatrix} = I$$

and $\det Q_\theta = c^2 + s^2 = 1$ hence $Q_\theta \in SO(2)$.

Now suppose $Q = [\mathbf{q}_1, \mathbf{q}_2] \in SO(2)$ where we know its columns have norm 1 $\|\mathbf{q}_k\| = 1$ and are orthogonal. Write $\mathbf{q}_1 = [c, s]$ where we know $c = \cos\theta$ and $s = \sin\theta$ for $\theta = \mathrm{atan}(s, c)$. Since $\mathbf{q}_1 \cdot \mathbf{q}_2 = 0$ we can deduce $\mathbf{q}_2 = \pm[-s, c]$. The sign is positive as $\det Q = \pm(c^2+s^2) = \pm 1$.

∎

We can rotate an arbitrary vector in $\mathbb{R}^2$ to the unit axis using rotations, which are useful in linear algebra decompositions. Interestingly it only requires basic algebraic functions (no trigonometric functions):

Proposition 3 (rotation of a vector) The matrix

$$Q = \frac{1}{\sqrt{a^2 + b^2}} \begin{bmatrix} a & b \\ -b & a \end{bmatrix}$$

is a rotation matrix ($Q \in SO(2)$) satisfying

$$Q \begin{bmatrix} a \\ b \end{bmatrix} = \sqrt{a^2 + b^2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Proof

The last equation is trivial so the only question is that it is a rotation matrix. This follows immediately:

$$Q^\top Q = \frac{1}{a^2 + b^2} \begin{bmatrix} a^2 + b^2 & 0 \\ 0 & a^2 + b^2 \end{bmatrix} = I$$

and $\det Q = 1$.

∎

3. Reflections

In addition to rotations, another type of orthogonal/unitary matrix are reflections:

Definition 5 (reflection matrix) Given a unit vector $\mathbf{v} \in \mathbb{C}^n$ (satisfying $\|\mathbf{v}\| = 1$), the *reflection matrix*

$$Q_{\mathbf{v}} := I - 2\mathbf{v}\mathbf{v}^\star$$

These are reflections in the direction of $\mathbf{v}$. We can show this as follows:

Proposition 4 (Householder properties) $Q_{\mathbf{v}}$ satisfies:

1. $Q_{\mathbf{v}} = Q_{\mathbf{v}}^\star$ (Symmetry)
2. $Q_{\mathbf{v}}^\star Q_{\mathbf{v}} = I$ (Orthogonality $Q_{\mathbf{v}} \in U(n)$)
3. $\mathbf{v}$ is an eigenvector of $Q_{\mathbf{v}}$ with eigenvalue -1
4. $Q_{\mathbf{v}}$ is a rank-1 perturbation of I
5. $\det Q_{\mathbf{v}} = -1$ ($Q_{\mathbf{v}} \notin SO(n)$)

Proof

Property 1 follows immediately. Property 2 follows from

$$Q_{\mathbf{v}}^\star Q_{\mathbf{v}} = Q_{\mathbf{v}}^2 = I - 4\mathbf{v}\mathbf{v}^\star + 4\mathbf{v}\mathbf{v}^\star\mathbf{v}\mathbf{v}^\star = I$$

Property 3 follows since

$$Q_{\mathbf{v}}\mathbf{v} = -\mathbf{v}$$

Property 4 follows since $\mathbf{v}\mathbf{v}^\top$ is a rank-1 matrix as all rows are linear combinations of each other. To see property 5, note there is a dimension $n-1$ space W orthogonal to $\mathbf{v}$, that is, for all $\mathbf{w} \in W$ we have $\mathbf{w}^\star \mathbf{v} = 0$, which implies that

$$Q_{\mathbf{v}}\mathbf{w} = \mathbf{w}$$

In other words, 1 is an eigenvalue with multiplicity $n-1$ and -1 is an eigenvalue with multiplicity 1, and thus the product of the eigenvalues is -1.

