Exercise 12

Due date:

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Grade : ________

Problem 1 Score: ________. The sphere is a smooth manifold
Let us turn $\mathcal{M} = \mathbb{S}^{d-1}$ into a smooth manifold. Let $p = (0, \cdots, 0, 1) \in \mathbb{R}^d$, and define

$$\mathcal{U}_+ = \mathbb{S}^{d-1} \setminus \{p\}, \quad \mathcal{U}_- = \mathbb{S}^{d-1} \setminus \{-p\},$$

$$\phi_+ : \mathcal{U}_+ \to \mathbb{R}^{d-1}, \quad \phi_+(x) = \left(\frac{x_1}{1-x_d}, \cdots, \frac{x_{d-1}}{1-x_d}\right)$$
$$\phi_- : \mathcal{U}_- \to \mathbb{R}^{d-1}, \quad \phi_-(x) = \left(\frac{x_1}{1+x_d}, \cdots, \frac{x_{d-1}}{1+x_d}\right).$$

(1) Show that $(\mathcal{U}_+, \phi_+)$ and $(\mathcal{U}_-, \phi_-)$ are each $(d-1)$-dimensional charts for $\mathbb{S}^{d-1}$.

(2) Show that the charts $(\mathcal{U}_+, \phi_+)$ and $(\mathcal{U}_-, \phi_-)$ are compatible.

(3) Deduce that $\mathcal{A} = \{(\mathcal{U}_+, \phi_+), (\mathcal{U}_-, \phi_-)\}$ is an atlas for $\mathbb{S}^{d-1}$.

(4) Let $\mathcal{A}^+$ be the maximal atlas abtained from $\mathcal{A}$. Show that the atlas topology associated to $\mathcal{A}^+$ is hausdorff and second-countable. Conclude that $\mathbb{S}^{d-1}$ is a smooth manifold.

Solution: (1) As $\mathcal{U}_+$ and $\mathcal{U}_-$ are open subsets of $\mathbb{S}^{d-1}$, and $\mathbb{R}^{d-1}$ is open, and ϕ_+ and ϕ_- are clearly smooth, it suffices to show that ϕ_+ and ϕ_- are bijections.
Let $x, y \in \mathcal{U}_+$, such that $\phi_+(x) = \phi_+(y)$. Taking the squared norm of $\phi_+(x)$, we have

$$\begin{aligned}
\|\phi_+(x)\|^2 &= \sum_{i=1}^{d-1} \left(\frac{x_i}{1-x_d}\right)^2 \\
&= \frac{\|x\|^2 - x_d^2}{(1-x_d)^2} \\
&= \frac{1-x_d^2}{(1-x_d)^2} \\
&= \frac{1+x_d}{1-x_d}.
\end{aligned}$$

Similarly, we have

$$\|\phi_+(y)\|^2 = \frac{1+y_d}{1-y_d}.$$

Since $\phi_+(x) = \phi_+(y)$, we have

$$\begin{aligned}
\|\phi_+(x)\|^2 &= \|\phi_+(y)\|^2 \\
\frac{1+x_d}{1-x_d} &= \frac{1+y_d}{1-y_d} \\
y_d - x_d &= x_d - y_d \\
x_d &= y_d.
\end{aligned}$$

Then we have $x = y$, which implies that ϕ_+ is injective.
Next, let $y \in \mathbb{R}^{d-1}$, and define x_d as

$$x_d = \frac{\|y\|^2 - 1}{\|y\|^2 + 1} \in [-1, 1),$$

and

$$(x_1, \cdots, x_{d-1}) = (1-x_d)y.$$

Then we have

$$\begin{aligned}
\|x\|^2 &= \|(x_1, \cdots, x_{d-1}, x_d)\|^2 \\
&= \|(1-x_d)y\|^2 + x_d^2 \\
&= \frac{4\|y\|^2}{(\|y\|^2+1)^2} + \frac{(\|y\|^2-1)^2}{(\|y\|^2+1)^2}
\end{aligned}$$

$$= \frac{(\|y\|^2+1)^2}{(\|y\|^2+1)^2}$$
$$= 1,$$

which implies that $x \in \mathcal{U}_+$. Therefore, ϕ_+ is surjective. Then ϕ_+ is a bijection with ϕ_+^{-1} given by

$$\phi_+^{-1}(y) = \left(\frac{2y_1}{\|y\|^2+1}, \cdots, \frac{2y_{d-1}}{\|y\|^2+1}, \frac{\|y\|^2-1}{\|y\|^2+1} \right).$$

