Nonconvergence of two-site population Lloyd iteration in every dimension from three onward

Abstract

For each dimension $n \geq 3$, we construct a centrally symmetric, smooth, positively curved body arbitrarily close to the Euclidean ball. For the uniform law on this body, exact two-site population Lloyd iteration can fail to converge. From one antipodal initialization, the unordered pairs accumulate on every axis of an equatorial hyperplane at a common radius. The entire cluster set is homeomorphic to $\mathbb{RP}^{n-2}$, and every member is stationary. The construction prescribes each discrete centroid direction through the first absolute projection moment of an actual probability law. It also works with a smooth isotropic strongly log-concave perturbation of a Gaussian and with a smooth compactly supported log-concave density. Ordinary and optimal equal-mass updates agree along these orbits. For centrally symmetric, absolutely continuous planar laws with finite first moment and a twice continuously differentiable angular moment, ordinary iteration converges from every nonzero antipodal start. The existence and low-dimensional results are also formalized in Lean.

1 The question and the result

In population Lloyd iteration, each of two distinct sites receives the points nearest to it and moves to their conditional mean. In the equal-mass variant, the source is optimally transported, with squared Euclidean cost, to atoms of mass $1/2$ at the two sites. The new sites are the barycentres of the assigned masses. We track the unordered pair with the Hausdorff distance on nonempty compact subsets of $\mathbb{R}^n$. A stationary pair is fixed by one update. Sequential convergence means that the entire sequence approaches a single pair.

Theorem 1 (Projective cluster set)**.** *Fix an integer $n \geq 3$, a derivative order $M \geq 0$ and $\varepsilon > 0$. There is a centrally symmetric compact body $K \subset \mathbb{R}^n$ with nonempty interior, C^∞ boundary and strictly positive principal curvatures. Its radial function can be chosen within ε of 1 in $C^M(\mathbb{S}^{n-1})$. For the uniform probability law on K there is a pair of distinct interior sites $\{y, -y\}$ such that the set of all subsequential limits of its unordered Lloyd iterates is exactly*

$$\big\{\{-c(w,0), c(w,0)\} : w \in \mathbb{S}^{n-2} \subset \mathbb{R}^{n-1}\big\}, \qquad c > 0. \tag{1}$$

Every member is stationary. The sites along the orbit span $\mathbb{R}^n$ and remain interior. Ordinary and optimal equal-mass Lloyd give the same sequence. With its subspace topology the cluster set is homeomorphic to $\mathbb{RP}^{n-2}$.

The same initial pair can be used for two further sources with the same normalized centroid update at every nonzero antipodal input. One has an everywhere positive smooth density ρ, mean zero, covariance I, and $-D^2 \log \rho \succeq I/2$. Its density equals the standard Gaussian off $1 < |x| < 2$. The other has a globally smooth log-concave density supported on the closed ball of radius three,

positive on its interior. Each has the cluster set (1) with its own radius c, the full spanning property, and agreement of both Lloyd rules.

For $n = 3$ the cluster set is a circle of unoriented axes in a plane. A product with independent centered coordinates of finite second moment immediately gives nonconvergence in higher dimension. For lifted sites $(y_i, 0)$ the extra squared distance is the same for each i, and the extra coordinates of both conditional means vanish. The lifted orbit stays in the original three-dimensional subspace and inherits the circle. In Theorem 1, already at $n = 4$ one orbit approaches every unoriented axis of a three-dimensional hyperplane. Its limit space has dimension two, and its sites span four dimensions.

Relation to convergence results

Portales, Cazelles and Pauwels distinguish stationarity of accumulation points from convergence of a whole sequence and identify the general sequential question in their introduction [10, Sec. 1]. Their Theorem 2.3 gives convergence for ordinary optimal quantization with an absolutely continuous, compactly supported law admitting a globally subanalytic density and with convex support (Assumption 2). Their Theorem 2.5 gives convergence for equal-mass quantization under Assumption 1, which retains the density and compactness conditions. Our uniform law has convex support. Its nonconvergent orbit therefore implies that its density has no globally subanalytic representative. The compact smooth density gives the same obstruction even when the support is a Euclidean ball. The term *uniform* in their second algorithm refers to the masses of the target sites.

