The Riemannian barycentre as a proxy for global optimisation

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Abstract. Let M be a simply-connected compact Riemannian symmetric space, and U a twice-differentiable function on M, with unique global minimum at $x^* \in M$. The idea of the present work is to replace the problem of searching for the global minimum of U, by the problem of finding the Riemannian barycentre of the Gibbs distribution $P_T \propto \exp(-U/T)$. In other words, instead of minimising the function U itself, to minimise $\mathcal{E}_T(x) = \frac{1}{2} \int d^2(x, z) P_T(dz)$, where $d(\cdot, \cdot)$ denotes Riemannian distance. The following original result is proved : if U is invariant by geodesic symmetry about x^* , then for each $\delta < \frac{1}{2}r_{cx}$ (r_{cx} the convexity radius of M), there exists T_{δ} such that $T \leq T_{\delta}$ implies \mathcal{E}_T is strongly convex on the geodesic ball $B(x^*, \delta)$, and x^* is the unique global minimum of \mathcal{E}_T . Moreover, this T_{δ} can be computed explicitly. This result gives rise to a general algorithm for black-box optimisation, which is briefly described, and will be further explored in future work.

Keywords: Riemannian barycentre \cdot black-box optimisation \cdot symmetric space.

It is common knowledge that the Riemannian barycentre \bar{x} , of a probability distribution P defined on a Riemannian manifold M, may fail to be unique. However, if P is supported inside a geodesic ball $B(x^*, \delta)$ with radius $\delta < \frac{1}{2}r_{cx}$ $(r_{cx}$ the convexity radius of M), then \bar{x} is unique and also belongs to $B(x^*, \delta)$. In fact, Afsari has shown this to be true, even when $\delta < r_{cx}$ (see [1][2]).

Does this statement continue to hold, if P is not supported inside $B(x^*, \delta)$, but merely concentrated on this ball? The answer to this question is positive, assuming that M is a simply-connected compact Riemannian symmetric space, and $P = P_T \propto \exp(-U/T)$, where the function U has unique global minimum at $x^* \in M$. This is given by Proposition 2, in Section 2 below.

Proposition 2 motivates the main idea of the present work: the Riemannian barycentre \bar{x}_T of P_T can be used as a proxy for the global minimum x^* of U. In general, \bar{x}_T only provides an approximation of x^* , but the two are equal if U is invariant by geodesic symmetry about x^* , as stated in Proposition 3, in Section 4 below.

The following Section 1 introduces Proposition 1, which estimates the Riemannian distance between \bar{x}_{τ} and x^* , as a function of T.

1 Concentration of the barycentre

Let P be a probability distribution on a complete Riemannian manifold M. A (Riemannian) barycentre of P is any global minimiser $\bar{x} \in M$ of the function

$$\mathcal{E}(x) = \frac{1}{2} \int_{M} d^{2}(x, z) P(dz) \quad \text{for } x \in M$$
(1)

The following statement is due to Karcher, and was improved upon by Afsari [1][2]: if P is supported inside a geodesic ball $B(x^*, \delta)$, where $x^* \in M$ and $\delta < \frac{1}{2}r_{cx}$ (r_{cx} the convexity radius of M), then \mathcal{E} is strongly convex on $B(x^*, \delta)$, and P has a unique barycentre $\bar{x} \in B(x^*, \delta)$.

On the other hand, the present work considers a setting where P is not supported inside $B(x^*, \delta)$, but merely concentrated on this ball. Precisely, assume P is equal to the Gibbs distribution

$$P_T(dz) = (Z(T))^{-1} \exp\left[-\frac{U(z)}{T}\right] \operatorname{vol}(dz) \; ; \; T > 0 \tag{2}$$

where Z(T) is a normalising constant, U is a C^2 function with unique global minimum at x^* , and vol is the Riemannian volume of M. Then, let \mathcal{E}_T denote the function \mathcal{E} in (1), and let \bar{x}_T denote any barycentre of P_T .

In this new setting, it is not clear whether \mathcal{E}_{τ} is differentiable or not. Therefore, statements about convexity of \mathcal{E}_{τ} and uniqueness of \bar{x}_{τ} are postponed to the following Section 2. For now, it is possible to state the following Proposition 1. In this proposition, $d(\cdot, \cdot)$ denotes Riemannian distance, and $W(\cdot, \cdot)$ denotes the Kantorovich (L^1 -Wasserstein) distance [3][4]. Moreover, (μ_{\min}, μ_{\max}) is any open interval which contains the spectrum of the Hessian $\nabla^2 U(x^*)$, considered as a linear mapping of the tangent space $T_{x^*}M$.

Proposition 1. assume M is an n-dimensional compact Riemannian manifold with non-negative sectional curvature. Denote δ_{x^*} the Dirac distribution at x^* . The following hold,

(i) for any $\eta > 0$,

$$W(P_T, \delta_{x^*}) < \frac{\eta^2}{(4\operatorname{diam} M)} \implies d(\bar{x}_T, x^*) < \eta$$
(3)

(ii) for $T \leq T_o$ (which can be computed explicitly)

$$W(P_T, \delta_{x^*}) \le \sqrt{2\pi} (\pi/2)^{n-1} B_n^{-1} (\mu_{\max}/\mu_{\min})^{n/2} (T/\mu_{\min})^{1/2}$$
(4)

where $B_n = B(1/2, n/2)$ in terms of the Beta function.

Proposition 1 is motivated by the idea of using \bar{x}_T as an approximation of x^* . Intuitively, this requires choosing T so small that P_T is sufficiently close to δ_{x^*} . Just how small a T may be required is indicated by the inequality in (4). This inequality is optimal and explicit, in the following sense. It is optimal because the dependence on $T^{1/2}$ in its right-hand side cannot be improved. Indeed, by the multi-dimensional Laplace approximation (see [5], for example), the left-hand side is equivalent to $L \cdot T^{1/2}$ (in the limit $T \to 0$). While this constant L is not tractable, the constants appearing in Inequality (4) depend explicitly on the manifold M and the function U. In fact, this inequality does not follows from the multi-dimensional Laplace approximation, but rather from volume comparison theorems of Riemannian geometry [6].

In spite of these nice properties, Inequality (4) does not escape the curse of dimensionality. Indeed, for fixed T, its right-hand side increases exponentially with the dimension n (note that B_n decreases like $n^{-1/2}$). On the other hand, although T_o also depends on n, it is typically much less affected by dimensionality, and decreases slower that n^{-1} as n increases.

2 Convexity and uniqueness

Assume now that M is a simply-connected, compact Riemannian symmetric space. In this case, for any T, the function \mathcal{E}_T turns out to be C^2 throughout M. This results from the following lemma.

Lemma 1. let M be a simply-connected compact Riemannian symmetric space. Let $\gamma : I \to M$ be a geodesic defined on a compact interval I. Denote $\operatorname{Cut}(\gamma)$ the union of all cut loci $\operatorname{Cut}(\gamma(t))$ for $t \in I$. Then, the topological dimension of $\operatorname{Cut}(\gamma)$ is strictly less than $n = \dim M$. In particular, $\operatorname{Cut}(\gamma)$ is a set with volume equal to zero.

Remark : the assumption that M is simply-connected cannot be removed, as the conclusion does not hold if M is a real projective space.

The proof of Lemma 1 uses the structure of Riemannian symmetric spaces, as well as some results from topological dimension theory [7] (Chapter VII). The notion of topological dimension arises because it is possible $\operatorname{Cut}(\gamma)$ is not a manifold. The lemma immediately implies, for all t,

$$\mathcal{E}_{T}(\gamma(t)) = \frac{1}{2} \int_{M} d^{2}(\gamma(t), z) P_{T}(dz) = \frac{1}{2} \int_{M-\operatorname{Cut}(\gamma)} d^{2}(\gamma(t), z) P_{T}(dz)$$

Then, since the domain of integration avoids the cut loci of all the $\gamma(t)$, it becomes possible to differentiate under the integral. This is used in obtaining the following (the assumptions are the same as in Lemma 1).