Same argument can be applied to ϕ_-, and we can show that ϕ_- is a bijection with ϕ_-^{-1} given by

$$\phi_-^{-1}(y) = \left(\frac{2y_1}{\|y\|^2+1}, \cdots, \frac{2y_{d-1}}{\|y\|^2+1}, \frac{1-\|y\|^2}{\|y\|^2+1} \right).$$

Therefore, $(\mathcal{U}_+, \phi_+)$ and $(\mathcal{U}_-, \phi_-)$ are each $(d-1)$-dimensional charts for $\mathbb{S}^{d-1}$.

(2) Note that $\phi_+(\mathcal{U}_+ \cap \mathcal{U}_-) = \phi_-(\mathcal{U}_+ \cap \mathcal{U}_-) = \mathbb{R}^{d-1} \setminus \{0\}$ which is open in $\mathbb{R}^{d-1}$. Moreover, for all $y \in \mathbb{R}^{d-1} \setminus \{0\}$, we have

$$\phi_+ \circ \phi_-^{-1}(y) = \phi_+ \left(\frac{2y_1}{\|y\|^2+1}, \cdots, \frac{2y_{d-1}}{\|y\|^2+1}, \frac{1-\|y\|^2}{\|y\|^2+1} \right)$$
$$= \left(\frac{y_1}{\|y\|^2}, \cdots, \frac{y_{d-1}}{\|y\|^2} \right)$$
$$= \frac{y}{\|y\|^2} \in C^\infty(\mathbb{R}^{d-1} \setminus \{0\}).$$

Similarly, we have $\phi_- \circ \phi_+^{-1}(y) = \frac{y}{\|y\|^2} \in C^\infty(\mathbb{R}^{d-1} \setminus \{0\})$.
Therefore, the charts $(\mathcal{U}_+, \phi_+)$ and $(\mathcal{U}_-, \phi_-)$ are compatible.

(3) Since $(\mathcal{U}_+, \phi_+)$ and $(\mathcal{U}_-, \phi_-)$ are compatible $(d-1)$-dimensional charts for $\mathbb{S}^{d-1}$, and $\mathcal{U}_+ \cup \mathcal{U}_- = \mathbb{S}^{d-1}$, we have $\mathcal{A} = \{(\mathcal{U}_+, \phi_+), (\mathcal{U}_-, \phi_-)\}$ is an atlas for $\mathbb{S}^{d-1}$.

(4)

□

Problem 2 Score: _________. Smooth functions on the sphere
Let $\mathcal{A}$ be the atlas for $\mathbb{S}^{d-1}$ from the previous exercise.

(1) Let $f : \mathbb{S}^{d-1} \to \mathbb{R}$ be a smooth function as seen through the charts of $\mathcal{A}$. Show that f has a smooth extension $\bar{f}$ to a neighborhood of $\mathbb{S}^{d-1}$ in $\mathbb{R}^d$.

If we make additional assumptions, then the intersection of two g-convex sets is g-convex. A subset $S \subseteq \mathcal{M}$ is geodesically strongly convex if for any two points $x, y \in S$, among all geodesics segments $\gamma : [0,1] \to S$ with $\gamma(0) = x$ and $\gamma(1) = y$, exactly one of them is minimizing and this minimizing geodesic lies entirely in S.

(2) Let $S_1, S_2 \subseteq \mathcal{M}$ be two geodesically strongly convex sets. Show that $S_1 \cap S_2$ is geodesically strongly convex.

Solution: (1) Since f is smooth, then for all $x \in \mathbb{S}^{d-1}$, there exists a chart $(\mathcal{U}, \phi)$ in $\mathcal{A}$ such that $x \in \mathcal{U}$ and $f \circ \phi^{-1} : \phi(\mathcal{U}) \to \mathbb{R}$ is smooth at $\phi(x)$.