Du, Emelianenko and Ju [2, Thm. 2.6] assume that the iterates stay in a compact set on which the Lloyd map is continuous. Their conclusion reads: "the algorithm is globally convergent to a critical point of H". The proof explicitly concludes convergence of the sequence Z_n. Their Section 5 also lists global convergence for general smooth densities in arbitrary dimension among the open questions. Emelianenko, Ju and Rand [3, Def. 2.1, Thm. 2.1, and Sec. 4] distinguish weak convergence from convergence to a single configuration. In their notation, the gradient of the quantization energy tends to zero and the distance to the fixed-point set tends to zero. They expressly ask what would ensure a single limit. Their Theorem 3.8 establishes weak convergence and nondegeneracy on bounded convex domains with positive integrable density.

The uniform example in Theorem 1 satisfies the compactness and continuity hypotheses. Its density is constant on the body. Write $H(u) = \mathbb{E}|u \cdot X|$ and let $m(u)$ be the updated positive site from a pair on axis u. Updated radii are bounded below by $\min_{\|u\|=1} H(u) > 0$, since $m(u) \cdot u = H(u)$, and above by the radius of an enclosing ball. The positive initial radius preserves separation as well. At each pair in the compact orbit closure the bisector has zero mass and each cell has mass $1/2$. If sites tend to such a pair, the cell indicators converge almost everywhere. Dominated convergence for masses and first moments gives continuity of the Lloyd map there. The unordered configurations have multiple limits, so even ordered convergence to a point is impossible. Every cluster configuration is stationary. Thus this orbit separates the literal single-point conclusion in the 2006 paper from the weak conclusion made explicit in 2008.

Pagès and Yu's published abstract describes pointwise convergence under a strict initial error threshold [8]. The example meets that threshold even for ordinary Lloyd. Write $H(u) = \mathbb{E}|X \cdot u|$ at its initial unit direction u. The best one-site squared error is $S = \mathbb{E}\|X\|^2$ by symmetry. The pair $\{\pm H(u)u\}$ has squared error $S - H(u)^2 < S$. Every positive radius gives the same first partition and hence the same subsequent orbit. For the near-ball body this seed is interior by taking the perturbation small. In the public preprint, Theorem 2.1(b) supplies boundedness under a splitting condition. Part (a) obtains a single limit under the further local-finiteness condition on stationary grids at the limiting error. Our stationary equator violates that condition. The comparison with

the theorem as printed in the journal remains open pending inspection of its full hypotheses. The starting error is also strictly above the two-site optimum. At the first step $m(u) \neq H(u)u$ because the direction changes. Replacing the two sites by their conditional means while keeping the old assignment lowers squared error by $\|m(u) - H(u)u\|^2$. Reassignment cannot raise it.

A smooth objective can support winding descent trajectories. Absil, Mahony and Andrews give a continuous gradient-flow example in [1, eqs. (2.8)–(2.9)] and a sampled sequence satisfying their descent conditions in [1, Sec. 3]. To realize such behavior for Lloyd iteration one must identify a probability source whose *exact discrete* centroid updates trace the prescribed path. Sections 2 and 3 do this using classical cosine-transform inversion and a scalar potential with a specified first derivative. In the public literature examined for this manuscript we did not locate the same two-site population counterexample, in dimension three or in its projective extension. This search does not establish historical priority.

How the construction arose. In a project on extracting reusable operations from public AI proofs, we revisited the midpoint coupling in OpenAI's Brenier stability manuscript [7, Sec. 4, Lem. 4.2]. A finite comparison of the first moments of two cell partitions shortened its proof and gave a computable error bound for approximate Lloyd steps. Small step error left a different question open: where can the exact sites go? For symmetric pairs their next sites depend on one directional moment. Prescribing this moment turned the question into the inverse problem in Sections 2–3. The finite comparison supplies the error certificate. The proof of Theorem 1 starts from the exact centroid identity. The orbit construction below is self-contained.