Corollary 1. for $x \in M$, let $G_x(z) = \nabla f_z(x)$ and $H_x(z) = \nabla^2 f_z(x)$, where f_z is the function $x \mapsto \frac{1}{2} d^2(x, z)$. The following integrals converge for any T

$$G_x = \int_{M-\operatorname{Cut}(x)} G_x(z) P_T(dz) \; ; \; H_x = \int_{M-\operatorname{Cut}(x)} H_x(z) P_T(dz)$$

and both depend continuously on x. Moreover,

$$\nabla \mathcal{E}_T(x) = G_x \text{ and } \nabla^2 \mathcal{E}_T(x) = H_x$$
 (5)

so that \mathcal{E}_T is C^2 throughout M.

With Corollary 1 at hand, it is possible to obtain Proposition 2, which is concerned with the convexity of \mathcal{E}_T and uniqueness of \bar{x}_T . In this proposition, the following notation is used

$$f(T) = (2/\pi) \left(\pi/8\right)^{n/2} \left(\mu_{\max}/T\right)^{n/2} \exp\left(-U_{\delta}/T\right)$$
(6)

where $U_{\delta} = \inf\{U(x) - U(x^*); x \notin B(x^*, \delta)\}$ for positive δ . The reader may wish to note the fact that f(T) decreases to 0 as T decreases to 0.

Proposition 2. let M be a simply-connected compact Riemannian symmetric space. Let κ^2 be the maximum sectional curvature of M, and $r_{cx} = \kappa^{-1} \frac{\pi}{2}$ its convexity radius. If $T \leq T_o$ (see (ii) of Proposition 1), then the following hold for any $\delta < \frac{1}{2}r_{cx}$.

(i) for all x in the geodesic ball $B(x^*, \delta)$,

$$\nabla^2 \mathcal{E}_T(x) \ge \operatorname{Ct}(2\delta) \left(1 - \operatorname{vol}(M)f(T)\right) - \pi A_M f(T) \tag{7}$$

where $\operatorname{Ct}(2\delta) = 2\kappa\delta \cot(2\kappa\delta) > 0$ and $A_M > 0$ is a constant given by the structure of the symmetric space M.

(ii) there exists T_{δ} (which can be computed explicitly), such that $T \leq T_{\delta}$ implies \mathcal{E}_{T} is strongly convex on $B(x^*, \delta)$, and has a unique global minimum $\bar{x}_{T} \in B(x^*, \delta)$. In particular, this means \bar{x}_{T} is the unique barycentre of P_{T} .

Note that (ii) of Proposition 2 generalises the statement due to Karcher [1], which was recalled in Section 1.

3 Finding T_o and T_δ

Propositions 1 and 2 claim that T_o and T_δ can be computed explicitly. This means that, with some knowledge of the Riemannian manifold M and the function U, T_o and T_δ can be found by solving scalar equations. The current section gives the definitions of T_o and T_δ .

In the notation of Proposition 1, let $\rho > 0$ be small enough, so that,

$$\mu_{\min} d^2(x, x^*) \le 2 \left(U(x) - U(x^*) \right) \le \mu_{\max} d^2(x, x^*)$$

whenever $d(x, x^*) \leq \rho$, and consider the quantity

$$f(T,m,\rho) = (2/\pi)^{1/2} (\mu_{\max}/T)^{m/2} \exp(-U_{\rho}/T)$$

where U_{ρ} is defined as in (6). Note that $f(T, m, \rho)$ decreases to 0 as T decreases to 0, for fixed m and ρ . Now, it is possible to define T_{ρ} as

$$T_{o} = \min \left\{ T_{o}^{1}, T_{o}^{2} \right\} \text{ where}$$

$$T_{o}^{1} = \inf \left\{ T > 0 : f(T, n - 2, \rho) > \rho^{2-n} A_{n-1} \right\}$$

$$T_{o}^{2} = \inf \left\{ T > 0 : f(T, n + 1, \rho) > (\mu_{\max} / \mu_{\min})^{n/2} C_{n} \right\}$$
(8)

Here, $A_n = E|X|^n$ for $X \sim N(0, 1)$, and $C_n = \omega_n A_n/(\operatorname{diam} M \times \operatorname{vol} M)$, where ω_n is the surface area of a unit sphere S^{n-1} .

With regard to Proposition 2, define T_{δ} as follows,

$$T_{\delta} = \min\left\{T_{\delta}^{1}, T_{\delta}^{2}\right\} - \varepsilon \tag{9}$$

for some arbitrary $\varepsilon > 0$. Here, in the notation of (4), (6) and (7),

$$T_{\delta}^{1} = \inf \left\{ T \leq T_{o} : \sqrt{2\pi} \left(T/\mu_{\min} \right)^{1/2} > \delta^{2} \left(\mu_{\min}/\mu_{\max} \right)^{n/2} D_{n} \right\}$$
$$T_{\delta}^{2} = \inf \left\{ T \leq T_{o} : f(T) > \operatorname{Ct}(2\delta) \left(\operatorname{Ct}(2\delta) \operatorname{vol}(M) + \pi A_{M} \right)^{-1} \right\}$$

where $D_n = (2/\pi)^{n-1} B_n / (4 \operatorname{diam} M)$.

4 Black-box optimisation

Consider the problem of searching for the unique global minimum x^* of U. In black-box optimisation, it is only possible to evaluate U(x) for given $x \in M$, and the cost of this evaluation precludes numerical approximation of derivatives. Then, the problem is to find x^* using successive evaluations of U(x) (hopefully, as few of these evaluations as possible).

Here, a new algorithm for solving this problem is described. The idea of this algorithm is to find \bar{x}_T using successive evaluations of U(x), in the hope that \bar{x}_T will provide a good approximation of x^* . While the quality of this approximation is controlled by Inequalities (3) and (4) of Proposition 1, in some cases of interest, \bar{x}_T is exactly equal to x^* , for correctly chosen T, as in the following proposition 3.

To state this proposition, let s_{x^*} denote geodesic symmetry about x^* (see [7]). This is the transformation of M, which leaves x^* fixed, and reverses the direction of geodesics passing through x^* .

Proposition 3. assume that U is invariant by geodesic symmetry about x^* , in the sense that $U \circ s_{x^*} = U$. If $T \leq T_{\delta}$ (see (ii) of Proposition 2), then $\bar{x}_T = x^*$ is the unique barycentre of P_T .

Proposition 3 follows rather directly from Proposition 2. Precisely, by (*ii*) of Proposition 2, the condition $T \leq T_{\delta}$ implies \mathcal{E}_T is strongly convex on $B(x^*, \delta)$, and $\bar{x}_T \in B(x^*, \delta)$. Thus, \bar{x}_T is the unique stationary point of \mathcal{E}_T in $B(x^*, \delta)$. But, using the fact that U is invariant by geodesic symmetry about x^* , it is possible to prove that x^* is a stationary point of \mathcal{E}_T , and this implies $\bar{x}_T = x^*$. The two following examples verify the conditions of Proposition 3.