∎

Example 3 (reflection through 2-vector) Consider reflection through $\mathbf{x} = [1, 2]^\top$. We first need to normalise $\mathbf{x}$:

$$\mathbf{v} = \frac{\mathbf{x}}{\|\mathbf{x}\|} = \begin{bmatrix} \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{bmatrix}$$

Note this indeed has unit norm:

$$\|\mathbf{v}\|^2 = \frac{1}{5} + \frac{4}{5} = 1.$$

Thus the reflection matrix is:

$$Q_{\mathbf{v}} = I - 2\mathbf{v}\mathbf{v}^\top = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} - \frac{2}{5}\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 3 & -4 \\ -4 & -3 \end{bmatrix}$$

Indeed it is symmetric, and orthogonal. It sends $\mathbf{x}$ to $-\mathbf{x}$:

$$Q_{\mathbf{v}}\mathbf{x} = \frac{1}{5}\begin{bmatrix} 3-8 \\ -4-6 \end{bmatrix} = -\mathbf{x}$$

Any vector orthogonal to $\mathbf{x}$, like $\mathbf{y} = [-2, 1]^\top$, is left fixed:

$$Q_{\mathbf{v}}\mathbf{y} = \frac{1}{5}\begin{bmatrix} -6-4 \\ 8-3 \end{bmatrix} = \mathbf{y}$$

Note that *building* the matrix $Q_{\mathbf{v}}$ will be expensive ($O(n^2)$ operations), but we can *apply* $Q_{\mathbf{v}}$ to a vector in $O(n)$ operations using the expression:

$$Q_{\mathbf{v}}\mathbf{x} = \mathbf{x} - 2\mathbf{v}(\mathbf{v}^\star\mathbf{x}) = \mathbf{x} - 2\mathbf{v}(\mathbf{v}\cdot\mathbf{x}).$$

Just as rotations can be used to rotate vectors to be aligned with coordinate axis, so can reflections, but in this case it works for vectors in $\mathbb{C}^n$, not just $\mathbb{R}^2$:

Definition 6 (Householder reflection, real case) For a given vector $\mathbf{x} \in \mathbb{R}^n$, define the Householder reflection

$$Q_{\mathbf{x}}^{\pm,\mathrm{H}} := Q_{\mathbf{w}}$$

for $\mathbf{y} = \mp\|\mathbf{x}\|\mathbf{e}_1 + \mathbf{x}$ and $\mathbf{w} = \frac{\mathbf{y}}{\|\mathbf{y}\|}$. The default choice in sign is:

$$Q_{\mathbf{x}}^{\mathrm{H}} := Q_{\mathbf{x}}^{-\mathrm{sign}(x_1),\mathrm{H}}.$$

Lemma 1 (Householder reflection maps to axis) For $\mathbf{x} \in \mathbb{R}^n$,

$$Q_{\mathbf{x}}^{\pm,\mathrm{H}}\mathbf{x} = \pm\|\mathbf{x}\|\mathbf{e}_1$$

Proof Note that

$$\|\mathbf{y}\|^2 = 2\|\mathbf{x}\|^2 \mp 2\|\mathbf{x}\|x_1,$$
$$\mathbf{y}^\top\mathbf{x} = \|\mathbf{x}\|^2 \mp \|\mathbf{x}\|x_1$$

where $x_1 = \mathbf{e}_1^\top\mathbf{x}$. Therefore:

$$Q_{\mathbf{x}}^{\pm,\mathrm{H}}\mathbf{x} = (I - 2\mathbf{w}\mathbf{w}^\top)\mathbf{x} = \mathbf{x} - 2\frac{\mathbf{y}\|\mathbf{x}\|}{\|\mathbf{y}\|^2}(\|\mathbf{x}\| \mp x_1) = \mathbf{x} - \mathbf{y} = \pm\|\mathbf{x}\|\mathbf{e}_1.$$