2 From a directional moment to a probability source

Let X have an even, absolutely continuous probability law with finite second moment. For $x \in \mathbb{R}^n$ put $H(x) = \mathbb{E}|\langle x, X\rangle|$. It is positive away from zero. For $\|u\| = 1$ and $r > 0$, distances to $\pm ru$ select the sign of $\langle u, X\rangle$, with null ties and halves of mass $1/2$. Differentiating under the expectation, dominated by $|X|$, shows that the next positive site is

$$m(u) = \nabla H(u) = \mathbb{E}[X \operatorname{sign}\langle u, X\rangle] = H(u)u + \nabla_S H(u).$$

The last identity follows from degree-one homogeneity and the radial-tangential decomposition of the Euclidean gradient. The two conditional means are opposites. The nearest assignment minimizes squared cost pointwise and has the prescribed half masses. Any optimal coupling must make that assignment almost everywhere, because any positive probability sent to the farther site gives strictly positive excess cost. Thus both algorithms have the same updates from these seeds. In particular, if $H|_{\mathbb{S}^{n-1}} = c\,e^f$ for $c > 0$, the next direction and site are

$$T_f(u) = \frac{u + \nabla_S f(u)}{\|u + \nabla_S f(u)\|}, \qquad m(u) = c\,e^{f(u)}(u + \nabla_S f(u)). \tag{2}$$

This normalization is the generalized power step on the unit sphere applied to the convex objective H [4, Alg. 1 and Sec. 3.3]. For an antipodal pair the squared quantization error is $\mathbb{E}\|X\|^2 + r^2 - 2rH(u)$, so H also determines the best radius at each fixed direction. Multiplying H by a positive constant rescales the updated radii and preserves the direction map. The derivative and ordinary centroid identities require only a finite first moment.

Lemma 2 (Local realization in dimension n)**.** *Let $n \geq 2$. Every smooth even h sufficiently close to 1 in $C^\infty(\mathbb{S}^{n-1})$ is realized as $H|_{\mathbb{S}^{n-1}} = ch$, $c > 0$, by a uniform centrally symmetric smooth*

positively curved body close to the ball. As $h \to 1$ its radial function tends to 1 in C^∞. A Gaussian shell perturbation as in Theorem 1 realizes the same h.

Proof. Write dS for area measure and $C_n q(u) = \int |\langle u, v\rangle| q(v)\, dS(v)$. On smooth even functions C_n is a continuous linear automorphism, including continuity of its inverse. See Klain [5, proof of Prop. 3.1] and Kuchment and Terzioglu [6, text following Thm. 2]. For uniform bodies, the radial moment formula below is Petty's [9, proof of Thm. (4.1), p. 1545]. His theorem establishes uniqueness. Near the ball, realization up to a positive factor follows directly from his formula and the classical smooth inverse. Let $a_n = C_n 1 > 0$, constant by rotation invariance. Define

$$q = 1 + a_n C_n^{-1}(h-1), \qquad r = q^{1/(n+1)}, \qquad K = \{sv : v \in \mathbb{S}^{n-1},\ 0 \le s \le r(v)\}.$$

Then $q \to 1$ smoothly, so $q > 0$ and $r \to 1$ smoothly. Polar integration gives

$$H_K(u) = \frac{1}{(n+1)|K|} \int_{\mathbb{S}^{n-1}} |\langle u, v\rangle|\, r(v)^{n+1} dS(v) = \frac{a_n}{(n+1)|K|} h(u).$$

The extra radial power comes from the linear integrand. For convexity set $J(x) = |x|^2 / r(x/|x|)^2$ off zero, $J(0) = 0$. On the unit sphere $D^2 J \to 2I$ uniformly by C^2 convergence, and this Hessian is homogeneous of degree zero. Hence $D^2 J \succeq I$ away from zero. The derivative extends continuously by zero at the origin, so restricting to lines also gives strong convexity across zero. On $J = 1$, $x \cdot \nabla J = 2$. The second fundamental form is the tangent restriction of $D^2 J / |\nabla J|$, hence positive definite everywhere.