Example 1: assume $M = \operatorname{Gr}(k, \mathbb{C}^n)$ is a complex Grassmann manifold. In particular, M is a simply-connected, compact Riemannian symmetric space. Identify M with the set of Hermitian projectors $x : \mathbb{C}^n \to \mathbb{C}^n$ such that $\operatorname{tr}(x) = k$, where tr denotes the trace. Then, define $U(x) = -\operatorname{tr}(Cx)$ for $x \in \operatorname{Gr}(k, \mathbb{C}^n)$, where C is a Hermitian positive-definite matrix with distinct eigenvalues. Now, the unique global minimum of U occurs at x^* , the projector onto the principal k-subspace of C. Also, the geodesic symmetry s_{x^*} is given by $s_{x^*} \cdot x = r_{x^*} x r_{x^*}$, where $r_{x^*} : \mathbb{C}^n \to \mathbb{C}^n$ denotes reflection through the image space of x^* . It is elementary to verify that U is invariant by this geodesic symmetry.

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Example 2: let M be a simply-connected, compact Riemannian symmetric space, and U_a a function on M with unique global minimum at $o \in M$. Assume moreover that U_o is invariant by geodesic symmetry about o. For each $x^* \in M$, there exists an isometry g of M, such that $x^* = g \cdot o$. Then, $U(x) = U_o(g^{-1} \cdot x)$ has unique global minimum at x^* , and is invariant by geodesic symmetry about x^* .

Example 1 describes the standard problem of finding the principal subspace of the covariance matrix C. In Example 2, the function U_{o} is a known template, which undergoes an unknown transformation g, leading to the observed pattern U. This is a typical situation in pattern recognition problems.

Of course, from a mathematical point of view, Example 2 is not really an example, since it describes the completely general setting where the conditions of Proposition 3 are verified. In this setting, consider the following algorithm.

Description of the algorithm:

(1) sample $z_n \sim q(z_{n-1}, z)$

$$\begin{array}{ll} - \text{ input}: T \leq T_{\delta} & \% \text{ to find such } T, \text{ see Section 3} \\ Q(x,dz) = q(x,z) \text{vol}(dz) & \% \text{ symmetric Markov kernel} \\ \hat{x}_0 = z_0 \in M & \% \text{ initial guess for } x^* \\ - \text{ iterate}: \text{ for } n = 1, 2, \dots \end{array}$$

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- (2) compute $r_n = 1 \min\{1, \exp[(U(z_{n-1}) U(z_n))/T]\}$
- (3) reject z_n with probability r_n % then, $z_n = z_{n-1}$ (4) $\hat{x}_n = \hat{x}_{n-1} \#_{\frac{1}{n}} z_n$ % see definition (10) below

– until: \hat{x}_n does not change sensibly

- output : \hat{x}_n

% approximation of x^*

The above algorithm recursively computes the Riemannian barycentre \hat{x}_n of the samples z_n generated by a symmetric Metropolis-Hastings algorithm (see [8]). Here, The Metropolis-Hastings algorithm is implemented in lines (1)--(3). On the other hand, line (4) takes care of the Riemannian barycentre. Precisely, if $\gamma: [0,1] \to M$ is a length-minimising geodesic connecting \hat{x}_{n-1} to z_n , let

$$\hat{x}_{n-1} \#_{\frac{1}{n}} z_n = \gamma \left(1/n \right) \tag{10}$$

This geodesic γ need not be unique.

The point of using the Metropolis-Hastings algorithm is that the generated z_n eventually sample from the Gibbs distribution P_T . The convergence of the distribution P_n of z_n to P_T takes place exponentially fast. Indeed, it may be inferred from [8] (see Theorem 8, Page 36)

$$\|P_n - P_T\|_{TV} \le (1 - p_T)^n \tag{11}$$

where $\|\cdot\|_{TV}$ is the total variation norm, and $p_T \in (0, 1)$ verifies

$$p_T \leq (\operatorname{vol} M) \inf_{x,z} q(x,z) \exp(-\sup_x U(x)/T)$$

so the rate of convergence is degraded when T is small.

Accordingly, the intuitive justification of the above algorithm is the following. Since the z_n eventually sample from the Gibbs distribution P_T , and the desired global minimum x^* of U is equal to the barycentre \bar{x}_T of P_T (by Proposition 3), then the barycentre \hat{x}_n of the z_n is expected to converge to x^* .

It should be emphasised that, in the present state of the literature, there is no rigorous result which confirms this convergence $z_n \to x^*$. It is therefore an open problem, to be confronted in future work.

For a basic computer experiment, consider $M = S^2 \subset \mathbb{R}^3$, and let

$$U(x) = -P_9(x^3)$$
 for $x = (x^1, x^2, x^3) \in S^2$ (12)

where P_9 is the Legendre polynomial of degree 9 [9]. The unique global minimiser of U is $x^* = (0, 0, 1)$, and the conditions of Proposition 3 are verified, since U is invariant by reflection in the x^3 axis, which is geodesic symmetry about x^* .

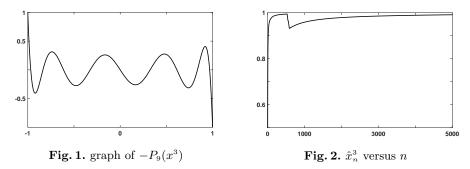


Figure 1 shows the dependence of U(x) on x^3 , displaying multiple local minima and maxima. Figure 2 shows the algorithm overcoming these local minima and maxima, and converging to the global minimum $x^* = (0, 0, 1)$, within n = 5000 iterations. The experiment was conducted with T = 0.2, and the Markov kernel Q obtained from the von Mises-Fisher distribution (see [10]). The initial guess $\hat{x}_0 = (0, 0, -1)$ is not shown in Figure 2.

In comparison, a standard simulated annealing method offered less robust performance, which varied considerably with the choice of annealing schedule.

5 Proofs

This section is devoted to the proofs of the results stated in previous sections.

As of now, assume that $U(x^*) = 0$. There is not loss of generality in making this assumption.

5.1 Proof of Proposition 1

Proof of (i): denote $f_x(z) = \frac{1}{2} d^2(x, z)$. By the definition of \mathcal{E}_T

$$\mathcal{E}_{T}(x) = \int_{M} f_{x}(z) P_{T}(dz)$$
(13a)

Moreover, let \mathcal{E}_0 be the function

$$\mathcal{E}_{0}(x) = \int_{M} f_{x}(z) \,\delta_{x^{*}}(dz) = \frac{1}{2} \,d^{2}(x, x^{*})$$
(13b)

For any x, it is elementary that $f_x(z)$ is Lipschitz continuous, with respect to z, with Lipschitz constant diam M. Then, from the Kantorovich-Rubinshtein formula [4],

$$|\mathcal{E}_{T}(x) - \mathcal{E}_{0}(x)| \leq (\operatorname{diam} M) W(P_{T}, \delta_{x^{*}})$$
(13c)

a uniform bound in $x \in M$. It now follows that

$$\inf_{x \in B(x^*,\eta)} \mathcal{E}_{T}(x) - \inf_{x \in B(x^*,\eta)} \mathcal{E}_{0}(x) \leq (\operatorname{diam} M) W(P_{T}, \delta_{x^*}) \quad \text{and} \qquad (13d)$$

$$\inf_{x \notin B(x^*,\eta)} \mathcal{E}_0(x) - \inf_{x \notin B(x^*,\eta)} \mathcal{E}_T(x) \leq (\operatorname{diam} M) W(P_T, \delta_{x^*})$$
(13e)

However, from (13b), it is clear that

$$\inf_{x \in B(x^*,\eta)} \mathcal{E}_{\scriptscriptstyle 0}(x) = 0 \quad \text{ and } \quad \inf_{x \notin B(x^*,\eta)} \mathcal{E}_{\scriptscriptstyle 0}(x) = \frac{\eta^2}{2}$$

To complete the proof, replace this into (13d) and (13e). Then, assuming the condition in (3) is verified,

$$\inf_{x \in B(x^*,\eta)} \mathcal{E}_T(x) < \frac{\eta^2}{4} < \inf_{x \notin B(x^*,\eta)} \mathcal{E}_T(x)$$
(13f)

This means that any global minimum \bar{x}_T of \mathcal{E}_T must belong to the open ball $B(x^*, \eta)$. In other words, $d(\bar{x}_T, x^*) < \eta$. This completes the proof of (3).

