Visualizing probabilistic models in Minkowski space: an analytical coordinate embedding

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Abstract

We show that the predicted probability distributions for any \(N\)-parameter statistical model taking the form of an exponential family can be explicitly and analytically embedded isometrically in a \(N+N\)-dimensional Minkowski space. That is, the model predictions can be visualized as control parameters are varied, preserving the natural distance between probability distributions. All pairwise distances between model instances are given by the symmetrized Kullback-Liebler divergence. We give formulas for these isKL coordinate embeddings, and illustrate the resulting visualizations with the coin toss problem, the ideal gas, \(n\) sided die, the nonlinear least squares fit, and the Gaussian fit. We conclude by visualizing the prediction space of the two-dimensional Ising model, where we examine the manifold behavior near its critical point.
I. CONTEXT

Many features of multiparameter models are best understood by studying the manifold of model predictions. The model’s parameters can be treated like the coordinates of a model manifold that traces out the predictions consistent with the model in the ‘behavior space’ of all possible predictions, e.g., experimental measurements or observables. Naively, embedding the predictions of a few-dimensional model in the infinite-dimensions of behavior space could lead to a curly tangle only described well in high dimensions. Surprisingly, model manifolds are usually observed to be well approximated by a relatively flat surface of lower dimension than the model, often forming flat hyperribbons with each successive cross sectional span geometrically smaller than the last [1, 2]. This has now been demonstrated rigorously for nonlinear least squares models [3], and helps explain the parameter indeterminacy or ‘sloppiness’ observed in systems biology [4] and other fields [5]. The hyperribbon geometry of the model manifold has inspired new algorithms for nonlinear least-squares fits [1, 2, 6, 7] and for the control of complex instrumentation such as particle accelerators [8].

Many statistical models are not of least-squares form. For example, the Ising model of magnetism and the ΛCDM model of the cosmic microwave background predict the distribution of results—not the explicit result—of an experiment. Local analysis of parameter sensitivity shows that the Ising model [9] and the ΛCDM model [10] are sloppy nonetheless, in the sense that they have a hierarchy of sensitivity eigenvalues spanning many decades. These local sensitivities are measured by the natural distance in the space of probability distributions, the Fisher Information Metric (FIM) [11].

In reference [10] it was shown that low-dimensional Euclidean embeddings indeed form a high-dimensional curly tangle in the space of probability distributions, but in the limit of zero data yield the ‘intensive’ isometric embedding InPCA into an infinite-dimensional Minkowski space. For a model whose parameters \( \theta = \{ \theta_\alpha \} \) predict that results \( x \) of an experiment will be distributed by \( P_\theta(x) \), InPCA allows visualization of the model manifold with pairwise distances given by the Bhattacharyya divergence [12]

\[
D_{Bhat}^2(P_\theta, P_\gamma) = -\log \left( \sum_x \sqrt{P_\theta(x)P_\gamma(x)} \right).
\]

For the Ising and ΛCDM models, \( x \) runs over spin configurations and observed spatial CMB maps, respectively. The InPCA manifold often forms a hyperribbon, thereby capturing most of the model variation with only a few principal components. This procedure of taking the limit of zero data can be applied using a more general class of pairwise distances given by the \( f \) divergences [13] and in return yields a collection of intensive distance measures, expressed as a linear combinations of
the Rényi divergences [14] (The details are provided in Appendix A). All Rényi divergences locally reproduce the FIM, so distances in behavior space reflect how sensitive the model predictions are to shifts in the model parameters.

Here we show, for a large class of important multiparameter models, that a different intensive embedding, built on the symmetrized Kullback-Liebler divergence [15]

\[
D_{sKL}^2(p_\theta, p_\gamma) = \sum_x (p_\theta(x) - p_\gamma(x)) \log(p_\theta(x)/p_\gamma(x))
\]

(2)
gerates an explicit, analytically tractable embedding in a Minkowski space of dimension equal to twice the number of parameters. We call this the isKL embedding (intensive symmetrized Kullback-Liebler, pronounced ‘icicle’), and provide the corresponding isKL coordinates in Sec. III. Our result is obtained for models which form the exponential families [16]:

\[
P_\theta(x) = h(x) \exp \left( \sum_\alpha \eta_\alpha(\theta) \Phi_\alpha(x) - A(\theta) \right),
\]

(3)
where \( h(x) \) is the base measure, the \( \eta_\alpha(\theta) \) are the natural parameters, the \( \Phi_\alpha(x) \) are the sufficient statistics, and \( A(\theta) \) is the log partition function. Most models in statistics and statistical mechanics form exponential families, e.g., the Boltzmann distribution defined on most Hamiltonians.

II. CURSE OF DIMENSIONALITY

Large data sets and multiparameter probabilistic models of large systems both suffer from the curse of dimensionality [17]: it is increasingly challenging to discriminate qualitatively close relations from distant relations as the amount of information per data point becomes large. This effect obscures meaningful features within the data set and renders contrast in distances between different data points nonexistent [18].

Intensive embeddings like inPCA and isKL break the curse of dimensionality for probabilistic models, allowing for low-dimensional projections of model manifolds in a suitable Minkowski space [10]. Big data applications have attempted to resolve this dimensionality issue by embedding the manifold in a curved space [19–21] or in an Euclidean space with an alternative distance measure [22–25], which can yield lower dimensional projections that capture dominant components of the variation in the data set. For example, reference [25] makes use of the potential distance to generate useful visualizations of large data sets for biological data in Euclidean space. Our methods suggest an alternative approach. We argue here that the use of Minkowski space is crucial – any general-purpose isometric embedding in an Euclidean space is doomed to a minimum practical
embedding dimension that scales with the number \( M \) of mutually distinguishable probability distributions. That is, any Euclidean embedding must have \( M - 1 \) important perpendicular coordinate axes to describe the qualitative model behavior.

We must mention an apparent counterexample to the argument that follows – an exception that proves the rule. A least-squares model (section \[VID\]) that fits a function \( f_i(\theta) \) to \( N \) experimental measurements \( d_i \) with normally distributed statistical errors has vector-valued predictions \( f(\theta) \) that sweep over a surface in \( \mathbb{R}^N \) \[1, 2\]. This is an intensive isometric embedding. Not only is the dimensionality of this manifold given by the number of data points (and not the number of distinguishable probability distributions), but (as mentioned above) this manifold generally forms a hyperribbon \[1, 2\], with rigorous bounds on spatial extent along a suitable set of perpendicular coordinate directions \[3\]. This hyperribbon structure is the behavior-space ramification of the parameter indeterminacy or ‘sloppiness’ observed as parameters are varied \[4, 5\]. Thus least-squares models do have low-dimensional representations of their model manifold in Euclidean space. We argue that this useful embedding cannot be extended to general probability distributions without making use of Minkowskian time-like coordinates. Indeed, the least-squares Euclidean embedding is reproduced by the Minkowski-space intensive embedding procedures described in section \[VID\]; the time-like coordinates happen to be zero for this particular case.

