GRAM-SCHMIDT ORTHANORMALISATION

An algorithm for 'orthanormalising' a set of vectors that are in $\mathbb{R}^n$

Takes a finite, linearly independent set $S = \{\underline{v}_1, \dots, \underline{v}_k\}$

Generates a finite, orthogonal set $S' = \{\underline{w}_1, \dots, \underline{w}_n\}$

NOTE: We must have $k \leq n$ or else not enough DOF.

How it works:

Define a projection operator $\text{proj}_{\underline{u}}(\underline{v}) = \dfrac{\langle \underline{v}, \underline{u} \rangle}{\langle \underline{u}, \underline{u} \rangle} \underline{u}$.

where $\langle \underline{u}, \underline{v} \rangle$ is usually just the dot product.

Then

$$\hat{\underline{w}}_1 = \underline{v}_1$$

$$\hat{\underline{w}}_2 = \underline{v}_2 - \text{proj}_{\underline{w}_1}(\underline{v}_2)$$

$$\hat{\underline{w}}_3 = \underline{v}_3 - \text{proj}_{\underline{w}_1}(\underline{v}_3) - \text{proj}_{\underline{w}_2}(\underline{v}_2).$$

$$\vdots$$

$$\hat{\underline{w}}_k = \underline{v}_k - \sum_{j=1}^{k-1} \text{proj}_{\underline{u}_j}(\underline{v}_j).$$

Then $w_i = \hat{\underline{w}}_i / \| \hat{w}_i \|$.

10b

EX. $\underline{v}_1 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$ $\quad \underline{v}_2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$

$$\hat{\underline{w}}_1 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

$$\hat{\underline{w}}_2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix} - \frac{\begin{pmatrix} -1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix}}{\begin{pmatrix} 2 \\ 3 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix}} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} + \frac{2}{13} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

$$= \begin{pmatrix} -1 \\ 0 \end{pmatrix} + \begin{pmatrix} 4/13 \\ 6/13 \end{pmatrix}$$

$$= \begin{pmatrix} -9/13 \\ 6/13 \end{pmatrix} = \begin{pmatrix} -9 \\ 6 \end{pmatrix} = \begin{pmatrix} -3 \\ 2 \end{pmatrix}$$

$$\hat{\underline{w}}_1 \cdot \hat{\underline{w}}_2 = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \cdot \begin{pmatrix} -9 \\ 6 \end{pmatrix} = -18 + 18 = 0 \quad \checkmark$$

$$\underline{w}_1 = \frac{1}{\sqrt{13}} \begin{pmatrix} 2 \\ 3 \end{pmatrix} \qquad \underline{w}_2 = \frac{1}{\sqrt{13}} \begin{pmatrix} -3 \\ 2 \end{pmatrix}$$

THE SINGULAR VALUE DECOMPOSITION

Very useful for overdetermined (rectangular/least square) problems.

$$\underline{\underline{A}}\,\underline{x} = \underline{b} \qquad \underline{\underline{A}} \in \mathbb{R}^{m \times n} \text{ with } m \geq n.$$

For any such matrix $\underline{\underline{A}}$ there exist a

$$\underline{\underline{U}} \in \mathbb{R}^{m \times m}, \quad \underline{\underline{V}} \in \mathbb{R}^{n \times n}, \quad \underline{\underline{\Sigma}} \in \mathbb{R}^{m \times n}$$

orthogonal $(\underline{\underline{A}}^T\underline{\underline{A}} = \underline{\underline{A}}\,\underline{\underline{A}}^T = \underline{\underline{I}})$.   diagonal

such that

$$\underline{\underline{A}} = \underline{\underline{U}}\,\underline{\underline{\Sigma}}\,\underline{\underline{V}}^T$$

and $\underline{\underline{\Sigma}} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$

NOTE: If $\sigma_r > 0$ is the smallest singular value greater than zero, then the matrix $\underline{\underline{A}}$ has rank r.

We call - the columns of $\underline{\underline{U}}$ the left singular vectors.