Proof of (*ii*): let $\rho \leq \min\{\inf x^*, \kappa^{-1} \frac{\pi}{2}\}$ where $\inf x^*$ is the injectivity radius of M at x^* , and κ^2 is an upper bound on the sectional curvature of M. Assume, in addition, ρ is small enough so

$$\mu_{\min} d^2(x, x^*) \le 2 \left(U(x) - U(x^*) \right) \le \mu_{\max} d^2(x, x^*)$$
(14a)

whenever $d(x, x^*) \leq \rho$. Further, consider the truncated distribution

$$P_T^{\rho}(dz) = \frac{\mathbf{1}_{B_{\rho}}(z)}{P_T(B_{\rho})} \cdot P_T(dz)$$
(14b)

where **1** denotes the indicator function, and B_{ρ} stands for the open ball $B(x^*, \rho)$. Of course, by the triangle inequality,

$$W(P_T, \delta_{x^*}) \le W(P_T, P_T^{\rho}) + W(P_T^{\rho}, \delta_{x^*})$$
(14c)

The proof relies on the following estimates, which use the notation of Section 3. First estimate: if $T \leq T_{\alpha}^{1}$, then

$$W(P_{\tau}, P_{\tau}^{\rho}) \le (\operatorname{diam} M \times \operatorname{vol} M) \ \frac{2}{\pi} \ \left(\frac{\pi}{8}\right)^{n/2} \left(\frac{\mu_{\max}}{T}\right)^{n/2} \exp\left(-U_{\rho}/T\right)$$
(14d)

Second estimate : if $T \leq T_o^1$, then

$$W(P_T^{\rho}, \delta_{x^*}) \le 2\sqrt{2\pi} \left(\frac{\pi}{2}\right)^{n-1} B_n^{-1} \left(\frac{\mu_{\max}}{\mu_{\min}}\right)^{n/2} \left(\frac{T}{\mu_{\min}}\right)^{1/2}$$
 (14e)

These two estimates are proved below. Assume now they hold true, and $T \leq T_o$. In particular, since $T \leq T_o^2$, the definition of T_o^2 implies

$$f(T, n+1, \rho) \le (\mu_{\max}/\mu_{\min})^{n/2} C_n$$

Recall the definition of C_n , and express ω_n and A_n in terms of the Gamma function [9]. The last inequality becomes

$$(\operatorname{diam} M \times \operatorname{vol} M) \ f(T, n+1, \rho) \le 2 (2\pi)^{n/2} B_n^{-1} \left(\mu_{\max} / \mu_{\min} \right)^{n/2}$$

This is the same as

$$(\operatorname{diam} M \times \operatorname{vol} M) \ \frac{1}{\pi} \ \left(\frac{\pi}{8}\right)^{n/2} f(T, n+1, \rho) \le \left(\frac{\pi}{2}\right)^{n-1} \ B_n^{-1} \ \left(\mu_{\max}/\mu_{\min}\right)^{n/2}$$

By the definition of $f(T, n + 1, \rho)$, it now follows the right-hand side of (14d) is less than half the right-hand side of (14e). In this case, (4) follows from the triangle inequality (14c).

Proof of first estimate : consider the coupling of P_T and P_T^{ρ} , provided by the probability distribution K on $M \times M$,

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$$K(dz_1 \times dz_2) = P_T^{\rho}(dz_1) \left[P_T(B_{\rho})\delta_{z_1}(dz_2) + \mathbf{1}_{B_{\rho}^c}(z_2)P_T(dz_2) \right]$$
(15a)

where B_{ρ}^{c} denotes the complement of B_{ρ} . Recall the definition of the Kantorovich distance (see [4]). Replacing (15a) into this definition, it follows that

$$W(P_T, P_T^{\rho}) \le (\operatorname{diam} M) P_T(B_{\rho}^c) \tag{15b}$$

Then, from the definition (2) of P_T ,

$$P_T(B_{\rho}^c) \le (Z(T))^{-1} (\operatorname{vol} M) \exp(-U_{\rho}/T)$$
 (15c)

Now, (14d) follows directly from (15b) and (15c), if the following lower bound on Z(T) can be proved,

$$Z(T) \ge \frac{\pi}{2} \left(\frac{8}{\pi}\right)^{n/2} \left(\frac{T}{\mu_{\max}}\right)^{n/2} \quad \text{for } T \le T_o^1 \tag{15d}$$

To prove this lower bound, note that

$$Z(T) \,=\, \int_M \,e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \,\,\geq\, \int_{B_\rho} \,e^{-\frac{U(z)}{T}} \operatorname{vol}(dz)$$

Using this last inequality and (14a), it is possible to write

$$Z(T) \ge \int_{B_{\rho}} e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \ge \int_{B_{\rho}} e^{-\frac{\mu_{\max}}{2T} d^{2}(x, x^{*})} \operatorname{vol}(dz)$$
(15e)

Writing this last integral in Riemannian spherical coordinates,

$$\int_{B_{\rho}} e^{-\frac{\mu_{\max}}{2T} d^2(x,x^*)} \operatorname{vol}(dz) = \int_0^{\rho} \int_{S^{n-1}} e^{-\frac{\mu_{\max}}{2T} r^2} \lambda(r,s) dr \,\omega_n(ds) \quad (15f)$$

where $\lambda(r, s)$ is the volume density in the Riemannian spherical coordinates, $r \geq 0$ and $s \in S^{n-1}$, and where $\omega_n(ds)$ is the area element of S^{n-1} . From the volume comparison theorem in [6] (see Page 129),

$$\lambda(r,s) \ge (\kappa^{-1}\sin(\kappa r))^{n-1} \ge ((2/\pi)r)^{n-1}$$
 (15g)

where the second inequality follows since $x \mapsto \sin(x)$ is concave for $x \in (0, \pi)$. Now, it follows from (15e) and (15f),

$$Z(T) \ge \omega_n \left(\frac{2}{\pi}\right)^{n-1} \int_0^\rho e^{-\frac{\mu_{\max}}{2T} r^2} r^{n-1} dr$$
(15h)

where ω_n is the surface area of S^{n-1} . Thus, the required lower bound (15d) follows by noting that

$$\int_{0}^{\rho} e^{-\frac{\mu_{\max}}{2T}r^{2}} r^{n-1} dr = (2\pi)^{1/2} \left(\frac{T}{\mu_{\max}}\right)^{n/2} A_{n-1} - \int_{\rho}^{\infty} e^{-\frac{\mu_{\max}}{2T}r^{2}} r^{n-1} dr$$

where $A_n = E|X|^n$ for $X \sim N(0, 1)$, and that

$$\int_{\rho}^{\infty} e^{-\frac{\mu_{\max}}{2T} r^2} r^{n-1} dr \le \rho^{n-2} \frac{T}{\mu_{\max}} e^{-\frac{\mu_{\max}}{2T} \rho^2} \le \rho^{n-2} \frac{T}{\mu_{\max}} e^{-\frac{U\rho}{T}}$$

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Indeed, taken together, these give

$$Z(T) \ge \omega_n \left(\frac{2}{\pi}\right)^{n-1} \left[(2\pi)^{1/2} \left(\frac{T}{\mu_{\max}}\right)^{n/2} A_{n-1} - \rho^{n-2} \frac{T}{\mu_{\max}} e^{-\frac{U\rho}{T}} \right]$$

Finally, (15d) can be obtained by noting the second term in square brackets is negligeable compared to the first, as T decreases to 0, and by expressing ω_n and A_{n-1} in terms of the Gamma function [9].

