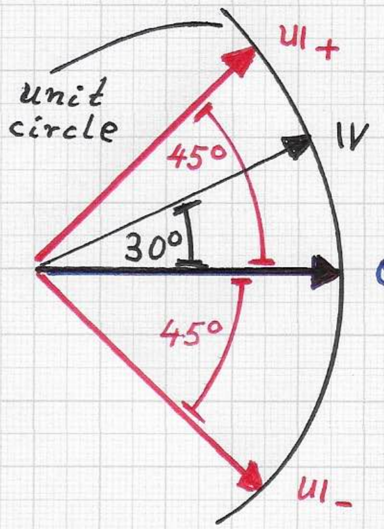
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



Simple 2D example. The resulting vectors are

$u1_+ = (\sqrt{2}/2, \sqrt{2}/2)^T$

and

$u1_- = (\sqrt{2}/2, -\sqrt{2}/2)^T$.

We compute the two possible values of $u1$ for the simple example sketched in the left figure. Using the formula provided on the previous page for the given vectors $e = (1,0)^T$ and $v = (\sqrt{3}/2, 1/2)^T$, one obtains

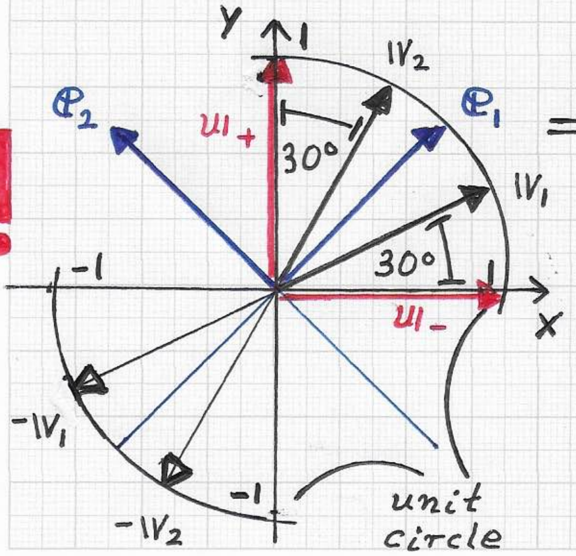
$$u1 = \frac{\sqrt{2}}{2}\left(e \; +/- \; \frac{v - (v \cdot e)\cdot e}{\sqrt{1-(v\cdot e)^2}}\right)$$

$$= \frac{\sqrt{2}}{2}\left(\begin{pmatrix}1\\0\end{pmatrix} +/- \frac{(\sqrt{3}/2, 1/2)^T - \sqrt{3}/2\,(1,0)^T}{\sqrt{1-(\sqrt{3}/2)^2}}\right)$$

$$= \frac{\sqrt{2}}{2}\left(\begin{pmatrix}1\\0\end{pmatrix} +/- \frac{(0, 1/2)^T}{\sqrt{1/4}}\right)$$

$$= \frac{\sqrt{2}}{2}\left(\begin{pmatrix}1\\0\end{pmatrix} +/- 2\begin{pmatrix}0\\1/2\end{pmatrix}\right)$$

$$= \frac{\sqrt{2}}{2}\begin{pmatrix}1\\+/-1\end{pmatrix} = \begin{pmatrix}\sqrt{2}/2\\+/-\sqrt{2}/2\end{pmatrix}$$



A more complicated example is shown in the left figure. Two unit non-orthogonal vectors are given, v_1 and v_2. Here, $v_1 = (\sqrt{3}/2, 1/2)^T$ and $v_2 = (1/2, \sqrt{3}/2)^T$. The desired pair of orthonormal vectors is given by $u1_- = (1,0)^T$ and $u1_+ = (0,1)^T$.

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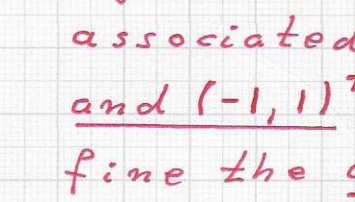
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks: ... In this 2D example, one must perform a principal components analysis (PCA) step, to calculate the necessary eigendirection vector $\mathbf{e}$ needed for the computation of $\mathbf{u}_-$ and $\mathbf{u}_+$. (PCA actually yields two orthogonal vectors; they are called $\mathbf{e}_1$ and $\mathbf{e}_2$, after normalization, in the bottom-left figure on the previous page.) PCA is applied to four vectors: $\mathbf{w}_1 = (\sqrt{3}/2, 1/2)^T$, $\mathbf{w}_2 = (1/2, \sqrt{3}/2)$, $-\mathbf{w}_1$ and $-\mathbf{w}_2$. For these four vectors PCA yields the eigenvalues $\lambda_1 = 2+\sqrt{3}$ and $\lambda_2 = 2-\sqrt{3}$ with associated orthogonal eigenvectors $(1,1)^T$ and $(-1,1)^T$. After normalization, they define the orthonormal vectors $\mathbf{e}_1 = (\sqrt{2}/2, \sqrt{2}/2)^T$ and $\mathbf{e}_2 = (-\sqrt{2}/2, \sqrt{2}/2)^T$. (PCA is performed for the matrix

$$\begin{pmatrix} \sqrt{3}/2 & 1/2 & -\sqrt{3}/2 & -1/2 \\ 1/2 & \sqrt{3}/2 & -1/2 & -\sqrt{3}/2 \end{pmatrix} \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \\ -1/2 & -\sqrt{3}/2 \end{pmatrix} = \begin{pmatrix} 2 & \sqrt{3} \\ \sqrt{3} & 2 \end{pmatrix}.)$$

