
Supplementary Material for: Unsupervised Riemannian Metric Learning for Histograms Using Aitchison Transformations*

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1 Proof for Proposition 1

The j^{th} component of the tangent vector of the positive sphere, mapped by a push-forward map F_* on a tangent vector $\mathbf{v} \in T_{\mathbf{x}}\mathbb{P}_n$

$$[F_*\mathbf{v}]_j = \frac{d}{dt} \sqrt{\frac{(\mathbf{x}_j + t\mathbf{v}_j)^{\alpha_j} \lambda_j}{\sum_{i=1}^{n+1} (\mathbf{x}_i + t\mathbf{v}_i)^{\alpha_i} \lambda_i}} \Big|_{t=0},$$

For simplify, let denote:

$$\begin{aligned} f_i(t) &= (\mathbf{x}_i + t\mathbf{v}_i)^{\alpha_i} \lambda_i, \\ h_i(t) &= \frac{df_i(t)}{dt} = (\mathbf{x}_i + t\mathbf{v}_i)^{\alpha_i-1} \lambda_i \alpha_i \mathbf{v}_i. \end{aligned}$$

So, we have:

$$[F_*\mathbf{v}]_j = \frac{h_j(t) \sum_{i=1}^{n+1} f_i(t) - f_j(t) \sum_{i=1}^{n+1} h_i(t)}{2 \sqrt{\frac{f_j(t)}{\sum_{i=1}^{n+1} f_i(t)} \left(\sum_{i=1}^{n+1} f_i(t) \right)^2}} \Big|_{t=0}$$

Since at $t = 0$, $f_i(0) = \mathbf{x}_i^{\alpha_i} \lambda_i$ and $h_i(0) = \mathbf{x}_i^{\alpha_i-1} \lambda_i \alpha_i \mathbf{v}_i$,

$$\begin{aligned} [F_*\mathbf{v}]_j &= \frac{1}{2} \mathbf{x}_j^{\frac{\alpha_j}{2}-1} \alpha_j \mathbf{v}_j \lambda_j^{\frac{1}{2}} \left(\sum_{\ell=1}^{n+1} \mathbf{x}_\ell^{\alpha_\ell} \lambda_\ell \right)^{-\frac{1}{2}} \\ &\quad - \frac{1}{2} \mathbf{x}_j^{\frac{\alpha_j}{2}} \lambda_j^{\frac{1}{2}} \frac{\sum_{\ell=1}^{n+1} \mathbf{x}_\ell^{\alpha_\ell-1} \alpha_\ell \mathbf{v}_\ell \lambda_\ell}{\left(\sum_{\ell=1}^{n+1} \mathbf{x}_\ell^{\alpha_\ell} \lambda_\ell \right)^{\frac{3}{2}}} \end{aligned}$$

Let apply $\mathbf{v} = \partial_i$, $1 \leq i \leq n$, the basis of the tangent space of the simplex $T_{\mathbf{x}}\mathbb{P}_n$

$$\begin{aligned} [F_*\partial_i]_j &= \frac{1}{2} \mathbf{x}_j^{\frac{\alpha_j}{2}-1} \alpha_j \lambda_j^{\frac{1}{2}} \left(\sum_{\ell=1}^{n+1} \mathbf{x}_\ell^{\alpha_\ell} \lambda_\ell \right)^{-\frac{1}{2}} (\delta_{j,i} - \delta_{j,n+1}) \\ &\quad - \frac{1}{2} \mathbf{x}_j^{\frac{\alpha_j}{2}} \lambda_j^{\frac{1}{2}} \frac{\mathbf{x}_i^{\alpha_i-1} \alpha_i \lambda_i - \mathbf{x}_{n+1}^{\alpha_{n+1}-1} \alpha_{n+1} \lambda_{n+1}}{\left(\sum_{\ell=1}^{n+1} \mathbf{x}_\ell^{\alpha_\ell} \lambda_\ell \right)^{\frac{3}{2}}}, \end{aligned}$$

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where $\delta_{j,i} = 1$ if $j = i$ and $\delta_{j,i} = 0$, otherwise.

