Bernd Hamann
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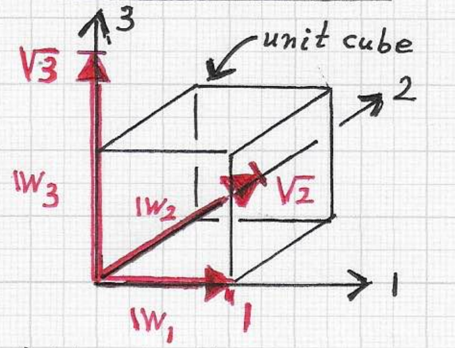
8/24/2023

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



After orthogonalization.

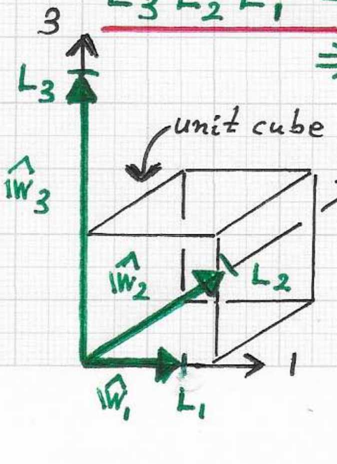
Applying the orthogonalization procedure to the given three vectors $\mathbb{v}_i$ shown in the figure on the previous page, one obtains the orthogonal vectors $\mathbb{w}_i$, sketched in the left figure. The lengths of these vectors are $\|\mathbb{w}_1\| = \|(1,0,0)^T\| = 1$, $\|\mathbb{w}_2\| = \|(0,\sqrt{2},0)^T\| = \sqrt{2}$ and $\|\mathbb{w}_3\| = \|(0,0,\sqrt{3})^T\| = \sqrt{3}$. Thus, these vectors define the same volume that the vectors $\mathbb{v}_i$ define, i.e., volume $= v = 1 \cdot \sqrt{2} \cdot \sqrt{3} = \sqrt{6}$. If length preservation (relative) of the original vectors $\mathbb{v}_i$ is desired, one will have to enforce the length ratio $\ell_3 / \ell_2 / \ell_1 = 3/2/1$ (or $3:2:1$). Thus, one must require that $L_3 : L_2 : L_1 = 3:2:1$. This requirement implies that $L_2 = 2L_1$ and $L_3 = 3L_1$. Therefore, the following volume equation must hold:

$$L_3 L_2 L_1 = 3L_1 \, 2L_1 \, L_1 = 6L_1^3 = \sqrt{6}$$

$$\Rightarrow L_1 = \sqrt[3]{\sqrt{6}/6} = 0.742$$

$$L_2 = 2L_1 = 1.484$$

$$L_3 = 3L_1 = 2.226$$



The left figure shows the resulting orthogonal vectors $\hat{\mathbb{w}}_i$ that have the same length ratio, i.e., $\|\mathbb{v}_1\| : \|\mathbb{v}_2\| : \|\mathbb{v}_3\|$.

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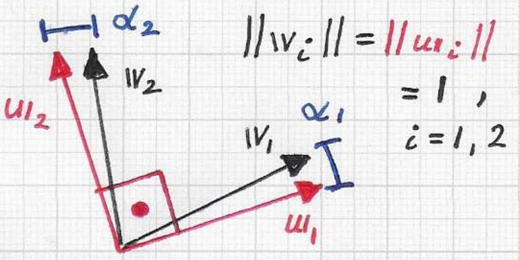
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



Orientation of pairs of vectors $\{\mathbb{w}_1, \mathbb{w}_2\}$ and $\{\mathbb{u}_1, \mathbb{u}_2\}$ minimizes angle sum $\alpha_1+\alpha_2$.

• **Note.** The methods described can be used to (i) perform orthogonalization; (ii) ensure length-ratio preservation of basis vectors; and (iii) guarantee hyper-volume preservation for parallelepipeds — in the general D-dimensional case. The top-left figure illustrates another goal that one should keep in mind when "optimally transforming" a set of non-orthogonal basis vectors to a set of orthogonal basis vectors: The figure shows a 2D example, where the goal is to map two given non-orthogonal vectors $\mathbb{w}_1$ and $\mathbb{w}_2$ to two orthogonal vectors $\mathbb{u}_1$ and $\mathbb{u}_2$, such that a measure for "overall orientation" is optimized. In other words, the transformation of $\mathbb{w}_1$ and $\mathbb{w}_2$ to $\mathbb{u}_1$ and $\mathbb{u}_2$ should minimally change the orientation of the given vectors $\mathbb{w}_1$ and $\mathbb{w}_2$. Formally, one can understand this problem as minimization of the angle sum $\alpha_1+\alpha_2$, or maximization of the sum of $\cos(\alpha_1)+\cos(\alpha_2)$. All vectors shown in the figure have length 1; considering only vectors of length 1 suffices, since the problem concerns orientation only.

