Unitary matrices from experiments

Aim lecture: We look at some applications of singular value decomposition.

Q Let $Q \in M_{nn}(\mathbb{C})$ be a matrix that we know from theory to be unitary. Suppose we have some experiment to determine its entries, and the resulting matrix is Q_0. With measurement error, it is unlikely that Q_0 is unitary. Can we guess Q from Q_0.

A Let $Q_0 = U_l D U_r^*$ be a singular value decomposition (SVD) of Q_0. Then $Q \approx U_l D U_r^* \implies D \approx U_l^* Q U_r$. Thus D is diagonal with non-negative entries & is approximately unitary so must be close to I_n. This suggests

Fact

The best unitary matrix approximating Q_0 is $U_l U_r^*$.

Least squares in the diagonal case

Suppose D is a real $m \times n$ diagonal matrix of the form $(d_{ij}) = D = \begin{pmatrix} D_+ & 0 \\ 0 & 0 \end{pmatrix}$, where D_+ is invertible $\rho \times \rho$ and the zero matrices have size $\rho \times (n-\rho), (m-\rho) \times \rho, (m-\rho) \times (n-\rho)$. Hence D_+ has non-zero diagonal entries $d_{11}, \dots, d_{\rho\rho}$.

Prop

A least squares solution to the eqn $D\mathbf{v} = \mathbf{w}$ is given by

1. any $\mathbf{v}$ with co-ord $v_1 = d_{11}^{-1} w_1, \dots, v_\rho = d_{\rho\rho}^{-1} w_\rho$ and $v_{\rho+1}, \dots, v_n$ arbitrary.
2. The solution $\mathbf{v}$ with minimal length $\|\mathbf{v}\|$ is $\mathbf{v} = (d_{11}^{-1} w_1, \dots, d_{\rho\rho}^{-1} w_\rho, 0, \dots, 0)^T$.

Proof. Defining $d_{ii} = v_i = 0$ if $i > n$, the least squares solns are those minimising

$$\|D\mathbf{v} - \mathbf{w}\|^2 = \sum_{i=1}^{m} (d_{ii} v_i - w_i)^2 = \sum_{i=1}^{\rho} (d_{ii} v_i - w_i)^2 + \sum_{i=\rho+1}^{m} w_i^2.$$

This is minimised precisely when $d_{ii} v_i - w_i = 0$ for $i = 1, \dots, \rho$.

Generalised inverses of diagonal matrices

Let D be the diagonal matrix on the last slide and consider the $n \times m$-diagonal matrix

$$D^- = \begin{pmatrix} D_+^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

We can restate Prop 2) as

Defn-Upshot

The unique minimal length least squares soln to $D\mathbf{v} = \mathbf{w}$ is $\mathbf{v} = D^-\mathbf{w}$. We call D^- the (Moore-Penrose) generalised inverse of D.

Note that
$DD^- =$

Q How do you extend this to arbitrary matrices?
A Consider the linear map $T_A : \mathbb{R}^n \longrightarrow \mathbb{R}^m$, and use an o/n change of co-ord on $\mathbb{R}^n, \mathbb{R}^m$ so that the representing matrix is diagonal, i.e. SVD.

Moore-Penrose generalised inverse

Let $A \in M_{mn}(\mathbb{R})$ and $A = U_l D U_r^*$ be a SVD for A.

Defn

The (Moore-Penrose) generalised inverse of A is $A^- = U_r D^- U_l^*$. (It turns out it does not depend on the SVD!).

E.g. Find the gen inverse of $A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Least squares and SVDs

Consider the SVD $A = U_l D U_r^*$ as above.

Prop

The least squares soln to $A\mathbf{v} = \mathbf{w}$ which has minimal length is $\mathbf{v} = A^- \mathbf{w}$.

Proof. We seek to minimise $\|A\mathbf{v} - \mathbf{w}\| = \|U_l D U_r^* \mathbf{v} - \mathbf{w}\| = \|D U_r^* \mathbf{v} - U_l^* \mathbf{w}\|$ since U_l is orthogonal. We change variables to $\mathbf{x} = U_r^* \mathbf{v}$ and seek to minimise $\|D\mathbf{x} - U_l^* \mathbf{w}\|$. Since U_r is orthogonal, the minimal length solns $\mathbf{x}$ correspond to the minimal length solns $\mathbf{v}$. This is given by

$$\mathbf{x} = D^- U_l^* \mathbf{w}.$$

Hence the minimal length least squares soln is

$$\mathbf{v} = U_r D^- U_l^* \mathbf{w} = A^- \mathbf{w}.$$