For the Gaussian source we use a separate radial shell perturbation. Write g_n for the standard Gaussian density and $g_* = \mathbb{E}|Z_1| = \sqrt{2/\pi}$. Take a nonnegative nonzero $\eta \in C_c^\infty((1,2))$. There is a signed $b(r) = \eta(r)(p_0 + p_1 r + p_2 r^2)$ with

$$\int_1^2 r^{n-1} b(r) dr = 0, \quad \int_1^2 r^n b(r) dr = 1, \quad \int_1^2 r^{n+1} b(r) dr = 0.$$

Indeed its moment matrix is the positive definite Gram matrix of $1, r, r^2$ for weight $r^{n-1}\eta$. Put $a = g_* C_n^{-1}(h-1)$, and define $\rho(x) = g_n(x) + b(|x|) a(x/|x|)$, setting the correction to zero near the origin. The three moments preserve mass and second moments and add $C_n a$ to H. Evenness preserves zero mean. The correction is small in C^2 on the fixed shell, where the Gaussian is bounded below. The logarithm and its first two derivatives converge uniformly there to those of g_n; outside the shell there is exact equality. This proves positivity and the claimed Hessian bound. For every unit u, $H_\rho(u) = g_* h(u)$.

The same shell correction gives a compactly supported smooth log-concave law. Use the normalized radial density proportional to $\exp[-|x|^2 - 1/(9 - |x|^2)]$ on $|x| < 3$, extended by zero, and replace g_* by its constant unit-direction moment. In the open ball the Hessian of the negative log of this baseline is bounded below by $2I$. The same three radial identities preserve normalization and the covariance of this baseline. A sufficiently small correction leaves the negative log-Hessian at least I on the shell. The density agrees with the baseline everywhere else. Extension by zero preserves log-concavity since the positive set is convex. □

3 An orbit visiting every equatorial direction

Proof of Theorem 1. Put $m = n - 2$. We first construct a smooth curve $a_0 : \mathbb{R} \to \mathbb{S}^m$ with bounded derivatives of every order and dense image after every time. Choose a sequence $(w_j)_{j \ge 1}$ repeating

each point of a countable dense subset infinitely often, a unit vector e, and a scalar smooth bump β supported in $(-1/4, 1/4)$ with $\beta(0) = 1$. For each j write $w_j = \cos\theta_j\, e + \sin\theta_j\, v_j$ with $v_j \perp e$, $\|v_j\| = 1$ and $0 \le \theta_j \le \pi$. At $w_j = \pm e$ any such v_j works. On $|t - j| < 1/4$ set

$$a_0(t) = \cos(\theta_j \beta(t-j))\, e + \sin(\theta_j \beta(t-j))\, v_j.$$

Set $a_0 = e$ elsewhere. Each arc agrees smoothly with e at its ends, and its rth derivative is bounded independently of j, since $\theta_j \in [0, \pi]$ and the bump is fixed. At the integers the curve visits every target in the sequence.

In a belt write $W(z, \xi) = (B(z)\xi, z)$, $B(z) = \sqrt{1 - z^2}$. Define U for $0 < z < 3/4$, and for $0 < z < 1/2$ define s, V by

$$a(z) = a_0(-\log z), \quad U(z) = W(z, a(z)), \quad s(z) = z - \delta e^{-1/z^2}, \quad V(z) = U(s(z)).$$

For all sufficiently small $\delta > 0$, $z/2 < s(z) < z$ and $D = \langle U, V\rangle > 1/2$ uniformly. Indeed $\|U'(z)\| = O(1/z)$ and $\|V - U\| = O(\delta e^{-1/z^2}/z)$. For small negative δ, s also stays positive and uniformly separated from 1 on the belt where we cut off; the perturbation is smooth across $\delta = 0$. Define at height z

$$G = V/D - U, \quad p = \langle G, (B'(z)a(z), 1)\rangle, \quad q = B(z)\big(G_{\mathrm{hor}} - \langle G_{\mathrm{hor}}, a(z)\rangle a(z)\big),$$

where G_{hor} is the first $n - 1$ coordinates. Then $G \perp U$ and normalizing $U + G$ gives exactly V. Take

$$A(z) = \int_0^z \big(p(t) + \langle q(t), a'(t)\rangle\big)\, dt, \qquad f_N(z, \xi) = A(z) + \langle q(z), \xi - a(z)\rangle.$$