Our argument that Minkowski space is important builds on the mathematical fact that the straightest path between two probability distributions \( P(x) \) and \( Q(x) \) in the space of all probability distributions is given by a linear interpolation \( \rho_\lambda(x) = \lambda P(x) + (1 - \lambda)Q(x) \) as \( \lambda \) ranges from zero to one. For simplicity, we consider discrete probability distributions, \( \sum_x P(x) = \sum_x Q(x) = 1 \). The length of this path integrating the metric of the statistical manifold, the Fisher Information Metric (FIM)

\[
I_{ij}(\theta) = \left< \frac{\partial^2 \log P(x)}{\partial \theta_i \partial \theta_j} \right>_x
\]

(4)
gives

\[
d_C(P,Q) = \int_0^1 \sqrt{\sum_x \frac{1}{p_\lambda(x)} \left( \frac{dp_\lambda(x)}{d\lambda} \right)^2} \ d\lambda.
\]

(5)

By letting \( p_\lambda(x) = y^2_\lambda(x) \) and realizing \( \sum_x p_\lambda(x) = \sum_x y^2_\lambda(x) = 1 \), Eq. \[5\] yields the arc length of a great circle connecting the two distributions,

\[
d_C(P,Q) = 2 \arccos \sum_x \sqrt{P(x)Q(x)}.
\]

(6)
**FIG. 1.**  (a) **Great circle path between probability distributions** is given by a linear interpolation $p_\lambda(x) = \lambda P(x) + (1 - \lambda)Q(x)$. As $0 \leq \lambda \leq 1$, the interpolation remains positive and normalized. The length of this path under the Fisher Information Metric (FIM) equals the arclength of the great circle, which is $d_{GC}(P, Q) = 2 \arccos \sum_x \sqrt{P(x)Q(x)}$. b) **Geodesic distance** between two Gaussian distribution with fixed $\sigma$ is given by sliding the Gaussian $\mu_P$ to $\mu_Q$, $d_G = \sigma^{-1} |\mu_P - \mu_Q|$. c) Here we illustrate three types of **distances in probability space.** The octant of the sphere schematically represents the space of all possible probability distributions. The great-circle distance $d_C$ is bounded by a quarter of the circumference of the sphere. The straight-line distance $d_S$ depends on the embedding. The geodesic distance $d_G$ is the minimum distance between the two distributions on a statistical manifold. When $d_G \gg d_C$, the path will curl around to fit inside the sphere.

For most models this path will leave the model manifold, since the average distribution is not an allowed model prediction: if $P$ and $Q$ are Gaussians of mean $\mu_P$ and $\mu_Q$, the geodesic path in the model manifold of Gaussians of fixed width $\sigma$ is given by sliding the Gaussian from $\mu_P$ to $\mu_Q$, while the shortest path in the space of all probability distributions is given by shrinking $P$ and growing $Q$ in place (see Fig. 1(a) and (b)).

The key point is that for any embedding that takes general families of probability distributions isometrically into a Euclidean space, no two points on the model manifold can be farther apart than $d_C$. In our simple example, if $\mu_P$ and $\mu_Q$ are many standard deviations apart, the geodesic path between them on the fixed-Gaussian model manifold has length

$$d_G = \int_{\mu_P}^{\mu_Q} \frac{d\mu}{\sigma} = \frac{|\mu_P - \mu_Q|}{\sigma}. \quad (7)$$

When $d_G \gg d_C$, the path must curl around to fit inside the sphere of radius 2, and low-dimensional projection will at best show a crumpled tangle that usually rapidly escapes into higher, undisplayed dimensions (see Fig. 1(c)). More generally, a useful low-dimensional projection should take
$M$ probability distributions with mutual near zero overlap and keep them separated by at least some minimum embedding-space distance $\Delta$, presumably comparable to the $d_C$. The minimum embedding dimension for such a set of points is given by the densest packing of spheres of diameter $\Delta$ into a sphere of diameter $d_G$ in $D$ dimensions. For the Hellinger embedding, or whenever $\Delta \sim d_C$, one needs $M - 1$ projection directions for $M$ mutually distinguishable predictions.

Note that in an Euclidean space, the embedding space distance (a straight line unconstrained by the manifold of probability distributions) is always smaller than the length of the straightest path on the manifold of probability distributions (bounded by $2\pi$, Eq. (6)), which is in turn shorter or equal to the geodesic length of the path $d_G$ constrained to lie on the particular model submanifold. We shall illustrate many times in the rest of this manuscript that this is not true of embeddings in Minkowski space. For example, Fig. 4 in reference [10] shows the inPCA model manifold for the coin-flip problem (different from the isKL embedding in section VIA). The straight-line distance between the two end-points (all heads and all tails) in Minkowski space goes to infinity, but the model manifold hugs a light cone, and the embedding distances from either endpoint to a fair coin is finite. As noted in [10], Minkowski space breaks the curse of dimensionality by violating the triangle inequality.

III. ISKL COORDINATES

In this section we derive the isKL coordinates for a general exponential family, giving an explicit isometric embedding of the probability distributions it predicts in Minkowski space.

Minkowski space in special relativity has three spatial coordinates and one time, with a metric $g_{\mu\nu} = \text{diag}(1,1,1,-c^2)$. Two points have zero distance if their squared spatial separation lies on the light cone $\Delta x^2 + \Delta y^2 + \Delta z^2 - c^2 \Delta t^2 = 0$. Our Minkowski space will have $N$ space-like and $N$ time-like coordinates, which we describe as an $N+N$-dimensional embedding space. We shall generate two coordinates $T^+_\alpha(\theta_\alpha)$ and $T^-_\alpha(\theta_\alpha)$ for each parameter $\theta_\alpha$, one space-like (with positive squared distance) and one time-like (with negative squared distance), such that

$$D^2_{sKL}(P_{\theta}, P_\gamma) = \sum_\alpha (T^+_\alpha(\theta_\alpha) - T^+_\alpha(\gamma_\alpha))^2 - (T^-_\alpha(\theta_\alpha) - T^-_\alpha(\gamma_\alpha))^2.$$  

(8)

The squared term with a positive sign is thus a space-like coordinate, and the term with a negative sign is the corresponding time-like coordinate. Since the symmetrized Kullback-Liebler distance is nonnegative, no pair of points can be time-like separated and we can expect the extent of the model manifold along the time-like coordinates will typically be smaller than its extent along the
space-like coordinates. However, the time-like coordinates are both physical and important, as we shall illustrate in particular using the 2D Ising model.