Proof of second estimate: the Kantorovich distance between P_T^{ρ} and the Dirac distribution δ_{x^*} is equal to the expectation of the distance to x^* , with respect to P_T^{ρ} [4]. Precisely,

$$W(P_T^{\rho}, \delta_{x^*}) = \int_M d(x^*, z) P_T^{\rho}(dz)$$

According to (2) and (14b), this is

$$W(P_T^{\rho}, \delta_{x^*}) = (P_T(B_{\rho})Z(T))^{-1} \int_{B_{\rho}} d(x^*, z) e^{-\frac{U(z)}{T}} \operatorname{vol}(dz)$$

Using (2) to express the probability $P_T(B_{\rho})$, this becomes

$$W(P_{T}^{\rho}, \delta_{x^{*}}) = \frac{\int_{B_{\rho}} d(x^{*}, z) e^{-\frac{U(z)}{T}} \operatorname{vol}(dz)}{\int_{B_{\rho}} e^{-\frac{U(z)}{T}} \operatorname{vol}(dz)}$$
(16a)

A lower bound on the denominator can be found from (15e) and subsequent inequalities, which were used to prove (15d). Precisely, these inequalities provide

$$\int_{B_{\rho}} e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \ge \frac{1}{2} \omega_n \left(\frac{2}{\pi}\right)^{n-1} (2\pi)^{1/2} A_{n-1} \left(\frac{T}{\mu_{\max}}\right)^{n/2}$$
(16b)

whenever $T \leq T_o^1$. For the numerator in (16a), it will be shown that, for any T,

$$\int_{B_{\rho}} d(x^*, z) \, e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \, \le \, \omega_n \, (2\pi)^{1/2} \, A_n \left(\frac{T}{\mu_{\min}}\right)^{(n+1)/2} \tag{16c}$$

Then, (14e) follows by dividing (16c) by (16b), and replacing in (16a), after noting that $A_n/A_{n-1} = \sqrt{2\pi} B_n^{-1}$. Thus, it only remains to prove (16c). Using (14a), it is seen that

$$\int_{B_{\rho}} d(x^*, z) \, e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \, \le \, \int_{B_{\rho}} d(x^*, z) \, e^{-\frac{\mu_{\min}}{2T} \, d^2(x, x^*)} \operatorname{vol}(dz)$$

By expressing this last integral in Riemannian spherical coordinates, as in (15f),

$$\int_{B_{\rho}} d(x^*, z) e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \leq \int_0^{\rho} \int_{S^{n-1}} r e^{-\frac{\mu_{\min}}{2T} r^2} \lambda(r, s) dr \,\omega_n(ds) \quad (16d)$$

From the volume comparison theorem in [6] (see Page 130), $\lambda(r,s) \leq r^{n-1}$. Therefore, (16d) becomes

$$\int_{B_{\rho}} d(x^*, z) e^{-\frac{U(z)}{T}} \operatorname{vol}(dz) \le \omega_n \int_0^{\rho} e^{-\frac{\mu_{\min}}{2T} r^2} r^n \, dr \le \omega_n \int_0^{\infty} e^{-\frac{\mu_{\min}}{2T} r^2} r^n \, dr$$

The right-hand side is half the *n*th absolute moment of a normal distribution. Expressing this in terms of A_n , and replacing in (16d), gives (16c).

6 Proof of Lemma 1

Denote G the connected component at identity of the group of isometries of M. It will be assumed that G is simply-connected and semisimple [7]. Any geodesic $\gamma: I \to M$ is of the form [7][11],

$$\gamma(t) = \exp(tY) \cdot x \tag{17a}$$

for some $x \in M$ and $Y \in \mathfrak{g}$, the Lie algebra of G, where $\exp : \mathfrak{g} \to G$ denotes the Lie group exponential mapping, and the dot denotes the action of G on M. For each $t \in I$, the cut locus $\operatorname{Cut}(\gamma(t))$ of $\gamma(t)$ is given by

$$\operatorname{Cut}(\gamma(t)) = \exp(tY) \cdot \operatorname{Cut}(x)$$
 (17b)

This is due to a more general result: let M be a Riemannian manifold and $g: M \to M$ be an isometry of M. Then, $\operatorname{Cut}(g \cdot x) = g \cdot \operatorname{Cut}(x)$ for all $x \in M$. This is because $y \in \operatorname{Cut}(x)$ if and only if y is conjugate to x along some geodesic, or there exist two different geodesics connecting x to y [6][11]. Both of these properties are preserved by the isometry g.

In order to describe the set $\operatorname{Cut}(x)$, denote K the isotropy group of x in G, and \mathfrak{k} the Lie algebra of K. Let $\mathfrak{g} = \mathfrak{k} + \mathfrak{p}$ be an orthogonal decomposition, with respect to the Killing form of \mathfrak{g} , and let \mathfrak{a} be a maximal Abelian subspace of \mathfrak{p} . Define $\mathcal{S} = K/C_{\mathfrak{a}}$ ($C_{\mathfrak{a}}$ the centraliser of \mathfrak{a} in K), and consider the mapping

$$\phi(s, a) = \exp\left(\operatorname{Ad}(s) a\right) \cdot x \quad \text{for } (s, a) \in \mathcal{S} \times \mathfrak{a}$$
(17c)

The set $\operatorname{Cut}(x)$ is the image under ϕ of a certain set $\mathcal{S} \times \partial Q$, which is now described, following [7][12].

Let Δ_+ be the set of positive restricted roots associated to the pair (G, K), (each $\lambda \in \Delta_+$ is a linear form $\lambda : \mathfrak{a} \to \mathbb{R}$). Then, let Q be the set of $a \in \mathfrak{a}$ such that $|\lambda(a)| \leq \pi$ for all $\lambda \in \Delta_+$, and ∂Q the boundary of Q. Then

$$\operatorname{Cut}(x) = \phi(\mathcal{S} \times \partial Q) \tag{17d}$$

Recapitulating (17b) and (17d),

$$\operatorname{Cut}(\gamma) = \varPhi(I \times \mathcal{S} \times \partial Q) \quad \text{where} \quad \varPhi(t, s, a) = \exp(tY) \cdot \phi(s, a) \tag{17e}$$

Lemma 1 states that the topological dimension of $\operatorname{Cut}(\gamma)$ is strictly less than dim M. This is proved using results from topological dimension theory [7][13].

Note that both I and S are compact. Indeed, S is compact since it is the continuous image of the compact group K under the projection $K \to K/C_{\mathfrak{a}}$. Also, ∂Q is compact in \mathfrak{a} , and $\partial Q = \bigcup_{\lambda} \partial Q_{\lambda}$ where $\partial Q_{\lambda} = \partial Q \cap \{\lambda(a) = \pm \pi\}$ for $\lambda \in \Delta_+$. Since $\{\lambda(a) = \pm \pi\}$ is the union of two (closed) hyperplanes in \mathfrak{a} , ∂Q_{λ} is compact. Now, each $I \times S \times \partial Q_{\lambda}$ is compact, and therefore closed. It follows from (17e) that (see [13], Page 30),

$$\dim \operatorname{Cut}(\gamma) = \dim \bigcup_{\lambda} \Phi(I \times \mathcal{S} \times \partial Q_{\lambda}) \le \max_{\lambda} \dim \Phi(I \times \mathcal{S} \times \partial Q_{\lambda}) \quad (17f)$$