Hence, we have $T = U(I - \beta\eta^T)D$.

Moreover, the metric on the positive sphere \mathbb{S}_n^+ is Euclidean. So, we have $J(\partial_i, \partial_j) = \langle F_*\partial_i, F_*\partial_j \rangle$. Consequently, we have the Gram matrix:

$$\mathcal{G} = TT^T = U(I - \beta\eta^T)D^2(I - \beta\eta^T)^T U^T.$$

2 Proof for Proposition 2

Let consider matrix $\beta\eta^T \in \mathbb{R}^{(n+1) \times (n+1)}$, and vector \mathbf{v} such that $\eta^T \mathbf{v} = 0$, so \mathbf{v} is a eigenvector of $\beta\eta^T$ with eigenvalue 0. There are n independent vectors $\{\mathbf{v}_i\}_{1 \leq i \leq n}$ such that $\eta^T \mathbf{v}_i = 0$. Moreover, $\text{trace}(\beta\eta^T) = \sum_{i=1}^{n+1} \beta_i \eta_i = 1$, or sum of the eigenvalues of $\beta\eta^T$ is 1. So, the last of $(n+1)$ eigenvalues is 1. On the other hand, $(\beta\eta^T)\beta = \beta(\eta^T\beta) = \beta$, or β is a eigenvector of $\beta\eta^T$ with eigenvalue 1. In summary, we have $\{(\mathbf{v}_i, 0)_{1 \leq i \leq n}, (\beta, 1)\}$ are eigenvectors and corresponding eigenvalues of $\beta\eta^T$. Let V be a matrix in $\mathbb{R}^{(n+1) \times (n+1)}$ whose columns are $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n, \beta\}$. So, we may express V as follow:

$$V = \begin{bmatrix} -\frac{\mathbf{x}_2 \alpha_1}{\alpha_2 \mathbf{x}_1} & \dots & -\frac{\mathbf{x}_{n+1} \alpha_1}{\alpha_{n+1} \mathbf{x}_1} & \mathbf{x}_1^{\alpha_1 - 1} \alpha_1 \lambda_1 \\ 1 & \dots & 0 & \mathbf{x}_1^{\alpha_2 - 1} \alpha_2 \lambda_2 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 1 & \mathbf{x}_{n+1}^{\alpha_{n+1} - 1} \alpha_{n+1} \lambda_{n+1} \end{bmatrix}.$$

Let Λ is a diagonal matrix in $\mathbb{R}^{(n+1) \times (n+1)}$ where $\Lambda_{ii} = 0$, for all $1 \leq i \leq n$, and $\Lambda_{(n+1)(n+1)} = 1$. We have $\beta\eta^T = V\Lambda V^{-1}$. Consequently, we have $I - \beta\eta^T = V(I - \Lambda)V^{-1}$. Since $I - \Lambda = \text{diag}(1, 1, \dots, 1, 0)$ and $I - \Lambda = (I - \Lambda)^2$, we may express $I - \beta\eta^T = \tilde{V}\tilde{V}^{-1}$, where $\tilde{V} \in \mathbb{R}^{(n+1) \times n}$ is the matrix V whose last column is removed, and $\tilde{V}^{-1} \in \mathbb{R}^{n \times (n+1)}$ is the matrix V^{-1} whose last row is removed.

Thus, we can express the Gram matrix \mathcal{G} as follow:

$$\begin{aligned} \mathcal{G} &= U\tilde{V}\tilde{V}^{-1}D^2(\tilde{V}\tilde{V}^{-1})^T U^T \\ &= (U\tilde{V})(\tilde{V}^{-1}D^2\tilde{V}^{-1})^T (U\tilde{V})^T \end{aligned}$$

We also note that $U\tilde{V}$ and $\tilde{V}^{-1}D^2\tilde{V}^{-1}$ are matrices in $\mathbb{R}^{n \times n}$. So, we have $\det \mathcal{G} = \det^2(U\tilde{V}) \det(\tilde{V}^{-1}D^2\tilde{V}^{-1})$.