For an exponential family, the last term in $D_{sKL}^2$ (Eq. (2)) is given by

$$\log(P_\theta(x)/P_\gamma(x)) = A(\gamma) - A(\theta) + \sum_\alpha (\eta(\gamma_\alpha) - \eta(\theta_\alpha))\Phi_\alpha(x).$$

(9)

The first terms of Eq. (9) give zero when inserted into $D_{sKL}^2$ (Eq. (2)):

$$\sum_x (P_\theta(x) - P_\gamma(x))(A(\gamma) - A(\theta)) = (A(\gamma) - A(\theta))(\sum_x P_\theta(x) - \sum_x P_\gamma(x))$$

= $(A(\gamma) - A(\theta))(1 - 1) = 0.

(10)

Hence for our general exponential family,

$$D_{sKL}^2(P_\theta, P_\gamma) = \sum_x (P_\theta(x) - P_\gamma(x))\sum_\alpha (\eta(\gamma_\alpha) - \eta(\theta_\alpha))\Phi_\alpha(x)$$

$$= \sum_\alpha (\eta(\gamma_\alpha) - \eta(\theta_\alpha))\sum_x (P_\theta(x) - P_\gamma(x))\Phi_\alpha(x)$$

$$= \sum_\alpha (\eta(\gamma_\alpha) - \eta(\theta_\alpha))(\langle\Phi_\alpha|x\rangle - \langle\Phi_\alpha|x\rangle)\gamma).$$

(11)

The key now is to notice that

$$(\eta(\gamma_\alpha) - \eta(\theta_\alpha))(\langle\Phi_\alpha|x\rangle - \langle\Phi_\alpha|x\rangle)\gamma)$$

$$= (1/4) ([\eta(\theta_\alpha) - \langle\Phi_\alpha|x\rangle] - [\eta(\gamma_\alpha) - \langle\Phi_\alpha|x\rangle])^2$$

$$- (1/4) ([\eta(\theta_\alpha) + \langle\Phi_\alpha|x\rangle] - [\eta(\gamma_\alpha) + \langle\Phi_\alpha|x\rangle])^2$$

$$= (T^+_\alpha(\theta_\alpha) - T^+_\alpha(\gamma_\alpha))^2 - (T^-_\alpha(\theta_\alpha) - T^-_\alpha(\gamma_\alpha))^2.$$

(12)

with the two Minkowski coordinates for $\theta_\alpha$ given by

$$T^+_\alpha(\theta_\alpha) = (1/2)(\eta(\theta_\alpha) - \langle\Phi_\alpha|x\rangle)$$

$$T^-_\alpha(\theta_\alpha) = (1/2)(\eta(\theta_\alpha) + \langle\Phi_\alpha|x\rangle)$$

(13)

now summing to $D_{sKL}^2(P_\theta, P_\gamma)$ as promised in Eq. (8). The terms quadratic in the parameters and quadratic in the expectation values all cancel, and the cross terms give the contribution of parameter $\alpha$ to $D_{sKL}^2$. This is our main result.

IV. FAMILIES OF EMBEDDINGS: ISOMETRIES OF MINKOWSKI SPACE

Our isKL embedding produces a rigid geometrical object representing the space of model predictions, but that object can be viewed from many perspectives. Any rotation or translation of an
object isometrically embedded in familiar 3D Euclidean space forms another isometric embedding: rotations and translations are isometries of Euclidean space. Correspondingly, there are a family of isKL embeddings formed by the isometries of Minkowski space. Translating the coordinates can be used to center the sampled points of the model manifold; certain boosts can be valuable in minimizing the total squared length of the coordinates (and hence reducing the importance of the time-like coordinates). The rotational isometries within the space-like and time-like subspaces can be used to focus attention on the directions of the model manifold that show the largest variations.

There is a close connection to principal component analysis (PCA) \[26\], and in particular to its generalization, multidimensional scaling (MDS) \[27\]. Principal component analysis uses the isometries of Euclidean space to optimally display data in a space of many dimensions. PCA translates the data to center it, then uses singular value decomposition to rotate and diagonalize the ‘moment of inertia’ tensor of the data set. The data remains many dimensional, but PCA allows one to examine the directions for which the data varies the most. The principal components are the orthogonal directions which best describe the data set – minimizing the sum of squared distances of the remaining data from an approximation restricted to the subspace they span.

Multidimensional scaling generalizes these ideas to situations where the data vectors are not known, but some measure of the pairwise distance is available. MDS generates a rigid, isometric embedding maintaining the pairwise distances, usually in a vector space of dimension equal to the number of data points. Again, this manifold can rotate or translate for a given system depending on the sampling used. Indeed, the eigensystem solved in MDS often has negative eigenvalues \[28–30\] corresponding to time-like coordinates, and changing the sampling can also induce Lorentz boosts. MDS, using the symmetrized Kullback-Liebler divergence $D^2_{sKL}$ as the pairwise distance, in fact produces an isKL embedding \[31\]. Our main result (Eq. (13)) implies that MDS applied with $D^2_{sKL}$ to high-dimensional data produced by an $N$-parameter exponential family will embed its predictions in a much smaller space, with only $N$ space-like and $N$ time-like non-zero coordinates. Furthermore, the resulting manifold will be given by the explicit isKL embedding of Eq. (13) up to isometries.

As a first step in considering the effects of these isometries, let us consider other embeddings, similar to Eq. (13), that also preserve pairwise distances. Clearly one can add a constant $C^\pm_\alpha$ to each coordinate (translations in Minkowski space). One also notes that the two terms $\eta(\theta)$ and $\langle \Phi_\alpha \rangle$ being subtracted may have different units. This can be fixed by rescaling these two terms up
and down by a scale factor $\lambda_\alpha$ with units $\sqrt{[\Phi_\alpha]/[\eta(\theta_\alpha)]:}$

$$T^+_{\alpha}(\theta_\alpha) = (1/2)(\lambda_\alpha \eta(\theta_\alpha) - (1/\lambda_\alpha)(\Phi_\alpha) \theta - C^+_{\alpha})$$

$$T^-_{\alpha}(\theta_\alpha) = (1/2)(\lambda_\alpha \eta(\theta_\alpha) + (1/\lambda_\alpha)(\Phi_\alpha) \theta - C^-_{\alpha}),$$

(14)

with different rescaling parameter $\lambda_\alpha$ and shifts $C^\pm_{\alpha}$ for each pair of coordinates.