But, for each λ ,

$$\Phi(I \times S \times \partial Q_{\lambda}) = \Phi(I \times S_{\lambda} \times \partial Q_{\lambda}) \subset \Phi(\mathbb{R} \times S_{\lambda} \times \{\lambda(a) = \pm \pi\})$$

where $S_{\lambda} = K/C_{\lambda}$ (C_{λ} the centraliser of $\{\lambda(a) = \pm \pi\}$ in K). The above inclusion implies (by [13], Page 26),

$$\dim \Phi(I \times \mathcal{S} \times \partial Q_{\lambda}) \leq \dim \Phi(\mathbb{R} \times \mathcal{S}_{\lambda} \times \{\lambda(a) = \pm \pi\})$$
(17g)

To conclude, note that the set $\mathbb{R} \times S_{\lambda} \times \{\lambda(a) = \pm \pi\}$ is a differentiable manifold. It follows that (see [7], Page 345),

$$\dim \Phi \left(\mathbb{R} \times \mathcal{S}_{\lambda} \times \{ \lambda(a) = \pm \pi \} \right) \leq \dim \left(\mathbb{R} \times \mathcal{S}_{\lambda} \times \{ \lambda(a) = \pm \pi \} \right)$$
(17h)

The right-hand side of this inequality is

$$\dim \left(\mathbb{R} \times \mathcal{S}_{\lambda} \times \{\lambda(a) = \pm \pi\}\right) = 1 + \dim \mathcal{S}_{\lambda} + \dim \mathfrak{a} - 1$$

since the dimension of a hyperplane in \mathfrak{a} is dim $\mathfrak{a} - 1$. In addition, according to [7] (Page 296), dim $S_{\lambda} < \dim S$. Thus,

$$\dim \left(\mathbb{R} \times \mathcal{S}_{\lambda} \times \{\lambda(a) = \pm \pi\}\right) = \dim \mathcal{S}_{\lambda} + \dim \mathfrak{a} < \dim M$$

since dim $M = \dim \mathcal{S} + \dim \mathfrak{a}$ [7]. Replacing this into (17h), it follows from (17f) and (17g) that dim $\operatorname{Cut}(\gamma) < \dim M$, as required.

7 Proof of Corollary 1

The corollary can be split into the two following claims, which will be proved separately.

First claim : both integrals G_x and H_x converge for any value of T.

Second claim: \mathcal{E}_{T} is C^{2} throughout M, with derivatives given by (5).

The fact that G_x and H_x depend continuously on x is contained in the second claim, since (5) states that G_x and H_x are the gradient and Hessian of \mathcal{E}_T at x.

In the following proofs, the notation D(x) = M - Cut(x) will be used, in order to avoid cumbersome expressions.

Proof of first claim : The convergence of the integral G_x is straightforward, since the integrand $G_x(z)$ is a smooth and bounded function, from D(x) to T_xM . This is because, by definition, $G_x(z)$ is given by

$$G_x(z) = -\operatorname{Exp}_x^{-1}(z) \tag{18}$$

where Exp is the Riemannian exponential mapping [6]. Therefore, $G_x(z)$ is smooth. In addition, $G_x(z)$ is bounded, in Riemannian norm, by diam M.

The convergence of the integral H_x is more difficult. While the integrand $H_x(z)$ is smooth on D(x), it is not bounded. It will be seen that H_x is an absolutely convergent improper integral.

Recall the mapping ϕ defined in (17c). Let D_+ be the set of points $a \in \mathfrak{a}$ which belong to the interior of Q, and which verify $\lambda(a) \geq 0$ for each $\lambda \in \Delta_+$. Let D^o_+ be the interior of D_+ . Then, ϕ maps $S \times D_+$ onto D(x), and is a diffeomorphism of $S \times D^o_+$ onto its image in D(x) [7][12] (see Chapter VII in [7]). Using Sard's theorem [14], it follows from the definition of H_x that

$$H_x = \int_{\mathcal{S}} \int_{D_+} H_x(\phi(s,a)) \, p_T(\phi(s,a)) \, J(a) \, da \, \omega(ds) \tag{19a}$$

where p_T denotes the density of P_T with respect to the Riemannian volume of M, and J(a) is the Jacobian determinant of ϕ , given by [7]

$$J(a) = \prod_{\lambda \in \Delta_+} (\sin \lambda(a))^{m_{\lambda}}$$
(19b)

with m_{λ} the multiplicity of the restricted root λ , and where $\omega(ds)$ is the invariant Riemannian volume induced on S from K.

Now, $H_x(\phi(s, a))$ can be expressed as follows (cot is the cotangent function)

$$H_x(\phi(s,a)) = \Pi_0(s) + \sum_{\lambda \in \Delta_+} \lambda(a) \cot \lambda(a) \Pi_\lambda(s)$$
(19c)

where $\Pi_0(s)$ and the $\Pi_{\lambda}(s)$ denote orthogonal projectors, onto the respective eigenspaces of $H_x(\phi(s, a))$.

According to this expression, $H_x(\phi(s, a))$ diverges to $-\infty$ whenever $\lambda(a) = \pi$. However, the product

$$H_x(\phi(s,a)) p_T(\phi(s,a)) J(a)$$

which appears under the integral in (19a), is clearly continuous and bounded on the domain of integration. Thus, the absolute convergence of the integral H_x follows immediately from (19a). It now remains to provide a proof of (19c). This is here only briefly indicated. Expression (19c) is a slight improvement of the one in [15] (see Theorem IV.1, Page 636), where it is enough to note that if R is the curvature tensor of M, then the operator $R_v(u) = R(v, u)v$ has the eigenvalues 0 and $(\lambda(a))^2$ for each $\lambda \in \Delta_+$, whenever $v, u \in T_x M \simeq \mathfrak{p}$ with $v = \operatorname{Ad}(s) a$ [7][12]. It is well-known, by properties of the Jacobi equation [6], that $H_x(\phi(s, a))$ has the same eigenspace decomposition as R_v , in this case. **Proof of second claim:** the proof of this claim relies in a crucial way on Lemma 1. To compute the gradient and Hessian of the function \mathcal{E}_T at $x \in M$, consider any geodesic $\gamma : I \to M$, defined on a compact interval $I = [-\tau, \tau]$, such that $\gamma(0) = x$. For each $t \in I$, by definition of the function \mathcal{E}_T ,

$$\mathcal{E}_{T}(\gamma(t)) = \frac{1}{2} \int_{M} d^{2}(\gamma(t), z) P_{T}(dz)$$
(20a)

However, Lemma 1 states that the set

$$\operatorname{Cut}(\gamma) = \bigcup_{t \in I} \operatorname{Cut}(\gamma(t))$$

has Riemannian volume equal to zero. From (2), it is clear that P_T is absolutely continuous with respect to Riemannian volume. Therefor, $Cut(\gamma)$ can be removed from the domain of integration in (20a). Then,

$$\mathcal{E}_{T}(\gamma(t)) = \frac{1}{2} \int_{\mathcal{D}(\gamma)} d^{2}(\gamma(t), z) P_{T}(dz)$$
(20b)

where $D(\gamma) = M - Cut(\gamma)$. Now, for each $z \in D(\gamma)$, the function

$$t \mapsto f_z(t) = \frac{1}{2} d^2(\gamma(t), z)$$

is twice continuously differentiable with respect to $t \in I$, with

$$\frac{df_z}{dt} = \left\langle G_{\gamma(t)}(z), \dot{\gamma} \right\rangle \quad \text{and} \quad \frac{d^2 f_z}{dt^2} = H_{\gamma(t)}(z) \left(\dot{\gamma}, \dot{\gamma} \right) \tag{20c}$$

where $\langle \cdot, \cdot \rangle$ denotes the Riemannian metric of M, and $\dot{\gamma}$ the velocity of the geodesic γ . Indeed, this holds because the geodesic γ does not intersect the cut locus $\operatorname{Cut}(z)$ (see [6]).