We can now perform the described "optimal orthonormalization" for the vectors $\mathbf{w}_1$ and $\mathbf{w}_2$ by using $\mathbf{e}_1$ as eigendirection $\mathbf{e}$ needed for the computation of $\mathbf{u}_-$ and $\mathbf{u}_+$. Further, we use vector $\mathbf{w}_1$ as $\mathbf{w}$-vector needed for the equation for $\mathbf{u}$ on page 10 (9/3/2023). The left figure shows these choices.



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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... In summary, we use the vectors $\mathbb{e} = (\sqrt{2}/2, \sqrt{2}/2)^T$ and $\mathbb{w} = (\sqrt{3}/2, 1/2)^T$ for the computation of the pair of orthonormal vectors $\mathbb{u}_{1+}$ and $\mathbb{u}_{1-}$. One obtains:

$$\mathbb{u}_1 = \frac{\sqrt{2}}{2}\left(\mathbb{e} +/- \frac{\mathbb{w} - (\mathbb{w}\bullet\mathbb{e})\cdot\mathbb{e}}{\sqrt{1-(\mathbb{w}\bullet\mathbb{e})^2}}\right)$$

$$= \frac{\sqrt{2}}{2}\left(\begin{pmatrix}\sqrt{2}/2\\ \sqrt{2}/2\end{pmatrix} +/- \frac{(\sqrt{3}/2, 1/2)^T - (\sqrt{3}/2, 1/2)^T\bullet(\sqrt{2}/2, \sqrt{2}/2)^T\,\mathbb{e}}{\sqrt{1-((\sqrt{3}/2, 1/2)^T\bullet(\sqrt{2}/2, \sqrt{2}/2)^T)^2}}\right)$$

= "complicated square roots" ...

$$= \begin{pmatrix}1/2\\ 1/2\end{pmatrix} +/- \frac{\sqrt{2}}{2}\cdot\frac{(\sqrt{3}/2, 1/2)^T - 0.965926\,(\sqrt{2}/2, \sqrt{2}/2)^T}{\sqrt{1-(0.965926)^2}}\Bigg)$$

$$= \begin{pmatrix}1/2\\ 1/2\end{pmatrix} +/- \frac{\sqrt{2}}{2}\left(3.863703\left(\begin{pmatrix}\sqrt{3}/2\\ 1/2\end{pmatrix} - 0.965926\begin{pmatrix}\sqrt{2}/2\\ \sqrt{2}/2\end{pmatrix}\right)\right)$$

$$= \begin{pmatrix}1/2\\ 1/2\end{pmatrix} +/- \frac{\sqrt{2}}{2}\left(3.863703\begin{pmatrix}0.183013\\ -0.183013\end{pmatrix}\right)$$

$$= \begin{pmatrix}1/2\\ 1/2\end{pmatrix} +/- \frac{\sqrt{2}}{2}\begin{pmatrix}\sqrt{2}/2\\ -\sqrt{2}/2\end{pmatrix} = \begin{pmatrix}1/2\\ 1/2\end{pmatrix} +/- \begin{pmatrix}1/2\\ -1/2\end{pmatrix} = \begin{pmatrix}1/2 +/- 1/2\\ 1/2 -/+ 1/2\end{pmatrix}$$

Thus, the two resulting $\mathbb{u}_1$-vectors are the vectors $(1,0)^T$ and $(0,1)^T$, as expected. One can define $\mathbb{u}_{1-} = (1,0)^T$ and $\mathbb{u}_{1+} = (0,1)^T$ (or vice versa). The construction of such an "optimal orthogonal basis vector set" must ultimately be performed for the D-dimensional setting.