We can view Eq. (14) as a composition of two transformations – a translation and a rescaling. The translation is of course one of our isometries. For brevity, the average of $\Phi_\alpha$ given parameters $\theta$ is written as $\langle \Phi_\alpha \rangle_\theta = \langle \Phi_\alpha \rangle$ in the subsequent discussion. Ignoring the translations, rescaling by $\lambda_\alpha$ corresponds to a Lorentz boost $t' = \gamma(t - vx)$, $x' = \gamma(x - vt)$ of our time-like and space-like coordinates $(t, x) = (T^-_{\alpha}, T^+_{\alpha})$, where $\gamma = 1/\sqrt{1-v^2}$:

$$t' = (1/2)\gamma ((\eta(\theta_\alpha) + \langle \Phi_\alpha \rangle) - v(\eta(\theta_\alpha) - \langle \Phi_\alpha \rangle))$$

$$= (1/2) (\gamma(1-v)\eta(\theta_\alpha) - \gamma(1+v)\langle \Phi_\alpha \rangle)$$

$$= (1/2) (\lambda_\alpha \eta(\theta_\alpha) - (1/\lambda_\alpha)(\Phi_\alpha)), \quad \tag{15}$$

$$x' = (1/2)\gamma ((\eta(\theta_\alpha) - \langle \Phi_\alpha \rangle) - v(\eta(\theta_\alpha) + \langle \Phi_\alpha \rangle))$$

$$= (1/2) (\gamma(1-v)\eta(\theta_\alpha) + \gamma(1+v)\langle \Phi_\alpha \rangle)$$

$$= (1/2) (\lambda_\alpha \eta(\theta_\alpha) + (1/\lambda_\alpha)(\Phi_\alpha)).$$

A natural criterion for a good viewpoint of the model manifold would be one which minimizes the sum of squares of the coordinates. In Euclidean space, this just translates the manifold so that its center of mass sits at the origin. Indeed, using $C^+_{\alpha}$ and $C^-_{\alpha}$ to shift our two coordinates to their centers of mass corresponds nicely to shifting the sampled parameters $\eta(\theta_\alpha) \rightarrow \eta(\theta_\alpha) - \overline{\eta(\theta_\alpha)}$ and resulting means $\langle \Phi_\alpha \rangle - \overline{\langle \Phi_\alpha \rangle}$ to their respective centers of mass. Now, presuming for simplicity that the data is centered, let us examine the sum of the squares of our two coordinates $T^+_{\alpha}$ and $T^-_{\alpha}$,

$$(T^+_{\alpha}(\theta_\alpha))^2 + (T^-_{\alpha}(\theta_\alpha))^2 = \frac{1}{2} \left( \lambda_\alpha^2 \eta^2(\theta_\alpha) + \frac{1}{\lambda_\alpha^2} \langle \Phi_\alpha \rangle^2 \right) \quad \tag{16}$$

To get a good point of view in Minkowski space, we seek to minimize the sum of squares of the coordinates by optimizing $\lambda_\alpha$. This yields $\lambda^4_{\alpha} = \langle \Phi_\alpha \rangle^2/\eta^2(\theta_\alpha)$. As the parameters are shifted with respect to their centers of mass, we can recast $\lambda_\alpha = (\text{Var}(\langle \Phi_\alpha \rangle)/\text{Var}(\eta(\theta_\alpha)))^{1/4}$, where the variance is averaged over the ensemble of parameters and the mean $\langle \Phi_\alpha \rangle$ is taken at a fixed parameter $\theta$.

V. CONNECTION TO MULTIDIMENSIONAL SCALING (MDS)

We can now establish a connection with MDS. For a sampling $d\mu(\theta)$ of parameter space, MDS generates an embedding whose $i$th projection is given by $\sqrt{\Lambda_i}v_i$, where $\Lambda_i$ and $v_i$ are the eigenvalue
and eigenvector of the double mean centered pairwise distance matrix, \( D^2_c = (1/2)PD^2P \), where \( P_{i,j} = 1/n - \delta_{i,j} \), \( D^2 \) is the pairwise distance matrix and \( n \) is the number of sampled points. Since the manifold width on each projection is associated with the square root of the MDS eigenvalues \( \sqrt{\Lambda_i} \), we posit that \( T^\pm_k(\theta_k) \) is a solution to the integral eigenvalue problem

\[
\int D^2_c(\theta, \gamma)T^\pm_k(\theta_k)d\mu(\theta) = \Lambda^\pm_kT^\pm_k(\gamma_k), \quad (17)
\]

a continuum version of MDS eigenvalue decomposition procedure, where \( D^2_c(\theta, \gamma) \) is the double mean-centered \( D^2_{sKL}(P_\theta, P_\gamma) \). Upon solving Eq. (17), we have \( \Lambda^\pm_k = -\lambda^2_k\Var(\eta(\theta_k)) \pm \Cov(\eta(\theta_k), \langle \Phi_k \rangle) \). In general, when the eigenvalues are degenerate, the eigenvectors of \( D^2_c \) are free to rotate within the degenerate spacelike and timelike subspaces, depending on \( d\mu \). Hence, the solution will be a linear combination of the degenerate coordinates described in Eq. (14), \( T^\pm(\theta) = \sum_i T^\pm_i(\theta_i) \) where \( T^\pm_i(\theta_i) \)s share the same eigenvalue. In all our examples except the generalized die, symmetry keeps rotations from mixing directions and the projection coordinates can be calculated from Eq. (14) regardless of degeneracy.

VI. EXAMPLES

To demonstrate how isKL embeddings optimize the total squared distance of coordinates to produce a good visualization, we consider several probabilistic models that form exponential families: the coin toss problem, the ideal gas model, the \( n \)-sided die, the nonlinear least square problem, Gaussian fits to data, and the two dimensional Ising model.