The claim that \mathcal{E}_{T} is twice differentiable, and has derivatives given by (5), follows from (20b) and (20c), by differentiation under the integral sign, provided it can be shown that the families of functions

$$\left\{ z \mapsto G_{\gamma(t)}(z) \, ; \, t \in I \right\}$$
 and $\left\{ z \mapsto H_{\gamma(t)}(z) \, ; \, t \in I \right\}$

which all have the common domain of definition $D(\gamma)$, are uniformly integrable with respect to P_T [14]. Roughly, uniform integrability means that the rate of absolute convergence of the following integrals does not depend on t,

$$G_{\gamma(t)} = \int_{\mathcal{D}(\gamma)} G_{\gamma(t)}(z) P_{T}(dz) \; ; \; H_{\gamma(t)} = \int_{\mathcal{D}(\gamma)} H_{\gamma(t)}(z) P_{T}(dz)$$

This is clear for the integrals $G_{\gamma(t)}$ because $G_{\gamma(t)}(z)$ is bounded in Riemannian norm by diam M, uniformly in t and z (see the proof of the first claim).

Then, consider the integral $H_x = H_{\gamma(0)}$, and recall Formulae (19a) and (19c). Each $z \in D(\gamma)$ can be written under the form $z = \phi(s, a)$ where $(s, a) \in \mathcal{S} \times D_+$. Accordingly, it follows from (19c) that

$$||H_x(z)||_F \le (\dim M)^{\frac{1}{2}} \max\{1, |\kappa(a) \cot \kappa(a)|\}$$
(20d)

where $\|\cdot\|_F$ is the Frobenius norm with respect to the Riemannian metric of M, and $\kappa \in \Delta_+$ is the highest restricted root [7] ($\kappa(a) \ge \lambda(a)$ for $\lambda \in \Delta_+$, $a \in D_+$).

The required uniform integrability is equivalent to the statement that

$$\lim_{K \to \infty} \int_{\mathcal{D}(\gamma)} \|H_x(z)\|_F \mathbf{1}\{\|H_x(z)\|_F > K\} P_T(dz) = 0$$
(20e)

where the rate of convergence to this limit does not depend on x. But, according to (20d), if K > 1, there exists $\epsilon > 0$ such that

$$\{ \|H_x(z)\|_F > K \} = \{ \kappa(a) > \pi - \epsilon \}$$

and $\epsilon \to 0$ as $K \to \infty$. In this case, the integral in (20e) is less than

$$(\dim M)^{\frac{1}{2}} \left(\sup_{z} p_{T}(z) \right) \int_{\mathcal{D}(\gamma)} |\kappa(a) \cot \kappa(a)| \mathbf{1} \{ \kappa(a) > \pi - \epsilon \} \operatorname{vol}(dz) \quad (20f)$$

Now, using the same integral formula as in (19a), this last integral is equal to

$$\int_{\mathcal{S}} \int_{D_{+}} |\kappa(a) \cot \kappa(a)| \mathbf{1} \{\kappa(a) > \pi - \epsilon\} J(a) da \,\omega(ds) = \omega(\mathcal{S}) \int_{D_{+}} [|\kappa(a) \cot \kappa(a)| J(a)] \mathbf{1} \{\kappa(a) > \pi - \epsilon\} da$$

In view of (19b), since $\kappa \in \Delta_+$, the function in square brackets is bounded on the closure of D_+ . In fact [7], its supremum is $\kappa^2 = (\kappa, \kappa)$ where (\cdot, \cdot) is the scalar product induced on \mathfrak{a}^* (the dual space of \mathfrak{a}) by the Killing form of \mathfrak{g} . Finally, by (20f), the integral in (20e) is less than

$$(\dim M)^{\frac{1}{2}} \left(\sup_{z} p_{T}(z) \right) \omega(\mathcal{S}) \kappa^{2} \int_{D_{+}} \mathbf{1} \left\{ \kappa(a) > \pi - \epsilon \right\} da$$

Since, $\kappa(a) \in [0, \pi)$ for $a \in D_+$, this last integral converges to 0 as $\epsilon \to 0$, at a rate which does not depend on x. This proves the required uniform integrability, so the proof is now complete.

8 Proof of Proposition 2

Remark : in the statement of Proposition 2, the notation κ^2 is used for the maximum sectional curvature of M. In the previous proof of Corollary 1, the same notation κ^2 was used for the squared norm of the highest restricted root. This is not an abuse of notation, since the two quantities are in fact equal [7] (see Page 334).

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Proof of (i): let $x \in B(x^*, \delta)$. By (5) of Corollary 1, $\nabla^2 \mathcal{E}_T(x)$ is equal to H_x . To obtain (7), decompose H_x into two integrals

$$H_x = \int_{B(x,r_{cx})} H_x(z) P_T(dz) + \int_{D(x) - B(x,r_{cx})} H_x(z) P_T(dz)$$
(21a)

This is possible since $B(x, r_{cx}) \subset D(x)$, where D(x) = M - Cut(x). The first integral in (21a) will be denoted I_1 , and the second integral I_2 .

With regard to I_1 , note the inclusions $B(x^*, \delta) \subset B(x, 2\delta) \subset B(x, r_{cx})$, which follow from the triangle inequality. In addition, note that $H_x(z) \geq 0$ (in the Loewner order [16]), for $z \in B(x, r_{cx})$. Therefore,

$$I_1 \ge \int_{B(x^*,\delta)} H_x(z) P_T(dz)$$
(21b)

However, from (19c) and the definition of $\kappa \in \Delta_+$,

$$H_x(z) \ge \kappa(a) \cot \kappa(a) \tag{21c}$$

for $z = \phi(s, a) \in D(x)$. Using the Cauchy-Scwharz inequality, $\kappa(a) \leq \kappa ||a||$. Moreover, (17c) implies ||a|| = d(x, z), since Ad(s) is an isometry. Accordingly, if $z \in B(x, 2\delta)$, it follows from (21c)

$$H_x(z) \ge \kappa(a) \cot \kappa(a) \ge 2\kappa \delta \cot(2\kappa \delta) = \operatorname{Ct}(2\delta) > 0$$
(21d)

where the last inequality is because $2\delta < r_{cx} = \kappa^{-1} \frac{\pi}{2}$. Replacing in (21b) gives

$$I_1 \geq \operatorname{Ct}(2\delta) P_T(B(x^*, \delta)) = \operatorname{Ct}(2\delta) \left[1 - P_T(B^c(x^*, \delta))\right]$$

Finally, (15c) and (15d) imply that $P_T(B^c(x^*, \delta)) \leq \operatorname{vol}(M) f(T)$, where f(T) was defined in (6) – Precisely, this follows after replacing ρ by δ in (15c). Thus,

$$I_1 \ge \operatorname{Ct}(2\delta) \left(1 - \operatorname{vol}(M)f(T)\right) \tag{21e}$$

The proof of (7) will be completed by showing

$$I_2 \ge -\pi A_M f(T) \tag{22a}$$

To show this, note using (21c) that

$$I_2 \ge \int_{\mathcal{D}(x) - B(x, r_{cx})} \kappa(a) \cot \kappa(a) P_T(dz)$$
(22b)

Now, $\kappa(\alpha) \cot \kappa(\alpha)$ is negative if and only if $\kappa(\alpha) \geq \frac{\pi}{2}$. However, the set of $z = \phi(s, a)$ where $\kappa(a) \geq \frac{\pi}{2}$ is a subset of $D(x) - B(x, r_{cx})$. Indeed, $\kappa(a) \geq \frac{\pi}{2}$ implies $||a|| \geq \kappa^{-1}\frac{\pi}{2} = r_{cx}$, by the Cauchy-Schwarz inequality, and this is the same as $d(x, z) \geq r_{cx}$, since ||a|| = d(x, z). Therefore, it follows from (22b),

$$I_2 \ge \int_{\mathcal{D}(x)} \mathbf{1}\{\kappa(a) \ge \pi/2\} \,\kappa(a) \cot \kappa(a) \, P_T(dz) \tag{22c}$$