At $\xi = a(z)$ the partial derivative in z with ξ fixed is $A' - \langle q, a'\rangle = p$. Along every unit-sphere tangent $v \perp a(z)$ the angular derivative is $\langle q, v\rangle = \langle G, (Bv, 0)\rangle$. Together with W_z the vectors $(Bv, 0)$ span the entire tangent space. Consequently $\nabla_S f_N(U) = G$. The term $\langle q, a'\rangle$ in the primitive is needed even though $q \perp a$.

For smoothness at the equator, $\partial_z^j U(z) = O_j(z^{-j})$ follows by the chain rule and bounded angular derivatives. Set $e = s - z$. In

$$V - U = e \int_0^1 U'(z + \lambda e)\, d\lambda$$

all derivatives of the integral, including parameter derivatives, are bounded by fixed inverse powers of z, uniformly for small $|\delta|$ and $0 \le \lambda \le 1$. The factor $e = -\delta e^{-1/z^2}$ and all its derivatives vanish faster than every such power. This proves joint flatness of $V - U$. Since $D - 1 = \langle U, V - U\rangle$ and D stays bounded below, the same bounds apply to G, p, q, $q \cdot a'$ and A. Thus f_N extends smoothly and flatly to $z = 0$, uniformly in angle in every smooth chart. Multiply it by a smooth cutoff equal to 1 on $0 \le z \le 1/5$ and zero for $z \ge 1/3$. Extend to the southern hemisphere by evenness and put $f = 0$ at the equator. At $\delta = 0$ the entire function is zero; joint smoothness on a compact sphere gives $h_\delta = e^f \to 1$ in every fixed C^M. Lemma 2 applies for small positive δ.

Choose $z_0 = 1/8$ and $z_{j+1} = s(z_j)$. Equation (2) gives $U(z_j) \mapsto U(z_{j+1})$ for the actual normalized update. The heights decrease to zero since a positive limit would have a positive decrement. The times $t_j = -\log z_j$ diverge and

$$t_{j+1} - t_j = -\log(1 - \delta e^{-1/z_j^2}/z_j) \longrightarrow 0.$$

For any $w \in \mathbb{S}^m$, choose $T_i \to \infty$ with $a_0(T_i) \to w$. At the first index j_i with $t_{j_i} \ge T_i$, one has $j_i \to \infty$ and $0 \le t_{j_i} - T_i \le t_{j_i} - t_{j_i - 1} \to 0$. Bounded speed gives $a_0(t_{j_i}) \to w$. All limit directions are

equatorial by $z_j \to 0$. On the equator $f = 0$ and $\nabla_S f = 0$. Hence every limit radius is c and every such pair is fixed, directly from $m(u) = ce^{f(u)}(u + \nabla_S f(u))$. Start at radius $1/4$, an interior seed by closeness to the ball. Later centroids are interior since a supporting hyperplane cannot contain a conditional positive-volume half of the source. The map $w \mapsto \{-c(w,0), c(w,0)\}$ is continuous in the Hausdorff metric and has precisely the fibers $\{w, -w\}$. It induces a continuous bijection from the compact antipodal quotient onto the Hausdorff cluster space, hence a homeomorphism. The span of the actual sites is a closed linear subspace. It contains the equatorial hyperplane by the limits just obtained, and also the initial site, whose final coordinate is positive. It is therefore all of $\mathbb{R}^n$. □