Before diving into the examples, it is worth highlighting that the finite embedding dimension for exponential families appears to be a unique feature of \( D^2_{sKL} \). As \( D^2_{sKL} \) is part of a family of intensive distance measures known as the Rényi divergence, we embed the coin toss manifold with other symmetrized Rényi divergences to illustrate this uniqueness. As shown in Fig. 2 (a), the embedding is sloppy for all \( \alpha \) (geometrically decreasing manifold widths that span several decades) but only for \( \alpha = 1 \) does it truncate after two dimensions. This exact truncation is true for all the probabilistic models considered in this paper. In principle, we could perform experiments or simulations without knowing the number of parameters the exponential family distribution needs to describe the behaviour. If the isKL embedding gives a cutoff after \( N + N \) dimensions it suggests that a hidden \( N \)-parameter exponential family describes the experiment.
**FIG. 2.** (a) Squared principal length of intensive embedding with different symmetrized Rényi choices for the coin toss manifold. \( \alpha = 1/2 \) corresponds to Bhattacharyya divergence and \( \alpha \to 1 \) leads to Symmetrized Kullback-Liebler divergence (SymKL). Throughout the models considered in subsequent sections, SymKL provides the lowest embedding dimension while other Rényi choices give infinite embedding dimension. This implies the sloppiness of the embedding is influenced by the choice of divergence used. (b) Model manifold for the Coin toss (Bernoulli Problem) is visualized with isKL. The analytical calculation matches well with the numerical result returned from MDS.

### A. Bernoulli Problem

The Bernoulli problem or coin tossing experiment is one of the simplest probabilistic models. As a function of the fairness parameter \( p \), the result \( x \in \{0,1\} \) of a coin toss is distributed by \( P_p(x) = p^x(1-p)^{1-x} \). This probability distribution can be written in the form of an exponential family with \( \eta(p) = \log(p/(1-p)) \), \( \Phi(x) = x \), \( h(x) = 1 \), and \( A(\theta) = \log(1-e^\theta) \). The FIM for this model is given by

\[
(ds)^2 = \frac{(dp)^2}{p(1-p)}
\]  

(18)

By defining \( p = \sin^2 \theta \), we have \( ds = 2d\theta \). This produces a one dimensional embedding onto a Hellinger quarter circle of radius 2 with \( \theta \in [0, \pi/2] \). Upon taking the limit of zero data, the Hellinger distance transforms into the Bhattacharyya divergence. It is known that with the Bhattacharyya divergence, the coin toss manifold is embedded into a Minkowski space of infinite dimension \([3]\). The InPCA projection coordinates can be obtained analytically and are discussed in Appendix B. With isKL embedding, the coin toss manifold can be isometrically embedded into \((1+1)\) dimensions. As
\(\langle \Phi \rangle = p\), its pairwise distance is given by

\[
D_{sKL}^2(p, a) = (p - a) \log \frac{p(1 - a)}{a(1 - p)}.
\]

To obtain the projection coordinates analytically, we use the Jeffrey’s prior sampling. The centers of mass are \(\eta = 0\) and \(\langle \Phi \rangle = 1/2\) respectively. Furthermore, \(\text{Var}(\eta) = \pi^2\) and \(\text{Var}(\langle \Phi \rangle) = 1/8\) we have \(\lambda = (\text{Var}(\langle \Phi \rangle)/\text{Var}(\eta))^{1/4} = (2^{3/4}\sqrt{\pi})^{-1}\). With these, the projection coordinates are calculated to be

\[
T^{\pm}(p) = \frac{1}{2} \left( \lambda(\eta - \eta) \pm \frac{1}{\lambda} (\Phi - \langle \Phi \rangle) \right)
= \frac{1}{2^{7/4}\sqrt{\pi}} \log \left( \frac{p}{1 - p} \right) \pm \frac{\sqrt{\pi}}{2^{1/4}} \left( p - \frac{1}{2} \right)
\]

Fig. 2 shows the coin toss manifold.

**B. Ideal gas**

The ideal gas is a model of noninteracting particles. At pressure \(P\) and temperature \(\beta^{-1}\), the probability that \(N\) particles will be found in a configuration with momenta \(P\), positions \(Q\), and container volume \(V\) is

\[
p(P, Q, V | P, \beta) = Z^{-1}(P, \beta) \exp (-\beta P^2/2m - \beta PV),
\]

where the partition function \(Z(P, \beta) = (2\pi m/\beta)^{3N/2}(\beta P)^{-(N+1)}\) normalizes the distribution. This probability distribution is in the from of an exponential family with \((\eta_1(\theta), \eta_2(\theta)) = (\beta, \beta P), (\Phi_1(x), \Phi_2(x)) = (P^2/2m, V), h(x) = 1\) and \(A(\theta) = \log(Z(P, \beta))\). Using the coordinates \((p, \beta)\), where \(p = \beta P\), its FIM is \((ds)^2 = (N + 1)(dp/p)^2 + (3N/2)(d\beta/\beta)^2\). The scalar curvature of the resulting manifold is zero everywhere, implying that it is a developable surface. Indeed, by defining a new pair of coordinates \((x, y) = (\sqrt{1 + N \log(p)}, \sqrt{3N/2 \log(\beta)})\) we have a two dimensional Euclidean embedding. However, the pairwise distance in this embedding is not given by \(D_{sKL}^2\) and in fact it is not obtainable from any symmetrized Rényi divergence [32].

IsKL isometrically embeds the ideal gas into \((2+2)\) dimensions. The ideal gas law \(PV = N/\beta\) yields the sufficient statistics \(\langle P^2/2m\rangle = N/\beta\) and \(\langle V\rangle = N/p\), and the pairwise KL divergence between two distributions is

\[
D_{sKL}^2(p_1, p_2, \beta_1, \beta_2) = N(p_1 - p_2)\left(\frac{1}{p_1} - \frac{1}{p_2}\right) + N(\beta_1 - \beta_2)\left(\frac{1}{\beta_1} - \frac{1}{\beta_2}\right).
\]
FIG. 3. **Model manifold for the ideal gas** - The flat ideal gas manifold is embedded into a (2+2) dimensional Minkowski space. The manifold is 'rolled' twice in the four dimensional space, giving it a torus appearance in Minkowski space. The Carnot cycle is illustrated on the manifold. The manifold projections are depicted in a descending order based on the manifold widths along the spacelike/timelike components. The spacelike directions are color coded in black while the timelike directions are color coded in red.

Letting the centers of mass be $\langle \eta \rangle = \langle \eta \rangle$ and $\langle \Phi \rangle = \langle \Phi \rangle$, the projection coordinates are given by

$$
T_p^\pm(p) = \frac{1}{2} \left( \lambda_p \left( p - \langle p \rangle \right) \pm N\lambda_p^{-1} \left( p^{-1} - \langle p^{-1} \rangle \right) \right) \\
T_\beta^\pm(\beta) = \frac{1}{2} \left( \lambda_\beta \left( \beta - \langle \beta \rangle \right) \pm N\lambda_\beta^{-1} \left( \beta^{-1} - \langle \beta^{-1} \rangle \right) \right)
$$

(23)

From Eq. 23, the coordinate pairs yield $(T_k^+ - C_k^+)^2 - (T_k^- - C_k^-)^2 = r^2$, where $k = \{p, \beta\}$, $r^2 = N$ and $C_k^\pm = (1/2) \left( -\lambda_k \langle k \rangle \pm N\lambda_k^{-1} \langle k^{-1} \rangle \right)$ are constants that depend on the sampling range. Therefore, the ideal gas manifold is a four dimensional Minkowskian torus (topologically a hyperboloid) with radii $r_1 = r_2 = \sqrt{N}$. Just as the 4D Euclidean torus has zero curvature [33], so it does in Minkowski space.