(2) Let $x, y \in S_1 \cap S_2$ and $\gamma : [0,1] \to S_1 \cap S_2$ be the unique geodesic segment with $\gamma(0) = x$ and $\gamma(1) = y$. Since S_1, S_2 are geodesically strongly convex, $\gamma(t) \in S_1$ and $\gamma(t) \in S_2$ for all $t \in [0,1]$. Therefore, $\gamma(t) \in S_1 \cap S_2$ for all $t \in [0,1]$, which implies that $S_1 \cap S_2$ is geodesically strongly convex.

□

Problem 3 Score: _________. Fréchet mean on hemisphere
Write some code to generate random points $x_1, \cdots, x_n$ on a hemisphere

$$\mathbb{S}_+^{d-1} := \{x = (x^{(1)}, \cdots, x^{(d)}) \in \mathbb{R}^d : x^{(d)} > 0, \|x\| = 1\}$$

near the north pole, and implement the cost function for the intrinsic averaging, that is

$$f : \mathbb{S}_+^{d-1} \to \mathbb{R}, \quad f(x) = \frac{1}{2n} \sum_{i=1}^{n} \operatorname{dist}(x, x_i)^2.$$

A global minimizer of f is called the Fréchet mean of $x_1, \cdots, x_n$.
Recall that the squared distance between two points $x, y \in \mathbb{S}_+^{d-1}$ is given by

$$\operatorname{dist}(x, y)^2 = \arccos^2(x^\top y),$$

and the Riemannian gradient of the squared distance is given by

$$\operatorname{grad}\left(x \mapsto \frac{1}{2}\operatorname{dist}(x, y)\right)(x) = \frac{\operatorname{dist}(x, y)}{\sin(\operatorname{dist}(x, y))}(\cos(\operatorname{dist}(x, y))x - y).$$

Problem 4 Score: _________. Robust covariance estimation
Consider n points $x_1, \cdots, x_n \in \mathbb{R}^d$ sampled independently and identically distributed from a distribution P with zero mean. We want to estimate the covariance matrix of P. If P is a zero-mean normal distribution with covariance $\Sigma_{true} \in \mathbb{R}^{d\times d}$, then the maximum likelihood estimation amounts to minimizing the negative log-likelihood

$$\Sigma \mapsto \log(\det \Sigma) + \frac{1}{n} \sum_{j=1}^{n} x_j^\top \Sigma^{-1} x_j$$

over the $d \times d$ positive definite matrices

$$\mathcal{P}_d = \{\Sigma \in \mathbb{R}^{d\times d} : \Sigma = \Sigma^\top, \Sigma \succ 0\}.$$

The sample covariance matrix $\Sigma^* = \frac{1}{n}\sum_{j=1}^{n} x_j x_j^\top$ is a minimizer of this nagetive log-likelihood.
The sample covariance is not robust to outliers. So if P is not normal but some heavy-tailed distribution, then the sample covariance is not suitable. We can obtain a robust estimation of the covariance by minimizing the function

$$f : \mathcal{P}_d \to \mathbb{R}, \quad f(\Sigma) = \log(\det \Sigma) + \frac{1}{n} \sum_{j=1}^{n} d \log(x_j^\top \Sigma^{-1} x_j),$$

which places less emphasis on outliers (points far from the mean). A minimizer of this function is called "Tyler's M-estimator of scatter". It does not have a closed form solution, and the cost function f is non-convex in the Euclidean sense. However, it is g-convex in an appropriate metric, and so a minimizer can be found efficiently(e.g., with RGD).
We consider $\mathcal{M} = \mathcal{P}_d$ as an open subset of the symmetric $d \times d$ matrices, and endow it with the Fisher-Rao metric

$$\langle \dot\Sigma_1, \dot\Sigma_2 \rangle_\Sigma = \operatorname{Tr}(\Sigma^{-1}\dot\Sigma_1\Sigma^{-1}\dot\Sigma_2),$$

for $\Sigma \in \mathcal{P}_d$ and $\dot\Sigma_1, \dot\Sigma_2 \in \mathrm{T}_\Sigma\mathcal{P}_d = \{\dot\Sigma \in \mathbb{R}^{d\times d} : \dot\Sigma = \dot\Sigma^\top\}$. In this Riemannian metric, $\mathcal{P}_d$ is complete and geodesically strongly convex. For every $\Sigma_0, \Sigma_1 \in \mathcal{P}_d$, there is a unique geodesic segment between them, given by

$$\gamma(t) = \Sigma_0^{1/2}(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})^t\Sigma_0^{1/2}, \quad t \in [0, 1].$$