Compute $\det(U\tilde{V})$: Since, we have

$$\begin{aligned} U\tilde{V} &= \begin{pmatrix} -\frac{\mathbf{x}_2 \alpha_1}{\alpha_2 \mathbf{x}_1} & \dots & -\frac{\mathbf{x}_n \alpha_1}{\alpha_n \mathbf{x}_1} & -\frac{\mathbf{x}_{n+1} \alpha_1}{\alpha_{n+1} \mathbf{x}_1} & -1 \\ 1 & \dots & 0 & -1 & \\ \vdots & \ddots & \vdots & \vdots & \\ 0 & \dots & 1 & -1 & \end{pmatrix} \\ &= \frac{\alpha_1}{\mathbf{x}_1} \begin{pmatrix} -\sum_{i=1}^{n+1} \frac{\mathbf{x}_i}{\alpha_i} & -\frac{\mathbf{x}_3}{\alpha_3} & \dots & -\frac{\mathbf{x}_n}{\alpha_n} & -\frac{\mathbf{x}_{n+1}}{\alpha_{n+1}} - \frac{\mathbf{x}_1}{\alpha_1} \\ 0 & 0 & \dots & 0 & -1 \\ 0 & 1 & \dots & 0 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -1 \end{pmatrix}. \end{aligned}$$

Therefore, $\det(U\tilde{V}) = (-1)^n \frac{\alpha_1}{\mathbf{x}_1} \sum_{i=1}^{n+1} \frac{\mathbf{x}_i}{\alpha_i}$.

Compute $\det(\widetilde{V}^{-1}D^2\widetilde{V}^{-1}{}^T)$: Let consider a $(n+1) \times (n+1)$ matrix

$$W = \begin{pmatrix} -\frac{\mathbf{r}_2}{\mathbf{r}_1} & \cdots & -\frac{\mathbf{r}_{n+1}}{\mathbf{r}_1} & \mathbf{c}_1 \\ 1 & \cdots & 0 & \mathbf{c}_2 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 1 & \mathbf{c}_{n+1} \end{pmatrix}$$

We have its inverse:

$$W^{-1} = \frac{1}{\langle \mathbf{r}, \mathbf{c} \rangle} \begin{pmatrix} -\mathbf{r}_1 \mathbf{c}_2 & \langle \mathbf{r}, \mathbf{c} \rangle - \mathbf{r}_2 \mathbf{c}_2 & -\mathbf{r}_3 \mathbf{c}_2 & \cdots & -\mathbf{r}_{n+1} \mathbf{c}_2 \\ -\mathbf{r}_1 \mathbf{c}_3 & -\mathbf{r}_2 \mathbf{c}_3 & \langle \mathbf{r}, \mathbf{c} \rangle - \mathbf{r}_2 \mathbf{c}_3 & \cdots & -\mathbf{r}_{n+1} \mathbf{c}_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathbf{r}_1 \mathbf{c}_{n+1} & -\mathbf{r}_2 \mathbf{c}_{n+1} & -\mathbf{r}_2 \mathbf{c}_{n+1} & \cdots & \langle \mathbf{r}, \mathbf{c} \rangle - \mathbf{r}_{n+1} \mathbf{c}_{n+1} \\ \mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3 & \cdots & \mathbf{r}_{n+1} \end{pmatrix},$$

where vector $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{n+1})$ and vector $\mathbf{c} = (\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_{n+1})$ are in \mathbb{R}^{n+1} .

Now, we apply for the matrix V where $\mathbf{r}_i = \frac{\mathbf{x}_i}{\alpha_i}$ and $\mathbf{c}_i = \mathbf{x}_i^{\alpha_i-1} \alpha_i \lambda_i$, for all $1 \leq i \leq (n+1)$, and remove the last row to form \widetilde{V}^{-1} . For simplicity, we denote a diagonal matrix $P \in \mathbb{R}^{n \times n}$ where $P_{ii} = \mathbf{x}_{i+1}^{\alpha_{i+1}-1} \alpha_{i+1} \lambda_{i+1}$, for all $1 \leq i \leq n$ and matrix $Q \in \mathbb{R}^{n \times (n+1)}$ as follow:

$$Q = \begin{pmatrix} -\frac{\mathbf{x}_1}{\alpha_1} & \sum_{\substack{1 \leq i \leq n+1 \\ i \neq 2}} \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\mathbf{x}_2^{\alpha_2-1} \alpha_2 \lambda_2} & -\frac{\mathbf{x}_3}{\alpha_3} & \cdots & -\frac{\mathbf{x}_{n+1}}{\alpha_{n+1}} \\ -\frac{\mathbf{x}_1}{\alpha_1} & -\frac{\mathbf{x}_2}{\alpha_2} & \sum_{\substack{1 \leq i \leq n+1 \\ i \neq 3}} \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\mathbf{x}_3^{\alpha_3-1} \alpha_3 \lambda_3} & \cdots & -\frac{\mathbf{x}_{n+1}}{\alpha_{n+1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{\mathbf{x}_1}{\alpha_1} & -\frac{\mathbf{x}_2}{\alpha_2} & -\frac{\mathbf{x}_3}{\alpha_3} & \cdots & \sum_{i=1}^n \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\mathbf{x}_{n+1}^{\alpha_{n+1}-1} \alpha_{n+1} \lambda_{n+1}} \end{pmatrix}.$$

So, we have

$$\widetilde{V}^{-1} = \frac{1}{\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \lambda_i} P Q.$$

Then, we can compute

$$\widetilde{V}^{-1}D = \frac{1}{2 \left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \lambda_i \right)^{\frac{3}{2}}} P \begin{pmatrix} -\sqrt{\mathbf{x}_1^{\alpha_1} \lambda_1} & \sum_{\substack{1 \leq i \leq n+1 \\ i \neq 2}} \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\sqrt{\mathbf{x}_2^{\alpha_2} \lambda_2}} & -\sqrt{\mathbf{x}_3^{\alpha_3} \lambda_3} & \cdots & -\sqrt{\mathbf{x}_{n+1}^{\alpha_{n+1}} \lambda_{n+1}} \\ -\sqrt{\mathbf{x}_1^{\alpha_1} \lambda_1} & \sqrt{\mathbf{x}_2^{\alpha_2} \lambda_2} & \sum_{\substack{1 \leq i \leq n+1 \\ i \neq 3}} \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\mathbf{x}_3^{\alpha_3-1} \alpha_3 \lambda_3} & \cdots & -\sqrt{\mathbf{x}_{n+1}^{\alpha_{n+1}} \lambda_{n+1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\sqrt{\mathbf{x}_1^{\alpha_1} \lambda_1} & \sqrt{\mathbf{x}_2^{\alpha_2} \lambda_2} & -\sqrt{\mathbf{x}_3^{\alpha_3} \lambda_3} & \cdots & \sum_{i=1}^n \frac{\mathbf{x}_i^{\alpha_i} \lambda_i}{\sqrt{\mathbf{x}_{n+1}^{\alpha_{n+1}} \lambda_{n+1}}} \end{pmatrix}.$$

Consequently, we have:

$$\widetilde{V}^{-1}D^2\widetilde{V}^{-1}{}^T = \frac{1}{4 \left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \lambda_i \right)^2} P (\widehat{Q} - \mathbf{1}_{n \times n}) P,$$

where \widehat{Q} is a diagonal matrix in $\mathbb{R}^{n \times n}$, $\widehat{Q}_{ii} = \sum_{j=1}^{n+1} \frac{\mathbf{x}_j^{\alpha_j} \lambda_j}{\mathbf{x}_{i+1}^{\alpha_{i+1}} \lambda_{i+1}}$ and $\mathbf{1}_{n \times n}$ is a matrix of 1 in $\mathbb{R}^{n \times n}$.

Moreover, $\det(\widehat{Q} - \mathbf{1}_{n \times n}) = \prod_{i=1}^n Q_{ii} - \sum_{i=1}^n \prod_{j \neq i} Q_{jj}$, following Lemma 2 of Lebanon (2005).