Interestingly, as a torus is given by the Cartesian product of two circles (gluing a flat sheet right and left edges as well as the top and bottom edges), we are able to provide a mapping to the Euclidean embedding discussed by shifting the coordinates, $T_k^\pm \rightarrow T_k^\pm - C_k^\pm$ and parameterizing the coordinate pairs as $(T_k^+, T_k^-) = (\sqrt{N} \cosh(\phi_k), \sqrt{N} \sinh(\phi_k))$, where $\phi_k = (1/2) \log(k\lambda_k/\sqrt{N})$. 

13
FIG. 4. **Model manifold for the three sided die** is embedded into (2+2) dimension with isKL embedding. Depicted also is the coin toss submanifold in red. The manifold projections are depicted in a descending order based on the manifold widths along the spacelike/timelike components. The spacelike directions are color coded in black while the timelike directions are color coded in red. We have permutation symmetry in \((T^+_p, T^-_p)\) coordinate pairs and reflection symmetry along the \(p_1 = p_2\) line (dotted line) in \((T^+_p, T^-_p)\) coordinate pairs.

\[ (x, y) = \left( \sqrt{1 + N} \left( \log \left( \frac{\sqrt{N}}{\lambda_p} \right) + 2\phi_p \right), \sqrt{\frac{3N}{2}} \left( \log \left( \frac{\sqrt{N}}{\lambda_\beta} \right) + 2\phi_\beta \right) \right) \tag{24} \]

where the 'circles' can be unwound to straight lines through the hyperbolic angle \(\phi_k\).

Fig. 2 shows the ideal gas manifold. Discussion of the ideal gas is often accompanied by that of the thermodynamic cycles with which it can be used to extract work from a heat bath. The Carnot cycle, which is often considered to cost no entropy, was recently shown \[33\] to have a subextensive entropy cost proportional to the arclength of the cycle’s path on the model manifold. This challenges Szilard’s argument that information entropy and thermodynamic entropy can be freely exchanged. The path of a Carnot cycle is shown on the model manifold in Fig. \[3\]

**C. The \(n\)-sided die**

The \(n\) sided die is a model for a process with \(n\) outcomes. It has a discrete probability distribution of \(n\) states, with \(p_i\) as the probability of the \(i\)th state. This distribution can be written as \(P_p(x) = \)
\[ \prod_{i=1}^{n} p_i^{[x=i]} \], where \([x = i]\) is the Iverson bracket which evaluates to 1 if \(x = i\), 0 otherwise and \(\sum_{i=1}^{n} p_i = 1\). The probability distribution can be written in the form of an exponential family with \(\eta_k(\theta) = \log(p_i/p_n)\), \(\Phi_i = [x]\), \(h(x) = 1\) and \(A(\theta) = \log(1 + \sum_{i=1}^{n-1} e^{\theta_i})\). Its FIM is \((ds)^2 = \sum_{i=1}^{n} (dp_i)^2/p_i\).

IsKL gives \((2+2)\) and \((3+3)\) dimensional embeddings in Minkowski space. There are only two \(k\) where \(k = 1, 2\) respectively. For \(k = 1\), \(\lambda_1(p) = \frac{1}{\log(p_1/p_n)}\), the pairwise KL divergence between \(P_p\) and \(P_a\) is
\[
D_{sKL}^2(p, a) = \sum_{i=1}^{n} (p_i - a_i) \log \left( \frac{p_i}{a_i} \right). \tag{25}
\]

By letting \(\langle \eta_k \rangle = \langle \eta_i \rangle\) and \(\langle \Phi_i \rangle = \langle \Phi_i \rangle\), the projection coordinates are
\[
T_{k}^{(\pm)}(p_1, \ldots, p_{n-1}) = \frac{1}{2} \lambda_k \left( \log \left( \frac{p_k}{p_n} \right) - \left( \log \left( \frac{p_k}{p_n} \right) \right) \right) \pm \frac{1}{\lambda_k} \left( p_k - \langle p \rangle \right) \tag{26}
\]
where \(k = 1, \ldots, n - 1\) and \(p_n = 1 - \sum_{i=1}^{n-1} p_i\). As examples, we consider three and four sided dice. IsKL gives \((2+2)\) and \((3+3)\) dimensional embeddings in Minkowski space. There are only two eigenvalues returned in both cases, signalling the existence of symmetries in our embeddings. With uniform sampling of the parameter space, for \(n = 3\),
\[
T_{k}^{(2)}(p_1, p_2) = \frac{1}{6^{1/4} \sqrt{\pi}} \log \left( \frac{p_k}{1 - p_1 - p_2} \right) \pm 6^{1/4} \sqrt{\pi} \left( p_k - \frac{1}{3} \right) \tag{27}
\]
where \(k = 1, 2\). For \(n = 4\),
\[
T_{k}^{(3)}(p_1, p_2, p_3) = \frac{1}{5^{1/4} \sqrt{\frac{3}{4} \pi}} \log \left( \frac{p_k}{1 - p_1 - p_2 - p_3} \right) \pm 5^{1/4} \sqrt{\frac{3}{4} \pi} \left( p_k - \frac{1}{4} \right) \tag{28}
\]
where \(k = 1, 2, 3\). Finally, the projection coordinates for \(n = 2\) (a coin toss) are
\[
T_{k}^{(2)}(p) = \frac{1}{\sqrt{2\pi}} \log \left( \frac{p}{1 - p} \right) \pm \sqrt{2\pi} \left( p - \frac{1}{2} \right). \tag{29}
\]
As expected, comparing Eq. \(\text{(29)}\) with Eq. \(\text{(20)}\), the form does not depend on the sampling choice while the constant \(\lambda_p\) does. Fig. \(4\) shows the model manifold for a three sided die. Unlike the Hellinger embedding, the lack of spherical symmetry is manifest. We do however see a permutation symmetry among \(p_i\)s and a reflection symmetry along \(T_{p_i}^{\pm} = T_{p_2}^{\pm}\) in the \((T_{p_1}^{\pm}, T_{p_2}^{\pm})\) coordinate pairs.
One can extract the sub-manifold of a coin toss problem by restricting $p_2 = 0$. This submanifold is shown by the red line in Fig. [4]. In general, any discrete probability distribution is a subset of the $n$ sided die distribution, implying that other discrete exponential family distributions may have hidden low dimensional representation within the $n$ sided die model manifold.