This geodesic segment is minimizing. Alternatively, for every $\Sigma_0, \Sigma_1 \in \mathcal{P}_d$, there exists an invertible $V \in \mathbb{R}^{d\times d}$ and a diagonal $D \in \mathcal{P}_d$ such that $\Sigma_0 = VV^\top, \Sigma_1 = VDV^\top$. In this case,

$$\gamma(t) = VD^tV^\top, \quad t \in [0, 1].$$

(1) Show that the function $\Sigma \mapsto \log(\det \Sigma)$ is g-convex.

(2) Show that if $g : \mathcal{P}_d \to \mathbb{R}$ is g-convex, then the function $h(\Sigma) = g(\Sigma^{-1})$ is g-convex.

(3) Show that if $x \in \mathbb{R}^d$, then the function $\Sigma \mapsto \log(x^\top \Sigma x)$ is g-convex.

(4) Conclude that the function f is g-convex.

Solution: (1) Let $\Sigma_0, \Sigma_1 \in \mathcal{P}_d$, then the unique geodesic segment between Σ_0 and Σ_1 is given by

$$\gamma(t) = \Sigma_0^{1/2}(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})^t\Sigma_0^{1/2}, \quad t \in [0,1].$$

For all $t \in [0,1]$, we have

$$\begin{aligned}
\log(\det \gamma(t)) &= \log(\det(\Sigma_0^{1/2}(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})^t\Sigma_0^{1/2})) \\
&= \log\left(\det(\Sigma_0^{1/2})\det(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})^t\det(\Sigma_0^{1/2})\right) \\
&= \log(\det(\Sigma_0)) + t\log(\det(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})) \\
&= \log(\det(\Sigma_0)) + t\log\left(\det(\Sigma_0^{-1/2})\det(\Sigma_1)\det(\Sigma_0^{-1/2})\right) \\
&= \log(\det(\Sigma_0)) + t\log(\det(\Sigma_1)) - t\log(\det(\Sigma_0)) \\
&= (1-t)\log(\det(\Sigma_0)) + t\log(\det(\Sigma_1))
\end{aligned}$$

Therefore, $\log(\det \Sigma)$ is g-convex. Moreover, it's g-affine.

(2) Let $\Sigma_0, \Sigma_1 \in \mathcal{P}_d$, then the unique geodesic segment between Σ_0 and Σ_1 is given by

$$\gamma(t) = \Sigma_0^{1/2}(\Sigma_0^{-1/2}\Sigma_1\Sigma_0^{-1/2})^t\Sigma_0^{1/2}, \quad t \in [0,1].$$

Let $g : \mathcal{P}_d \to \mathbb{R}$ be g-convex, then for all $t \in [0,1]$, we have

$$\begin{aligned}
h(\gamma(t)) &= g(\gamma(t)^{-1}) \\
&\leq (1-t)g(\Sigma_0^{-1}) + tg(\Sigma_1^{-1}) \\
&= (1-t)h(\Sigma_0) + th(\Sigma_1).
\end{aligned}$$

Therefore, h is g-convex.

(3) Fix $x \in \mathbb{R}^d \setminus \{0\}$ and $F : \mathcal{P}_d \to \mathbb{R}$ given by $F(\Sigma) = \log(x^\top \Sigma x)$. Let $\Sigma \in \mathcal{P}_d$ and $\dot{\Sigma} \in \mathrm{T}_\Sigma\mathcal{P}_d$, then the differential of F at Σ in the direction $\dot{\Sigma}$ is given by

$$\begin{aligned}
DF(\Sigma)(\dot{\Sigma}) &= \frac{d}{dt}\log(x^\top(\Sigma + t\dot{\Sigma})x)\bigg|_{t=0} \\
&= (x^\top\Sigma x)^{-1}x^\top\dot{\Sigma}x \\
&= (x^\top\Sigma x)^{-1}\operatorname{Tr}(\dot{\Sigma}xx^\top).
\end{aligned}$$