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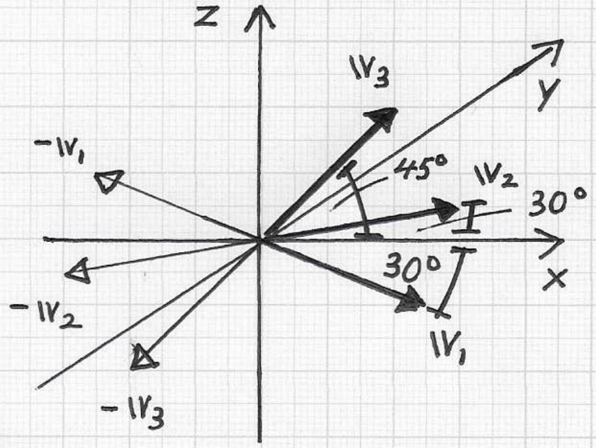
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... We consider a 3D example next. Here, we are using as input for the approach three normalized non-orthogonal basis vectors. The goal is the construction of three orthonormal basis vectors that approximate the given three vectors "optimally" — in the same way as described for the 2D case. We use a 3D example that uses vectors and angles similar to those used in the 2D examples. The left figure provides a sketch: The three given normalized non-orthogonal vectors are $\mathbb{v}_1 = (\sqrt{3}/2, -1/2, 0)^T$, $\mathbb{v}_2 = (\sqrt{3}/2, 1/2, 0)^T$ and $\mathbb{v}_3 = (\sqrt{2}/2, 0, \sqrt{2}/2)^T$.



PCA is applied to six vectors: $\mathbb{v}_1, \mathbb{v}_2, \mathbb{v}_3, -\mathbb{v}_1, -\mathbb{v}_2$ and $-\mathbb{v}_3$. The covariance matrix for which one must compute eigenvalues and eigenvectors is the matrix

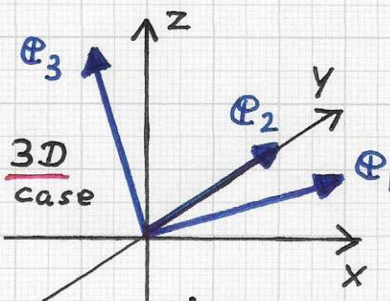
$$\underbrace{\begin{bmatrix} \sqrt{3}/2 & \sqrt{3}/2 & \sqrt{2}/2 & -\sqrt{3}/2 & -\sqrt{3}/2 & -\sqrt{2}/2 \\ -1/2 & 1/2 & 0 & 1/2 & -1/2 & 0 \\ 0 & 0 & \sqrt{2}/2 & 0 & 0 & -\sqrt{2}/2 \end{bmatrix}}_{M} \cdot M^T = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} = C.$$

The three eigenvalues and eigenvectors of C are $\lambda_1 = (5+\sqrt{13})/2$, $\lambda_2 = 1$ and $\lambda_3 = (5-\sqrt{13})/2$, and $\mathbb{e}_1 = ((3+\sqrt{13})/2, 0, 1)^T$, $\mathbb{e}_2 = (0, 1, 0)^T$ and $\mathbb{e}_3 = ((3-\sqrt{13}, 0, 1)^T$, respectively.

...

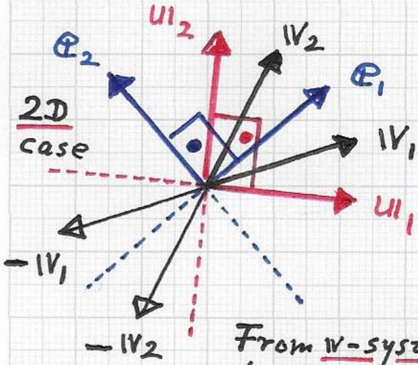
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** After normalization, the values of these three eigenvectors are approximately $\mathbf{e}_1 = (0.957092, 0, 0.289784)^T$, $\mathbf{e}_2 = (0, 1, 0)^T$ and $\mathbf{e}_3 = (-0.289784, 0, 0.957092)^T$. (Of course, the vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ are mutually orthogonal.) The objective is the construction of an orthonormal basis vector set from the PCA-generated orthonormal eigenvectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$, see left figure.



eigensystem

{ • **Note.** In the 2D case, one can understand the needed $\mathbf{u}$-vectors as vectors that are "dual" to the $\mathbf{e}$-eigenvectors defined by two normalized, non-orthogonal vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, see left figure. Here, PCA is applied to the four vectors $\mathbf{v}_1$, $\mathbf{v}_2$, $-\mathbf{v}_1$ and $-\mathbf{v}_2$. The two resulting eigenvectors (after normalization) are $\mathbf{e}_1$ and $\mathbf{e}_2$. The "optimal $\mathbf{u}$-system" is defined by the normalized, orthogonal vectors $\mathbf{u}_1$ and $\mathbf{u}_2$. The vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ are "dual" to $\mathbf{e}_1$ and $\mathbf{e}_2$, since one can obtain $\mathbf{u}_1$ and $\mathbf{u}_2$ by rotating $\mathbf{e}_1$ and $\mathbf{e}_2$ by $+/- 45°$ $(+/- \pi/4)$, or by calculating $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_1 - \mathbf{e}_2$ to define $\mathbf{u}_1$- and $\mathbf{u}_2$-directions.}...



From $\mathbf{v}$-system to $\mathbf{e}$-system to $\mathbf{u}$-system.