## ■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The four points $(0, \pm 1)^T$ and $(\pm 1, 0)^T$ are merely "candidate locations" — where $f(x,y)$ might have a local extremum. The "bordered Hessian determinant" test can be used to determine whether $f(x,y)$ is indeed locally extremal at these points (relative to / on the unit circle) and — if $f$ is extremal at these points — whether an extremum is a minimum or maximum of $f$. The bordered Hessian matrix $H_B$ is defined by first- and second-derivative behavior of the function $F(x,y,\lambda) = f(x,y) - \lambda \cdot (s(x,y) - 1)$. The derivatives of $F(x,y,\lambda)$ are called $F_x$, $F_y$, $F_{xx}$, $F_{xy}$, $F_{yx}$ and $F_{yy}$. The expression $(s(x,y)-1)$ defines the contour / level set $x^2+y^2-1=0$ in our example. The matrix $H_B$ is the 3-by-3 matrix

$$H_B = \begin{bmatrix} 0 & s_x & s_y \\ s_x & F_{xx} & F_{xy} \\ s_y & F_{yx} & F_{yy} \end{bmatrix} = \begin{bmatrix} 0 & 2x & 2y \\ 2x & 2-2\lambda & 0 \\ 2y & 0 & -2-2\lambda \end{bmatrix},$$

where $s = x^2+y^2$ and $F = (x^2-y^2) - \lambda \cdot (x^2+y^2-1)$.

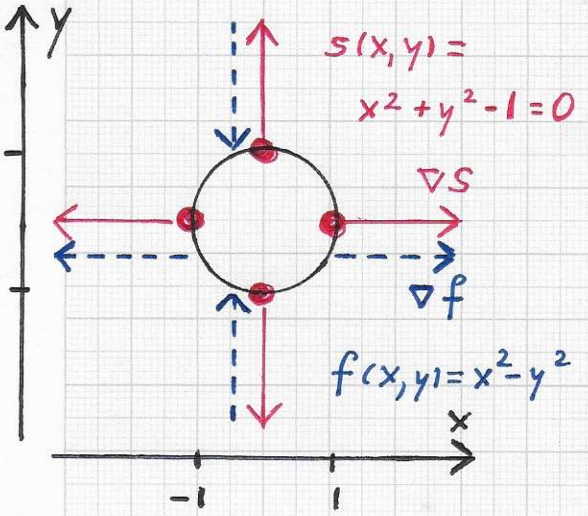
Thus, $F_{xx} = (2x - 2\lambda x)_x = 2 - 2\lambda$, $F_{xy} = F_{yx} = 0$ and $F_{yy} = (-2y - 2\lambda y)_y = -2 - 2\lambda$; $s_x = 2x$ and $s_y = 2y$.

$$\Rightarrow \det H_B = \begin{vmatrix} 0 & 2x & 2y \\ 2x & 2-2\lambda & 0 \\ 2y & 0 & -2-2\lambda \end{vmatrix} = 8\left((x^2-y^2) + \lambda(x^2+y^2)\right).$$

The type of an extremum (candidate) can (sometimes) be determined by the sign of $|H_B| = \det H_B$. ...

## ■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks: ...




We summarize the data needed for and resulting from the application of the bordered Hessian determinant test for our example and the four candidate extremal points '•' shown in the left figure. The value of $|H_B|$ indicates this:

(i) $|H_B| > 0 \Rightarrow (x,y)^T$ Local maximum;

(ii) $|H_B| < 0 \Rightarrow (x,y)^T$ Local minimum;

(iii) $|H_B| = 0 \Rightarrow$ test is inconclusive.

| $(x,y)^T$ | $\nabla s$ | $\nabla f$ | $\lambda$ | $\lvert H_B \rvert$ |
|---|---|---|---|---|
| $(-1,0)^T$ | $(-2,0)$ | $(-2,0)$ | 1 | 16 |
| $(1,0)^T$ | $(2,0)$ | $(2,0)$ | 1 | 16 |
| $(0,-1)^T$ | $(0,-2)$ | $(0,2)$ | -1 | -16 |
| $(0,1)^T$ | $(0,+2)$ | $(0,-2)$ | -1 | -16 |

When evaluating $|H_B| = 8\left((x^2-y^2)+\lambda(x^2+y^2)\right)$ for the four candidate points, one obtains the values 16 and -16, shown in the last table column. Thus, $(+/-1,0)^T$ are local maxima and $(0,+/-1)^T$ are local minima of $f(x,y)$ restricted to the unit circle. Case (iii) makes more tests necessary.