∎

Why do we choose the the opposite sign of x_1 for the default reflection? For stability. We demonstrate the reason for this by numerical example. Consider $\mathbf{x} = [1, h]$, i.e., a small perturbation from $\mathbf{e}_1$. If we reflect to $\mathrm{norm}(\mathbf{x})\mathbf{e}_1$ we see a numerical problem:

In [6]:
```
h = 10.0^(-10)
x = [1,h]
y = -norm(x)*[1,0] + x
w = y/norm(y)
Q = I - 2w*w'
Q*x
```

Out[6]:
```
2-element Vector{Float64}:
  1.0
 -1.0e-10
```

It didn't work! Even worse is if `h = 0`:

In [7]:
```
h = 0
x = [1,h]
y = -norm(x)*[1,0] + x
w = y/norm(y)
Q = I - 2w*w'
Q*x
```

Out[7]:
```
2-element Vector{Float64}:
 NaN
 NaN
```

This is because `y` has large relative error due to cancellation from floating point errors in computing the first entry `x[1] - norm(x)`. (Or has norm zero if `h=0`.) We avoid this cancellation by using the default choice:

In [8]:
```
h = 10.0^(-10)
x = [1,h]
y = sign(x[1])*norm(x)*[1,0] + x
w = y/norm(y)
Q = I - 2w*w'
Q*x
```

Out[8]:
```
2-element Vector{Float64}:
 -1.0
  0.0
```

We can extend this definition for complexes:

Definition 7 (Householder reflection, complex case) For a given vector $\mathbf{x} \in \mathbb{C}^n$, define the Householder reflection as

$$Q_{\mathbf{x}}^{\mathrm{H}} := Q_{\mathbf{w}}$$

for $\mathbf{y} = \mathrm{csign}(x_1)\|\mathbf{x}\|\mathbf{e}_1 + \mathbf{x}$ and $\mathbf{w} = \frac{\mathbf{y}}{\|\mathbf{y}\|}$, for $\mathrm{csign}(z) = \mathrm{e}^{\mathrm{i}\arg z}$.

Lemma 2 (Householder reflection maps to axis, complex case) For $\mathbf{x} \in \mathbb{C}^n$,

$$Q_{\mathbf{x}}^{\mathrm{H}}\mathbf{x} = -\mathrm{csign}(x_1)\|\mathbf{x}\|\mathbf{e}_1$$

Proof Denote $\alpha := \mathrm{csign}(x_1)$. Note that $\bar{\alpha}x_1 = \mathrm{e}^{-\mathrm{i}\arg x_1}x_1 = |x_1|$. Now we have

$$\begin{aligned}
\|\mathbf{y}\|^2 &= (\alpha\|\mathbf{x}\|\mathbf{e}_1 + \mathbf{x})^\star(\alpha\|\mathbf{x}\|\mathbf{e}_1 + \mathbf{x}) = |\alpha|\|\mathbf{x}\|^2 + \|\mathbf{x}\|\alpha\bar{x}_1 + \bar{\alpha}x_1\|\mathbf{x}\| + \|\mathbf{x}\|^2 \\
&= 2\|\mathbf{x}\|^2 + 2|x_1|\|\mathbf{x}\| \\
\mathbf{y}^\star\mathbf{x} &= \bar{\alpha}x_1\|\mathbf{x}\| + \|\mathbf{x}\|^2 = \|\mathbf{x}\|^2 + |x_1|\|\mathbf{x}\|
\end{aligned}$$

Therefore:

$$Q_{\mathbf{x}}^{\mathrm{H}}\mathbf{x} = (I - 2\mathbf{w}\mathbf{w}^\star)\mathbf{x} = \mathbf{x} - 2\frac{\mathbf{y}}{\|\mathbf{y}\|^2}(\|\mathbf{x}\|^2 + |x_1|\|\mathbf{x}\|) = \mathbf{x} - \mathbf{y} = -\alpha\|\mathbf{x}\|\mathbf{e}_1.$$

∎