Hence, we have:

$$\det(\widehat{Q} - \mathbf{1}_{n \times n}) = \frac{\left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \boldsymbol{\lambda}_i \right)^{n-1}}{\prod_{j=1}^{n+1} \mathbf{x}_j^{\alpha_j} \boldsymbol{\lambda}_j} (\mathbf{x}_1^{\alpha_1} \boldsymbol{\lambda}_1)^2.$$

Consequently, we have

$$\begin{aligned} \det\left(\widetilde{V}^{-1} D^2 \widetilde{V}^{-1 T}\right) &= \frac{1}{4^n \left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \boldsymbol{\lambda}_i \right)^{2n}} \det^2(P) \det(\widehat{Q} - \mathbf{1}_{n \times n}). \end{aligned}$$

Since $\det(P) = \prod_{j=2}^{n+1} \mathbf{x}_j^{\alpha_j - 1} \alpha_j \boldsymbol{\lambda}_j$, we have:

$$\det\left(\widetilde{V}^{-1} D^2 \widetilde{V}^{-1 T}\right) = \frac{\left(\frac{\mathbf{x}_1}{\alpha_1} \right)^2 \left(\prod_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i - 2} \alpha_i^2 \boldsymbol{\lambda}_i \right)}{4^n \left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \boldsymbol{\lambda}_i \right)^{n+1}}.$$

$$\text{Hence, we have: } \det \mathcal{G} = \frac{\left(\sum_{i=1}^{n+1} \frac{\mathbf{x}_i}{\alpha_i} \right)^2 \left(\prod_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i - 2} \alpha_i^2 \boldsymbol{\lambda}_i \right)}{4^n \left(\sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \boldsymbol{\lambda}_i \right)^{n+1}}.$$

3 Proof for Proposition 3

The partial derivative of the objective function \mathcal{F} with respect to $\boldsymbol{\lambda}$ is:

$$\begin{aligned} \frac{\partial \mathcal{F}}{\partial \boldsymbol{\lambda}} &= \frac{1}{m} \sum_{i=1}^m \frac{\partial \log \text{dvol} g^{-1}(\mathbf{x}_i)}{\partial \boldsymbol{\lambda}} \\ &\quad - E \left(\frac{\partial \log \text{dvol} g^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} \right)_{p(\mathbf{x})} \end{aligned}$$

Since we have

$$\begin{aligned} &\frac{\partial \log \int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \text{d}\mathbf{x}}{\partial \boldsymbol{\lambda}} \\ &= \frac{1}{\int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \text{d}\mathbf{x}} \frac{\partial \int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \text{d}\mathbf{x}}{\partial \boldsymbol{\lambda}} \\ &= \frac{1}{\int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \text{d}\mathbf{x}} \int_{\mathbb{P}_n} \frac{\partial \text{dvol} J^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} \text{d}\mathbf{x} \\ &= \frac{1}{\int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \text{d}\mathbf{x}} \int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{x}) \frac{\partial \log \text{dvol} g^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} \text{d}\mathbf{x} \\ &= \int_{\mathbb{P}_n} \frac{\text{dvol} J^{-1}(\mathbf{x})}{\int_{\mathbb{P}_n} \text{dvol} J^{-1}(\mathbf{z}) \text{d}\mathbf{z}} \frac{\partial \log \text{dvol} g^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} \text{d}\mathbf{x} \\ &= E \left(\frac{\partial \log \text{dvol} J^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} \right)_{p(\mathbf{x})}. \end{aligned}$$

and

$$\frac{\partial \log \text{dvol} J^{-1}(\mathbf{x})}{\partial \boldsymbol{\lambda}} = \frac{n+1}{2 \sum_{i=1}^{n+1} \mathbf{x}_i^{\alpha_i} \boldsymbol{\lambda}_i} [\mathbf{x}_j^{\alpha_j}]_{1 \leq j \leq n+1}.$$

So, we have the proof for $\frac{\partial \mathcal{F}}{\partial \lambda}$.

Similarly, we also obtain the proof for $\frac{\partial \mathcal{F}}{\partial \alpha}$.

References

G. Lebanon. *Riemannian Geometry and Statistical Machine Learning*. PhD thesis, CMU, 2005.