4 The threshold for symmetric starts

Theorem 3. *Let μ be a centrally symmetric, absolutely continuous probability with finite first moment, and initialize ordinary two-site Lloyd at $(x, -x)$, $x \neq 0$. In dimension one the first update is fixed. In dimension two assume in addition that $h(\theta) = \mathbb{E}|\langle X, (\cos\theta, \sin\theta)\rangle|$ is C^2. Then the ordered pairs converge. With finite second moment, every selection of optimal equal-mass updates has the same respective property.*

Proof. In one dimension the dividing point is zero. Each conditional mean lies strictly on its respective side, so both cells are unchanged after the first update. In the plane let $u = (\cos\theta, \sin\theta)$ and $u' = (-\sin\theta, \cos\theta)$. The signed first moment is $hu + h'u'$ with $h > 0$. The ordinary direction update lifts to

$$T(\theta) = \theta + \arctan(h'/h), \qquad T'(\theta) = \frac{h(h + h'')}{h^2 + (h')^2}.$$

Positivity of h follows from absolute continuity. The function $t \mapsto H(u+tu')$ is convex, and it equals $\sqrt{1+t^2}\, h(\theta + \arctan t)$. Its second derivative at $t = 0$ equals $h + h''$. Hence T is nondecreasing. Any maximum of h gives a fixed angle. Its 2π-translates enclose the starting angle in a closed interval whose endpoints are fixed. Monotonicity keeps the iterates in that interval and, after comparing the initial angle to its image, orders all subsequent iterates in the same direction. They converge. Continuity of $hu + h'u'$ then gives convergence of both site locations. The pointwise assignment argument of Section 2 gives the equal-mass assertion for finite quadratic cost. □

Under these symmetry and moment conditions, three is the smallest dimension admitting a nonconvergent antipodal orbit. The higher-dimensional theorem makes an existential assertion about initialization.

5 Formal verification

A separate Lean project proves the following theorem.

`LloydNDVerified.projective_lloyd`

Its inputs are $k, M \in \mathbb{N}$ and $\varepsilon > 0$, with ambient dimension $k + 3$. Its witnesses are a uniform body, two densities and one common seed. For each it proves (1) in both directions, the quotient homeomorphism, stationarity, full span and agreement of all optimal equal-mass choices with ordinary Lloyd. The normalized updates agree across the three sources for every antipodal input. The formal radial closeness estimate controls derivatives up to M of an extension of the radius, uniformly on $\{|x| > 1/2\}$. Theorem 3 is checked by separate declarations for dimensions one and two.

Both proofs use smooth excursions to repeated dense targets. The paper uses time $-\log z$. Lean uses reciprocal height $z = 1/T$ and

$$T_0 = 8, \qquad T_{j+1} = T_j + \delta \exp(-\delta^2 - T_j^2).$$

It constructs a smooth even ambient potential with the required derivative on the orbit and proves directional-moment realization for smooth parameter families by a Fourier right inverse. A coordinate permutation moves the equatorial normal from the last coordinate in the paper to the first in Lean. The optional finite numerical checks test the local directional formula on example paths. The infinite-time conclusions come from the proofs.

Use of artificial intelligence

A human initiator proposed extracting reusable mathematics from long AI-generated proofs and asked for an extension of the Lloyd example to all higher dimensions. The development was steered to preserve the original hypotheses, test reuse in an independent problem, separate established ingredients from the proposed orbit construction, and check the formal theorem against the stated mathematical claims. OpenAI Codex developed the counterexample and cluster-set proof, wrote the exposition and Lean code, compared sources, and ran the checks. The project records identify Codex but do not establish a specific model version for each historical run. A GPT-6-based Codex agent prepared the publication drafts. The attribution proposed for review concerns the prescribed exact orbit and its exhaustive cluster set. Historical priority for the separate Gaussian-shell construction and the earlier transport comparison is unassessed.

The recorded Lean 4.34.1 build and kernel replay cover 106 local modules. The main endpoint has 66 local modules in its import closure. Its reported axiom dependencies are `propext`, `Classical.choice`, and `Quot.sound`. The historical comparisons and the modified-radius starting-error calculation are written arguments. Independent human mathematical review has not been confirmed.

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