Pseudo-algorithm
Principal Curve for Spherical Modelling

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Algorithm 1 : Principal Curve - Spherical Modelling

Input parameters:

$\boldsymbol{Z} \in \mathbb{R}^{M \times N}$, max-min azimuthal angles i.e., $\varphi_{\max}, \varphi_{\min}$ and sphere radius r.

Output parameters:

Ordered $\boldsymbol{Z}$, $\boldsymbol{s}$, and principal curve function $\boldsymbol{f}(\cdot) \mapsto \mathbb{R}^N$, $\operatorname{supp}(f(\cdot)) \in [0,1]$.

$h(x) = x(\varphi_{\max} - \varphi_{\min}) + \varphi_{\min}$ ▷ $x \in [0,1]$ and $h(s) \in [\varphi_{\min}, \varphi_{\max}]$

$\boldsymbol{f}^{(0)}(\cdot) = [r\cos(h(\cdot)), r\sin(h(\cdot)), \mathbb{0}]^\intercal$ ▷ $\mathbb{0} \in \mathbb{R}^{(N-2)}$, vector of zeros

$\Delta d = \infty$

$i = 1$

$\mathrm{tol} = 10^{-5}$

$\mathrm{iterations} = 100$

while $\Delta d > \mathrm{tol}$ **and** $i < \mathrm{iterations}$ **do**

  $(\boldsymbol{s}^{(i)}, d^{(i)}) \leftarrow \lambda^{(i)}(\boldsymbol{Z}^{(i)})$ ▷ Projection operator procedure

  $(\boldsymbol{s}^{(i)}, \boldsymbol{Z}^{(i)}) \leftarrow \textsc{sort}(\boldsymbol{s}^{(i)}, \boldsymbol{Z}^{(i)})$ ▷ sort $\boldsymbol{s}^{(i)}$, and $\boldsymbol{Z}^{(i)}$ matrix-rows, w.r.t. $\boldsymbol{s}^{(i)}$-values

  $\boldsymbol{p}^{(i)} = \boldsymbol{f}^{(i)}(\boldsymbol{s}^{(i)})$ ▷ Orthogonal points to the principal curve $\boldsymbol{f}^{(i)}(\cdot)$

  $\boldsymbol{s}^{(i)} \leftarrow \textsc{unit\_speed\_transform}(\boldsymbol{p}^{(i)})$

  $\boldsymbol{s}^{(i+1)} = \boldsymbol{s}^{(i)}$

  $\boldsymbol{Z}^{(i+1)} = \boldsymbol{Z}^{(i)}$

  $\Delta d = ||d^{(i)} - d^{(i-1)}||$

  $i = i + 1$

  $\boldsymbol{f}^{(i)}(\cdot) = [\hat{f}_1^{(i)}(\cdot)(\cdot \mid \boldsymbol{s}^{(i-1)}, \boldsymbol{z}_{(*,1)}^{(i-1)}), \ldots, \hat{f}_N^{(i)}(\cdot)(\cdot \mid \boldsymbol{s}^{(i-1)}, \boldsymbol{z}_{(*,N)}^{(i-1)})]^\intercal$

    ▷ where, $\hat{f}_k^{(i)}(\cdot \mid \boldsymbol{s}^{(i-1)}, \boldsymbol{z}_{(*,k)}^{(i-1)}) \mapsto \mathbb{R} \; \forall \; k = \{1, \ldots, N\}$ is an univariate spline function fitted with data values $\boldsymbol{s}^{(i-1)}$ as inputs, and the k^{th} column-vector of $\boldsymbol{Z}^{(i-1)}$ as outputs, i.e., $\boldsymbol{z}_{(*,k)}^{(i-1)}$.

end while

return $(\boldsymbol{Z}^{(i)}, \; \boldsymbol{s}^{(i)}, \boldsymbol{f}^{(i)}(\cdot))$

procedure $\lambda^{(i)}(\boldsymbol{Z}^{(i)})$: ▷ Projection operator (23), i.e., $\lambda^{(i)}(\cdot) \equiv \lambda_{\boldsymbol{f}^{(i)}(\cdot)}(\cdot)$

  $\Psi = \{s : s = \frac{n}{100}, n \in \{0, \ldots, 100\}\}$ ▷ Helper vector to segment the principal curve

  $\boldsymbol{s}^{(i)} = \mathbb{0} \in \mathbb{R}^M$ ▷ Empty 0's vector.

  $d^{(i)} = 0$

  for k **in** $\{1, \ldots, M\}$ **do**

    ▷ Search the closest segmented curve point.

    $s_{\text{init}} = \underset{s}{\operatorname{argmin}} \, ||\boldsymbol{z}_{(k,*)}^{(i)} - \boldsymbol{f}^{(i)}(\Psi)||^2$ ▷ $\boldsymbol{z}_{(k,*)}^{(i)}$ is k^{th} row-vector of $\boldsymbol{Z}^{(i)}$.

    ▷ Find the orthogonal projection to the principal curve

    ▷ solving the non-convex problem with initialization s_{init}:

    $s_k^{(i)} \leftarrow \underset{s}{\operatorname{argmin}} \, ||\boldsymbol{z}_{(k,*)}^{(i)} - \boldsymbol{f}^{(i)}(s)||^2, \quad \text{s.t. } 0 \leq s \leq 1.$ ▷ $s_k^{(i)}$ refers to elements of $\boldsymbol{s}^{(i)}$.

    $\Delta d = ||\boldsymbol{z}_{(k,*)}^{(i)} - \boldsymbol{f}^{(i)}(s_k)||$

    $d^{(i)} = d^{(i)} + \Delta d$

  end for

end procedure

procedure $\textsc{unit\_speed\_transform}(\boldsymbol{p}^{(i)})$ ▷ Constant curve speed, i.e., $||\boldsymbol{f'}^{(i)}(s)|| \equiv 1$

  $\Delta r_l = ||p_{l+1}^{(i)} - p_l^{(i)}|| \quad \forall \; l = \{1, \ldots, (M-1)\}$ ▷ $p_l^{(i)}$ refers to elements of $\boldsymbol{p}^{(i)}$.

  $\boldsymbol{s}^{(i)} = \mathbb{0} \in \mathbb{R}^M$ ▷ Empty 0's vector.

  $s_n^{(i)} \leftarrow \sum_{l=1}^{n} \Delta r_l / \sum_{l=1}^{M-1} \Delta r_l \quad \forall \; n = \{2, \ldots, M\}$ ▷ $s_n^{(i)}$ refers to elements of $\boldsymbol{s}^{(i)}$.

end procedure