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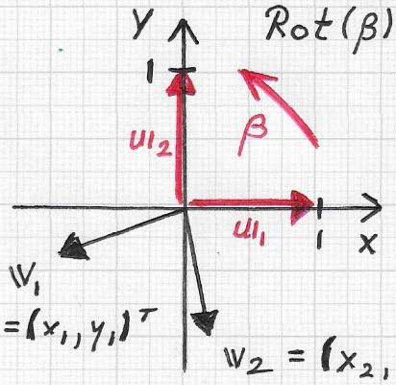
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks: ...



$$Rot(\beta) = R(\beta) = R = \begin{bmatrix} c\beta & -s\beta \\ s\beta & c\beta \end{bmatrix}$$

Rotating orthonormal basis vector pair u_1, u_2.

Concerning the two-dimensional ($D=2$) case, one can understand this optimization problem as the problem of calculating the optimal rotation angle β, see left figure. Given the orthonormal basis vector pair u_1, u_2, in initial orientation $u_1 = (1,0)^T$ and $u_2 = (0,1)^T$, one must determine the angle β for a rotation matrix $Rot(\beta) = R(\beta) = R$ that – when applied to the initial values of u_1 and u_2 – maximizes the value of $\cos(\alpha_1) + \cos(\alpha_2)$. Thus, we can tackle a univariate optimization problem that is defined as follows:

$$\begin{bmatrix} c\beta & -s\beta \\ s\beta & c\beta \end{bmatrix} \cdot \begin{bmatrix} u_1, & u_2 \end{bmatrix} = \begin{bmatrix} c\beta & -s\beta \\ s\beta & c\beta \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} c\beta & -s\beta \\ s\beta & c\beta \end{bmatrix}$$

$$\Rightarrow R \cdot u_1 = (c\beta, s\beta)^T, \quad R \cdot u_2 = (-s\beta, c\beta)^T$$

$$\Rightarrow \langle R u_1, w_1 \rangle = \langle (c\beta, s\beta)^T, (x_1, y_1)^T \rangle = x_1 c\beta + y_1 s\beta \,;$$
$$\langle R u_2, w_2 \rangle = \langle (-s\beta, c\beta)^T, (x_2, y_2)^T \rangle = -x_2 s\beta + y_2 c\beta$$

$$\Rightarrow \cos(\alpha_1) + \cos(\alpha_2) = x_1 c\beta + y_1 s\beta - x_2 s\beta + y_2 c\beta$$

$$\Rightarrow \text{Maximize } C(\beta) = \cos(\alpha_1(\beta)) + \cos(\alpha_2(\beta)) = x_1 c\beta + y_1 s\beta - x_2 s\beta + y_2 c\beta, \quad \beta \in [0, 2\pi].$$

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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... To maximize the value of $C(\beta)$, we must consider its derivative:

$$d/d\beta\ C(\beta) = -x_1 s\beta + y_1 c\beta - x_2 c\beta - y_2 s\beta \quad , \beta \in [0, 2\pi]$$

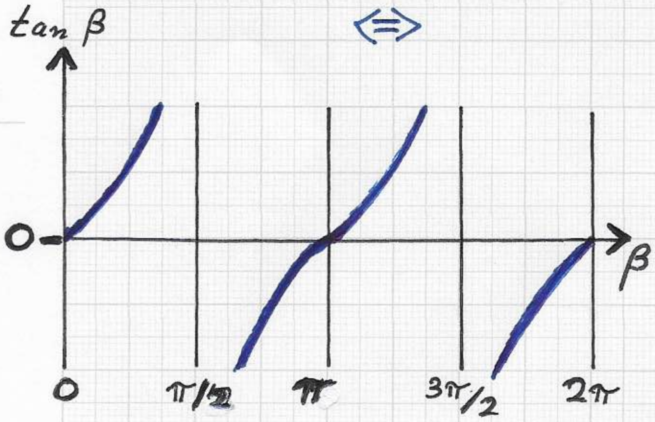
$$\Rightarrow \quad C' = -x_1 s\beta + y_1 c\beta - x_2 c\beta - y_2 s\beta = 0$$

$$\Leftrightarrow \quad (-x_1 - y_2)\, s\beta + (y_1 - x_2)\, c\beta = 0$$

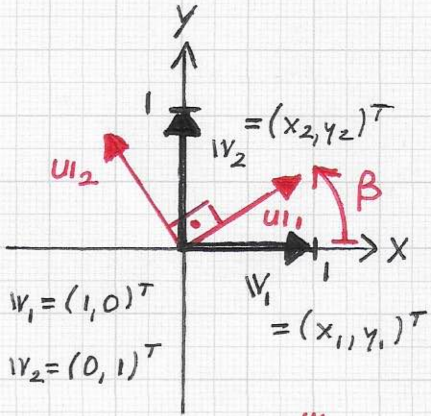
$$\Leftrightarrow \quad (x_1 + y_2)\, s\beta = (y_1 - x_2)\, c\beta$$