### D. Nonlinear least square models

Nonlinear least square models are ubiquitous in fitting deterministic models to data with noise. These models take the form of a nonlinear vector-valued function $f_i(\theta)$ predicting the value of experimental data points $x_i$ with uncertainties $\sigma_i$. Their associated probability distribution is

$$
P(x|\theta) = \prod_i \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp \left( \frac{\sum_i (f_i(\theta) - x_i)^2}{2\sigma_i^2} \right). \tag{30}$$

This probability distribution takes the form of an exponential family with $\eta_i(\theta) = f_i(\theta)/\sigma_i$, $\Phi(x) = x_i/\sigma_i$, $h(x) = \sum_i x_i^2/\sigma_i^2$ and $A(\theta) = \sum_i f_i^2(\theta)/2\sigma_i^2 - \log(2\pi\sigma_i^2)/2$. Unlike the other models discussed, which have the same number of natural parameters $\eta_i$ and model parameters $\theta_\alpha$, here the number of natural parameters is given by the number of data points being fit. The FIM is given by $J^\top_{\beta i}J_{i\alpha}$, where $J_{i\alpha} = \partial f_i(\theta)/\partial \theta_\alpha$ is the Jacobian.

Least-squares models with $N$ data points have a natural ‘prediction embedding’ into $N$-dimensional Euclidean space with one coordinate per data point $x_i$ given by the error-normalized model prediction $f_i(\theta)/\sigma_i$. While the number of data points can be much larger than the number of parameters, this embedding remains valuable because the model predictions are surprisingly often well approximated by low-dimensional, flat model manifolds we call hyperribbons [1–3]. Hyperribbons have a hierarchy of manifold widths—like a ribbon, their dimensions (length, width, thickness, ... ) become geometrically smaller—yielding predictions that depend mostly on the first few principal components. Our least-squares model has $N$ natural parameters, so isKL will produce an embedding into an $N + N$ dimensional Minkowski space. Can we find one that makes the time-like distances equal to zero, reproducing the $N$-dimensional prediction embedding?

The symmetrized Kullback–Liebler divergence between two models is indeed given by the Euclidean distance between the two model predictions:

$$
D_{isKL}^2(\theta_1, \theta_2) = \sum_{i=1}^N \frac{(f_i(\theta_1) - f_i(\theta_2))^2}{\sigma_i^2}. \tag{31}
$$

This appears promising: the isKL distance is the same as that of the prediction embedding above. Interestingly, any Rényi divergence (such as the Bhattacharyya distance used by inPCA [10]) gives
FIG. 5. **Model manifold for the muon lifetime**, our two-parameter least-squares model, evaluated at three time points. The isKL embedding is confined to three Euclidean dimensions, with the three time-like coordinates identically zero. The model manifold is bounded with four edges at $\theta_k = 0$ and $\theta_k = \infty$ and a tight fold along $\theta_1 = \theta_2$. Depicted also is the experimental data point in red which is in close proximity to the $\theta_1 = \theta_2$ boundary. See [1, Fig. 1].

By taking $\lambda = 1$ the time-like coordinates vanish and we reproduce the $N$-dimensional prediction embedding.

Figure 5 shows this prediction embedding for the classical nonlinear least squares model of two exponential decays, here in the context of a cosmic muon lifetime experiment. Approximately half of muons generated by cosmic ray collisions are negative muons which can be captured by a proton of host nuclei. The effective negative muon lifetime $1/\theta_2$ (including capture) is therefore expected to be shorter than the decay-only lifetime of positive muons $1/\theta_1$. The model prediction for the number of muons surviving after some time $N(t)$ is thus the sum of two exponentials. Mathematically, we have

$$\hat{N}(\theta_1, \theta_2, r, t) = \frac{1}{1 + r} \left( r e^{-\theta_1 t} + e^{-\theta_2 t} \right)$$

where $\hat{N}(t)$ is the normalized number of muons and $r = N_{\mu^+}/N_{\mu^-} = 1.18 \pm 0.12$ is the ratio of
FIG. 6. Viewing Heaven and Hell in Minkowski Space - Escher’s art - Circle Limit IV which is also known as Heaven and Hell is used to decorate Gaussian fit manifold. The embedding dimension is (2+2). The manifold projections are depicted in a descending order based on the manifold widths along the spacelike/timelike components. The spacelike directions are color coded in black while the timelike directions are color coded in red. Reflection symmetry is illustrated with a dashed line along projections with a $\mu/\sigma^2$ component. The submanifold of a least square model with a single Gaussian distribution of fixed $\sigma^2 = 1$ is depicted in green.

incident positive muons to negative muons formed by the cosmic rays [36]. Fig. 5 shows the muon lifetime model manifold via the isKL embedding (identical to the prediction embedding), with three sampled time points. The projection coordinates are $\hat{N}(t_i)/\sigma_i$. Since $r \approx 1$, there is a tight fold in the model manifold along $\theta_1 = \theta_2$. The experimental data point is close to the manifold fold, implying the negative muon capture event only leads to a slight change in negative muon lifetime.

E. Gaussian fits to data

The Gaussian distribution is an exceptionally good approximation for many physical problems and thus serves as a good model to explore in the context of manifold visualization. For example the distribution of women’s heights with mean height $\mu$ and variance in height $\sigma^2$ in a country is fitted to a normal (Gaussian) distribution. The Gaussian distribution $P(x|\mu, \sigma) = (2\pi\sigma^2)^{-1/2} \exp(-(x-\mu)^2/2\sigma^2)$ has two parameters, the mean $\mu$ and the variance $\sigma^2$. It can be written in the form of an exponential family with $(\eta_1(\theta), \eta_2(\theta)) = (\mu/\sigma^2, -1/2\sigma^2)$, $(\Phi_1(x), \Phi_2(x)) = (x, x^2)$, $h(x) = (2\pi)^{-1/2}$.
and \(A(\theta_1, \theta_2) = -\theta_1^2/4\theta_2 - (1/2) \log (-2\theta_2)\). Its FIM is given by \((ds)^2 = \sigma^{-2}((d\mu)^2 + 2(d\sigma)^2)\).