Then the Euclidean gradient of F at Σ is given by

$$\operatorname{grad}_\mathcal{E} F(\Sigma) = \frac{xx^\top}{x^\top\Sigma x}.$$

The Euclidean Hessian of F at Σ is given by

$$\begin{aligned}
\operatorname{Hess}_\mathcal{E} F(\Sigma)(\dot{\Sigma}) &= D\operatorname{grad}_\mathcal{E} F(\Sigma)(\dot{\Sigma}) \\
&= D\left(\frac{xx^\top}{x^\top\Sigma x}\right)(\dot{\Sigma}) \\
&= -\frac{xx^\top x^\top\dot{\Sigma}x}{(x^\top\Sigma x)^2}.
\end{aligned}$$

Then the Riemannian Hessian of F at Σ is given by

$$\begin{aligned}
\operatorname{Hess}_\mathcal{M} F(\Sigma)(\dot{\Sigma}) &= \Sigma\operatorname{Hess}_\mathcal{E} F(\Sigma)(\dot{\Sigma})\Sigma + \frac{\dot{\Sigma}\operatorname{grad}_\mathcal{E} F(\Sigma)\Sigma + \Sigma\operatorname{grad}_\mathcal{E} F(\Sigma)\dot{\Sigma}}{2} \\
&= -\frac{\Sigma xx^\top x^\top\dot{\Sigma}x\Sigma}{(x^\top\Sigma x)^2} + \frac{\dot{\Sigma}xx^\top\Sigma + \Sigma xx^\top\dot{\Sigma}}{2x^\top\Sigma x} \\
&= \frac{1}{2x^\top\Sigma x}(\dot{\Sigma}xx^\top\Sigma + \Sigma xx^\top\dot{\Sigma} - \frac{2\Sigma xx^\top x^\top\dot{\Sigma}x\Sigma}{x^\top\Sigma x}).
\end{aligned}$$

To show the Riemannian Hessian is positive semidefinite,

$$
\begin{aligned}
\langle \operatorname{Hess}_{\mathcal{M}} F(\Sigma)(\dot{\Sigma}), \dot{\Sigma}\rangle_{\Sigma} &= \operatorname{Tr}\left(\Sigma^{-1} \operatorname{Hess}_{\mathcal{M}} F(\Sigma)(\dot{\Sigma})\Sigma^{-1}\dot{\Sigma}\right) \\
&= \frac{1}{2x^\top \Sigma x} \operatorname{Tr}\left(\Sigma^{-1}(\dot{\Sigma}xx^\top\Sigma + \Sigma xx^\top\dot{\Sigma} - \frac{2\Sigma xx^\top x^\top\dot{\Sigma}x\Sigma}{x^\top\Sigma x})\Sigma^{-1}\dot{\Sigma}\right) \\
&= \frac{1}{2x^\top \Sigma x} \operatorname{Tr}\left(\Sigma^{-1}\dot{\Sigma}xx^\top\dot{\Sigma} + xx^\top\dot{\Sigma}\Sigma^{-1}\dot{\Sigma} - \frac{2xx^\top x^\top\dot{\Sigma}x\dot{\Sigma}}{x^\top\Sigma x}\right) \\
&= \frac{1}{x^\top \Sigma x}\left(x^\top\dot{\Sigma}\Sigma^{-1}\dot{\Sigma}x - \frac{(x^\top\dot{\Sigma}x)^2}{x^\top\Sigma x}\right) \\
&= \frac{1}{(x^\top\Sigma x)^2}\left[(x^\top\Sigma x)(x^\top\dot{\Sigma}\Sigma^{-1}\dot{\Sigma}x) - (x^\top\dot{\Sigma}x)^2\right] \geq 0.
\end{aligned}
$$

Therefore, $F(\Sigma) = \log(x^\top\Sigma x)$ is g-convex.

(4) As shown in (1), (2), and (3), the functions $\log(\det\Sigma)$, $\log(\det\Sigma^{-1})$, and $\log(x^\top\Sigma x)$ are g-convex. Therefore, the function f is g-convex as a non-negative combination of g-convex functions.

$\square$