$$\Leftrightarrow \quad s\beta / c\beta = (y_1 - x_2)/(x_1 + y_2)$$

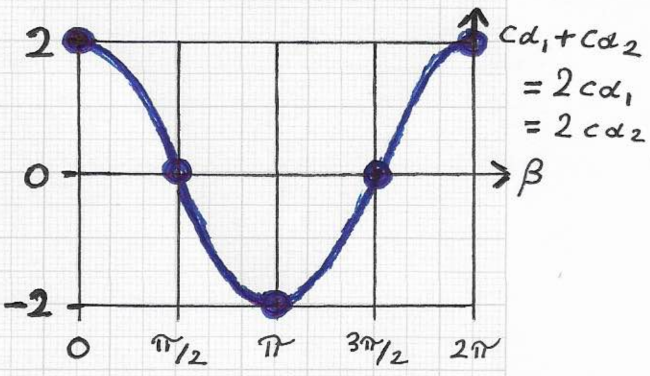
$$\Leftrightarrow \quad \tan\beta = \frac{y_1 - x_2}{x_1 + y_2} \ .$$

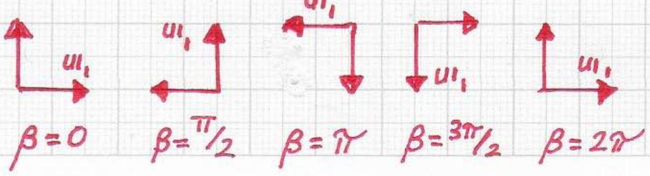


The left figure shows a qualitative sketch of the graph of the tan function. In the interval $[0, 2\pi]$, $\tan\beta = 0$ holds for $\beta \in \{0, \pi, 2\pi\}$.



β	$c\alpha_1$	$c\alpha_2$
0	1	1
$\pi/2$	0	0
π	-1	-1
$3\pi/2$	0	0
2π	1	1





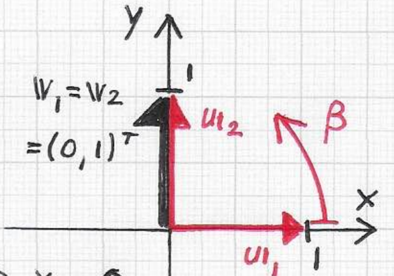
These figures and the table consider the simple example $\mathbb{v}_1 = (1,0)^T$ and $\mathbb{v}_2 = (0,1)^T$, i.e., a case where $\mathbb{v}_1$ and $\mathbb{v}_2$ are orthogonal. ...

$\Rightarrow$ **Extrema:** $\tan\beta = \dfrac{y_1 - x_2}{x_1 + y_2} = 0$

$\Rightarrow \beta = 0, \pi, 2\pi$.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The simple scenario illustrated and discussed at the bottom of the previous page uses vectors $\mathbb{V}_1$ and $\mathbb{V}_2$ that are already orthogonal. Thus, the optimal solution vectors are $\mathbb{u}_1 = \mathbb{V}_1$ and $\mathbb{u}_2 = \mathbb{V}_2$. Algebraically, $\tan\beta = (y_1 - x_2)/(x_1 + y_2)$ must hold to define an extremum of the function $C(\beta) = \cos(\alpha_1) + \cos(\alpha_2)$. Here, $\tan\beta = (0-0)/(1+1) = 0$. Further, $\tan\beta$ takes on the value 0 for $\beta = 0, \pi, 2\pi$. Due to the cyclic/periodic nature of the $\tan\beta$ function, one must only determine whether the desired maximum is associated with $\beta = 0$ or $\beta = \pi$. When evaluating $C(\beta)$ for $\beta = 0$ and $\beta = \pi$, one obtains the C-values 2 and -2, respectively. Therefore, $\beta = 0$ defines the maximal C-value – and, as expected, $\mathbb{u}_1 = \mathbb{V}_1$ and $\mathbb{u}_2 = \mathbb{V}_2$.



$\Rightarrow x_1 = 0$
$y_1 = 1$
$x_2 = 0$
$y_2 = 1$

"Limit": $\mathbb{V}_1 = \mathbb{V}_2$.

$\Rightarrow \tan\beta = \dfrac{y_1 - x_2}{x_1 + y_2} = 1$

$\Rightarrow \beta = \pi/4, 5\pi/4$.

We briefly discuss a "limit case" shown in the left figure, where $\mathbb{V}_1$ and $\mathbb{V}_2$ are equal; specifically, $\mathbb{V}_1 = \mathbb{V}_2 = (0,1)^T$. In this case, $\tan\beta = (y_1 - x_2)/(x_1 + y_2) = 1$.

β	0	$\pi/2$	π	$3\pi/2$	2π
$c\alpha_1$	0	1	0	-1	0
$c\alpha_2$	1	0	-1	0	1

Thus, $C(\beta)$ is extremal for $\beta = \pi/4$ and $\beta = 5\pi/4$. The maximal C-value is $C(\frac{\pi}{4}) = \sqrt{2}$.

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