- ———— " —— $\underline{\underline{V}}$ — " — right —— " ——
- the diagonal entries of $\underline{\underline{\Sigma}}$ are the singular values of $\underline{\underline{A}}$

How do we find $\underline{\underline{U}}$, $\underline{\underline{\Sigma}}$ and $\underline{\underline{V}}$?

1) Compute Eig vals and vecs of $\underline{\underline{A}}\underline{\underline{A}}^T$
2) Orthonormalise the Eig. vecs.
3) The columns of $\underline{\underline{U}}$ are these vectors ordered by size of Eigvals.
4) Compute Eig vals and vecs of $\underline{\underline{A}}^T\underline{\underline{A}}$
5) Orthonormalise the Eig vecs.
6) The columns of $\underline{\underline{V}}$ are these vectors organised
7) $\underline{\underline{S}}$ is diagonal with entries $\sqrt{\text{Eigvals}}$ ordered.

EX $\quad \underline{\underline{A}} = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} \qquad \underline{\underline{A}}\underline{\underline{A}}^T = \begin{pmatrix} 11 & 1 \\ 1 & 11 \end{pmatrix}$

Eigs of $\underline{\underline{A}}\underline{\underline{A}}^T$: $(11-\lambda)^2 - 1 = 0 \Rightarrow 11-\lambda = \pm 1$

$$\Rightarrow \boxed{\lambda = 10, 12.}$$

$\lambda = 10$: $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \underline{0} \Rightarrow \boxed{x_1 = -x_2.}$

$\lambda = 12$: $\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \underline{0} \Rightarrow \boxed{x_1 = x_2}$

Thus: $\lambda = 10$ $\underline{x} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\lambda = 12$ $\underline{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\hat{\underline{\underline{u}}} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \hat{\underline{u}}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \hat{\underline{u}}_2 = \begin{pmatrix} +1 \\ -1 \end{pmatrix}$$

$$\underline{w}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \underline{w}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

CHECK $\underline{w}_1 \cdot \underline{w}_2 = 0$.

$$\underline{\underline{u}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

$$\underline{\underline{A}}^T\underline{\underline{A}} = \begin{pmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{pmatrix} \qquad \lambda(\lambda-10)(\lambda-12) = 0$$

$$\Rightarrow \boxed{\lambda = 0, 10, 12}$$

Thus $\lambda = 12$ $\underline{x} = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}$, $\lambda = 10$ $\underline{x} = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}$

$\lambda = 0$ $\underline{x} = \begin{pmatrix} 1 \\ 2 \\ -5 \end{pmatrix}$

$$\hat{\underline{\underline{V}}} = \begin{pmatrix} 1 & 2 & 1 \\ 2 & -1 & 2 \\ 1 & 0 & -5 \end{pmatrix} \qquad \hat{\underline{V}}_1 = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} \qquad \hat{\underline{V}}_2 = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix} \qquad \hat{\underline{V}}_3 = \begin{pmatrix} 1 \\ 2 \\ -5 \end{pmatrix}$$

$$\underline{\underline{V}} = \begin{pmatrix} 1/\sqrt{6} & 2/\sqrt{6} & 1/\sqrt{6} \\ 2/\sqrt{5} & -1/\sqrt{5} & 0 \\ 1/\sqrt{30} & 2/\sqrt{30} & -5/\sqrt{30} \end{pmatrix}.$$

$$S = \begin{pmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{pmatrix}.$$

CHECK: $A = U S V^T$ ✓.

Why is this useful?

1) It allows us to easily compute the pseudo-inverse

If $A = U \Sigma' V^T$ Then $A^+ \leftarrow$ the pseudoinverse of A

$$A^+ = V \Sigma'^+ U^T$$

and Σ'^+ is computed by each non-zero diagonal entry of Σ' with its reciprocal. and then transposing.

2) least square minimization.

This can be use for finding a 'best fit' to data

$$\min_x \| A x - b \|$$

a soln is given by $A^+ b = x$

3) Approximating the condition number.

$$\mathrm{cond}(\underline{A}) = \|\underline{A}\|\,\|\underline{A}^{+}\|. \quad (= \|\underline{A}\|\,\|\underline{A}^{-1}\|.)$$

$$\mathrm{cond}(\underline{A}) \approx \sigma_1 / \sigma_r$$