Using the same integral formula as in (19a), this last integral is equal to

$$\int_{\mathcal{S}} \int_{D_{+}} \mathbf{1}\{\kappa(a) \ge \pi/2\} \, \kappa(a) \cot \kappa(a) \, p_{\tau}(\phi(s,a)) \, J(a) \, da \, \omega(ds) \ge - \int_{\mathcal{S}} \int_{D_{+}} \mathbf{1}\{\kappa(a) \ge \pi/2\} \, \kappa(a) \, p_{\tau}(\phi(s,a)) \, da \, \omega(ds)$$

because the product $\cot \kappa(a) J(a) \ge -1$ for all $a \in D_+$. Using this last inequality, and the fact that $\kappa(a) \le \pi$ for all $a \in D_+$, it follows from (22c),

$$I_2 \geq -\pi \int_{\mathcal{S}} \int_{D_+} \mathbf{1}\{\kappa(a) \geq \pi/2\} p_T(\phi(s,a)) \, da \, \omega(ds) \tag{22d}$$

Recall that $\{\kappa(a) \geq \pi/2\} \subset B^c(x, r_{cx})$, as discussed before (22c). In particular, this implies $\{\kappa(a) \geq \pi/2\} \subset B^c(x^*, \delta)$. However, by (2) and (15d), $p_T(z) \leq f(T)$ for all $z \in B^c(x^*, \delta)$. Returning to (22d), this gives

$$I_2 \ge -\pi f(T) \int_{\mathcal{S}} \int_{D_+} da \,\omega(ds) \tag{22e}$$

The double integral on the right-hand side is a constant which depends only on the structure of the symmetric space M. Denoting this constant by A_M gives the required lower bound (22a), and completes the proof of (7).

Proof of (*ii*): fix $\delta < \frac{1}{2}r_{cx}$, and let T_{δ} be given by (9). If $T \leq T_{\delta}$, then $T < T_{\delta}^2$, so the definition of T_{δ}^2 implies

$$f(T) < \frac{\operatorname{Ct}(2\delta)}{\operatorname{Ct}(2\delta)\operatorname{vol}(M) + \pi A_M}$$
(23a)

Now, by (7),

$$\nabla^2 \mathcal{E}_T(x) \ge \operatorname{Ct}(2\delta) \left(1 - \operatorname{vol}(M)f(T)\right) - \pi A_M f(T)$$
(23b)

for all $x \in B(x^*, \delta)$. However, it is clear from (23a), that the right-hand side of this inequality is strictly positive. It follows that \mathcal{E}_T is strongly convex on $B(x^*, \delta)$. Thus, to complete the proof, it only remains to show that any global minimum \bar{x}_T of \mathcal{E}_T must belong to $B(x^*, \delta)$. Indeed, since \mathcal{E}_T is strongly convex on $B(x^*, \delta)$, it has only one local minimum in $B(x^*, \delta)$. Therefore, \mathcal{E}_T can have only one global minimum \bar{x}_T .

By (i) of Proposition 1, to prove that $\bar{x}_T \in B(x^*, \delta)$, it is enough to prove

$$W(P_T, \delta_{x^*}) < \frac{\delta^2}{(4\operatorname{diam} M)}$$
(23c)

However, if $T \leq T_{\delta}$, then $T < T_{o}$. Therefore, by *(ii)* of Proposition 1, $W(P_{T}, \delta_{x^{*}})$ satisfies inequality (4). Furthermore, because $T < T_{\delta}^{1}$, it follows from the definition of T_{δ}^{1} that

$$\sqrt{2\pi} (T/\mu_{\min})^{1/2} < \delta^2 (\mu_{\min}/\mu_{\max})^{n/2} D_n$$

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or, by replacing the expression of D_n , and simplifying

$$\sqrt{2\pi} (\pi/2)^{n-1} B_n^{-1} (\mu_{\max}/\mu_{\min})^{n/2} (T/\mu_{\min})^{1/2} < \frac{\delta^2}{(4\operatorname{diam} M)}$$
(23d)

Thus, (23c) follows from (4) and (23d). This proves that \bar{x}_T belongs to $B(x^*, \delta)$, and therefore \bar{x}_T is the unique global minimum of \mathcal{E}_T . But this is equivalent to saying that \bar{x}_T is the unique barycentre of P_T .

9 Proof of Proposition 3

fix $\delta < \frac{1}{2}r_{cx}$, and let T_{δ} be given by (9). By (*ii*) of Proposition 2, if $T \leq T_{\delta}$, then \mathcal{E}_{T} is strictly convex on $B(x^*, \delta)$, with unique global minimum $\bar{x}_{T} \in B(x^*, \delta)$. By definition, this unique global minimum \bar{x}_{T} is the unique barycentre of P_{T} .

Accordingly, to prove that $\bar{x}_T = x^*$, it is enough to prove that x^* is a stationary point of \mathcal{E}_T . Indeed, as \mathcal{E}_T is strictly convex on $B(x^*, \delta)$, it can have only one stationary point in $B(x^*, \delta)$. This stationary point is then identical to \bar{x}_T .

The fact that x^* is a stationary point of \mathcal{E}_T will follow because U is invariant by geodesic symmetry about x^* . This invariance will be seen to imply

$$ds_{x^*} \cdot G_{x^*} = G_{x^*} \tag{24a}$$

which is equivalent to $G_{x^*} = 0$, since the derivative ds_{x^*} is equal to minus the identity, on the tangent space $T_{x^*}M$ [7]. By (5) of Corollary 1, this shows that $\nabla \mathcal{E}_{\mathcal{T}}(x^*) = 0$, so x^* is indeed a stationary point of $\mathcal{E}_{\mathcal{T}}$.

To obtain (24a), it is possible to write, from the definition of G_{x^*} ,

$$ds_{x^*} \cdot G_{x^*} = ds_{x^*} \cdot \int_{\mathcal{D}(x)} G_{x^*}(z) P_T(dz)$$
 (24b)

where D(x) = M - Cut(x). From (18), since s_{x^*} is an isometry, and reverses geodesics passing through x^* ,

$$ds_{x^*} \cdot G_{x^*}(z) = G_{x^*}(s_{x^*}(z))$$

Replacing this into (24b), and using $w = s_{x^*}(z)$ as a new variable of integration, it follows that

$$ds_{x^*} \cdot G_{x^*} = \int_{\mathcal{D}(x)} G_{x^*}(w) \left(P_T \circ s_{x^*} \right) (dw)$$
(24c)

because $s_{x^*}^{-1} = s_{x^*}$ and s_{x^*} maps D(x) onto itself. Now, note that $P_T \circ s_{x^*} = P_T$. This is clear, since from (2),

$$(P_T \circ s_{x^*})(dw) = (Z(T))^{-1} \exp\left[-\frac{(U \circ s_{x^*})(w)}{T}\right] (\text{vol} \circ s_{x^*})(dw)$$

However, by assumption, $U \circ s_{x^*}(w) = U(w)$. Moreover, since s_{x^*} is an isometry, it preserves Riemannian volume, so $(vol \circ s_{x^*})(dw) = vol(dw)$. Thus, (24c) reads

$$ds_{x^*} \cdot G_{x^*} = \int_{\mathcal{D}(x)} G_{x^*}(w) P_T(dw)$$

By definition, the right-hand side is G_{x^*} , so (24a) is obtained.

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