- **Note.** One can also represent the unit circle via explicit representations $y(x) = \ldots$ and $x(y) = \ldots$ and use them to define $f(x,y)$ as a univariate function, i.e., $f(x,y) = f(x, y(x)) = f(x)$ or $f(x,y) = f(x(y),y) = f(y)$. We describe this possibility for the same example.

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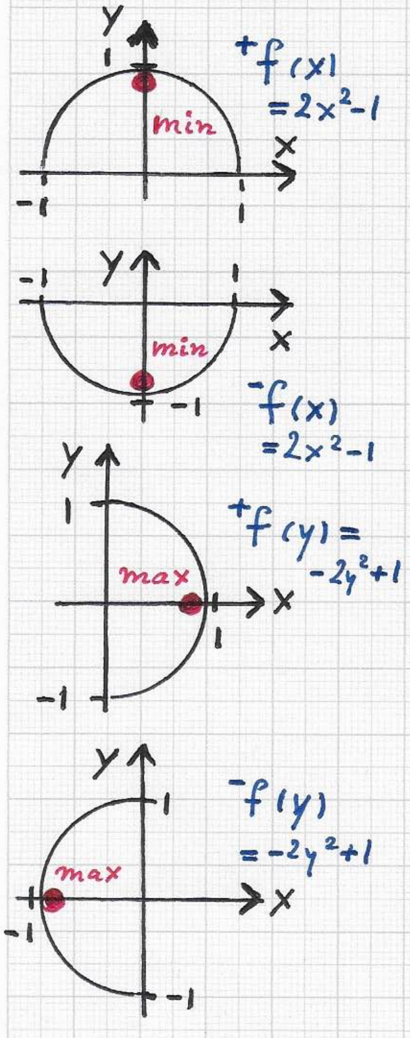
## OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...




Piecewise definition of unit circle via four explicit functions.

The four sketches of graphs in the left figure show how one can represent the unit circle — defined implicitly as $s(x,y) = x^2+y^2-1=0$ — via four univariate functions; the shown four semi-circles are defined in explicit form as

$$^{+}y=(1-x^2)^{1/2},\quad ^{-}y=-(1-x^2)^{1/2},$$

where $-1<x<1$, and

$$^{+}x=(1-y^2)^{1/2},\quad ^{-}x=-(1-y^2)^{1/2},$$

where $-1<y<1$. One can now use these functions as substitutes for the variables $y$ and $x$ in the definition of the bivariate function $f(x,y) = x^2-y^2$. One obtains

$$f(x,y) = x^2-y^2 = x^2-(1-x^2) = +2x^2-1 = {}^{+}f(x) = {}^{-}f(x),$$

since $(^{+}y)^2 = (^{-}y^2) = (1-x^2)$, and

$$f(x,y) = x^2-y^2 = (1-y^2)-y^2 = -2y^2+1 = {}^{+}f(y) = {}^{-}f(y),$$

since $(^{+}x)^2 = (^{-}x)^2 = (1-y^2)$. The first derivatives of these functions are $\frac{d}{dx}\,{}^{+}f(x) = \frac{d}{dx}\,{}^{-}f(x) = 4x$ and $\frac{d}{dy}\,{}^{+}f(y) = \frac{d}{dy}\,{}^{-}f(y) = -4y$. Thus, the extrema of these functions are defined by the requirements $4x=0 \Rightarrow x=0$ and $-4y=0 \Rightarrow y=0$. The second derivatives are $\frac{d^2}{dx^2}\,{}^{+}f(x) = \frac{d^2}{dx^2}\,{}^{-}f(x) = 4$ and $\frac{d^2}{dy^2}\,{}^{+}f(y) = \frac{d^2}{dy^2}\,{}^{-}f(y) = -4$. ...

## OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks:... Since the value of the second derivative of ${}^{+}f(x)$ and ${}^{-}f(x)$ (at $x=0$) is 4 ($>0$) and the value of the second derivative of ${}^{+}f(y)$ and ${}^{-}f(y)$ (at $y=0$) is $-4$ ($<0$), $f(x,y)$ has local minima at the points $(0,1)^T$ and $(0,-1)^T$ and local maxima at the points $(1,0)^T$ and $(-1,0)^T$ — as indicated in the figure on the previous page. Our problem — the calculation of a set of $D$ mutually orthogonal and normalized basis vectors being a best approximation of a given set of $D$ non-orthogonal, normalized basis vectors — can be understood as a constrained optimization problem. The given set $\{\mathbf{v}_i\}_{i=1}^{D}$ of basis vectors must be optimally approximated by the set $\{\mathbf{w}_i\}_{i=1}^{D}$ of orthonormal vectors. Thus, one must define this optimization problem via a (cost) function $f(x_1,\ldots,x_D)$, restricted to the unit hyper-sphere $s(x_1,\ldots,x_D) = x_1^2+\ldots+x_D^2-1=0$ (defined implicitly as a contour). Using the Lagrange multiplier method or an approach that defines the unit hyper-sphere in a piece-wise manner via multiple explicit functions are two possibilities to solve our optimization problem.

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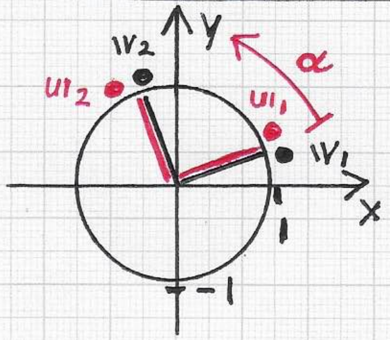
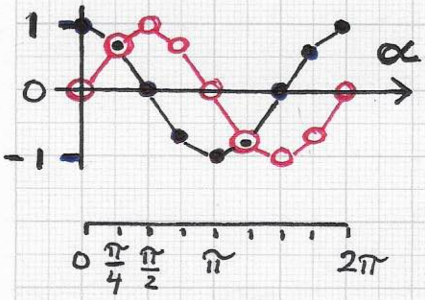
## ■ OBJECTS AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...




One can think of the orthonormalization problem as follows, when using a rotation as the underlying method used for optimization: The left figure shows an "initial configuration," i.e., two unit vectors $w_1$ and $w_2$ that are already orthogonal and thus optimal, and two orthonormal vectors $u_1$ and $u_2$ that must be rotated by an optimal angle $\alpha$ to approximate the pair $w_1$ and $w_2$ in a best-approximation way.

| $\alpha\,[\cdot\frac{\pi}{4}]$ | $u_1 \cdot w_1$ | $u_1 \cdot w_2$ | $u_2 \cdot w_1$ | $u_2 \cdot w_2$ | $C_1$ | $C_2$ |
|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 0 | 1 | 2 | 2 |
| 1 | $\sqrt{2}/2$ | $\sqrt{2}/2$ | $-\sqrt{2}/2$ | $\sqrt{2}/2$ | 0 | 0 |
| 2 | 0 | 1 | −1 | 0 | 2 | 2 |
| 3 | $-\sqrt{2}/2$ | $\sqrt{2}/2$ | $-\sqrt{2}/2$ | $-\sqrt{2}/2$ | 0 | 0 |
| 4 | −1 | 0 | 0 | −1 | 2 | 2 |
| 5 | $-\sqrt{2}/2$ | $-\sqrt{2}/2$ | $\sqrt{2}/2$ | $-\sqrt{2}/2$ | 0 | 0 |
| 6 | 0 | −1 | 1 | 0 | 2 | 2 |
| 7 | $\sqrt{2}/2$ | $-\sqrt{2}/2$ | $\sqrt{2}/2$ | $\sqrt{2}/2$ | 0 | 0 |
| 8 | 1 | 0 | 0 | 1 | 2 | 2 |
| | ↑ a | ↑ b | ↑ A | ↑ B | | |

For this "initial configuration," $\alpha \in \{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}, 2\pi\}$ is an optimal angle. We can define a cost function to be optimized via the scalar products $a = u_1 \cdot w_1$, $b = u_1 \cdot w_2$, $A = u_2 \cdot w_1$, $B = u_2 \cdot w_2$. For example, one could use

$C_1 = \left((a^2-b^2)^2 + (B^2-A^2)^2\right)$ or

$C_2 = \big|\,|a|-|b|\,\big| + \big|\,|B|-|A|\,\big|$.

The left table provides the resulting data for $\alpha = i\frac{\pi}{4}$, $i = 0, 1, \ldots, 8$.

...