The Gaussian distribution FIM has a close resemblance to the Poincaré half plane metric \((ds)^2 = y^{-2}((dx)^2 + (dy)^2)\) both of which have a constant negative scalar curvature: -1/2 and -2, respectively. In differential geometry, it is known \(^{37}\) that the Poincaré half plane has an isometric canonical embedding into \((2+1)\) dimensional Minkowski space and takes the form of an imaginary sphere with radius squared equal to minus one. By rescaling, the corresponding embedding for the Gaussian fit manifold is therefore an imaginary sphere of radius squared equal to -2. Its spacelike components are given by \(X^+_1(\mu, \sigma) = (\mu^2 + 2\sigma^2 + 2)/2\sqrt{2}\sigma^2\), \(X^+_2(\mu, \sigma) = \mu/\sigma\) and its timelike component is given by \(X^-_3(\mu, \sigma) = (\mu^2 + 2\sigma^2 - 2)/(2\sqrt{2}\sigma^2)\). The pairwise distance which generates such an embedding is therefore

\[
D^2(\mu_1, \sigma_1, \mu_2, \sigma_2) = \frac{(\mu_1 - \mu_2)^2 + 2(\sigma_1 - \sigma_2)^2}{2\sigma_1\sigma_2}
\]

(34)

However, there is no obvious way of writing Eq. (34) in terms of \(P_0(x)\).

With the isKL embedding, the Gaussian distribution can be isometrically embedded into \((2+2)\) dimensions. As \(\langle \Phi_1(x) \rangle = \mu\) and \(\langle \Phi_2(x) \rangle = \mu^2 + \sigma^2\), the pairwise distance is given by

\[
D^2_{sKL}(\mu_1, \mu_2, \sigma_1^2, \sigma_2^2) = \left(\frac{\mu_1}{\sigma_1^2} - \frac{\mu_2}{\sigma_2^2}\right)^2 (\mu_1 - \mu_2) - \frac{1}{2} \left(\frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2}\right) \left(\mu_1^2 + \sigma_1^2 - \mu_2^2 + \sigma_2^2\right)
\]

(35)

Letting \(\bar{\eta} = \langle \eta \rangle\) and \(\bar{\Phi} = \langle \Phi \rangle\), the coordinates are given by

\[
T^{\pm}_{\text{odd}}(\mu, \sigma^2) = \frac{1}{2} \left(\lambda_{\text{odd}} \left(\frac{\mu}{\sigma^2} - \frac{\mu}{\sigma^2}\right) \pm \frac{1}{\lambda_{\text{odd}}} (\mu - \langle \mu \rangle)\right)
\]

\[
T^{\pm}_{\text{even}}(\mu, \sigma^2) = \frac{1}{2} \left(\lambda_{\text{even}} \left(\frac{1}{\sigma^2} - \frac{1}{\sigma^2}\right) \pm \frac{1}{\lambda_{\text{even}}} (\mu^2 + \sigma^2 - \langle \mu^2 + \sigma^2 \rangle)\right).
\]

(36)

Upon closer inspection, the coordinate pairs can be written as

\[
(T^{+}_{\text{odd}} - C^+_{\text{odd}})^2 - (T^{-}_{\text{odd}} - C^-_{\text{odd}})^2 - (T^{+}_{\text{even}} - C^+_{\text{even}})^2 + (T^{-}_{\text{even}} - C^-_{\text{even}})^2 = 1
\]

(37)

where \(C^\pm\) are constants. This suggests the isKL embedding is a 4 dimensional hyperboloid in Minkowski space. To get a good pictorial sense of how the probability distributions are arranged, we embedded ‘Heaven and Hell’ (Escher’s Circle Limit IV 1960- depicting a Poincaré disk) in Minkowski space via our isKL embedding (Fig. 3). The probabilistic manifold projection along \((\mu/\sigma^2, -1/2\sigma^2), (\mu/\sigma^2, -1/2\sigma^2), (\mu^2 + 2\sigma^2, \mu/\sigma^2)\) and \((-1/2\sigma^2, \mu/\sigma^2)\) components a exhibit reflection symmetry about \(\mu = 0\), manifesting the even parity coordinates. Moreover, the bats become stretched as \(\sigma^2 \to 0\), along the projected edge of the Poincaré disk. The submanifold of a least square model with a single Gaussian distribution of fixed \(\sigma^2 = 1\) from Sec. II is shown in green.
FIG. 7. **Two dimensional Ising Model isKL embedding** used to illustrate the geometric structure of statistical models with a phase transition. The manifold is embedded into $(2+2)$ dimensions and the manifold projections are shown in a descending order based on the manifold width along the spacelike/timelike directions. The spacelike direction are color coded in black while the timelike directions are color coded in red. Reflection symmetry is illustrated with a dotted line along projections with an $h$ component. For $\beta > \beta_c$, this is an opening on the manifold due to the spontaneous magnetization. The two arms illustrated correspond to $M(\beta, h) = \pm n$ with $\beta > \beta_c$ are lightlike. The values of $E$ and $M$ used were estimated from simulations with $n = 128 \times 128$ spins. The exact solution at zero field is depicted by the black line.

**F. 2D Ising model**

Most statistical mechanics models form an exponential family, and of particular interest is the behavior of their model manifolds near phase transitions. Here we show how the two dimensional Ising model manifold is embedded using our method. The Ising model is a model of magnetism comprised of a lattice of $n$ spins that can take the values $\pm 1$, “pointing up” or “pointing down.” At temperature $\beta^{-1}$ and in an external magnetic field $H$, the probability of observing a particular configuration $s = (s_1, \ldots, s_n)$ of the spins is given by the Boltzmann distribution

$$P(s|\beta, h) = \frac{\exp(\beta \sum_{i,j} s_i s_j + h \sum_i s_i)}{Z(\beta, h)}$$

(38)

where $h = \beta H$, $\langle ij \rangle$ denotes a sum over neighboring sites, and the partition function $Z(\beta, h)$ normalizes the distribution. The Ising model is an exponential family with $(\eta_1(\theta), \eta_2(\theta)) = (\beta, h)$, $(\Phi_1(s), \Phi_2(s)) = (\sum_{i,j} s_i s_j, \sum_i s_i)$, $h(s) = 1$, and $A(\theta) = -\log Z$. The Fisher information metric
is given by the mixed partial derivatives \( g_{ij} = \partial_i \partial_j \log Z \) with \( i, j \in \{\beta, h\} \).

The Hellinger embedding of the Ising model manifold is 2\( n \) dimensional. The curse of dimensionality manifests through an increase of ‘wrapping’ around the unit hypersphere as the number of spins increases, rendering low dimensional projections increasingly useless for visualization \[3\]. The ‘wrapping’ phenomenon can be ameliorated by using the InPCA embedding. Though InPCA embeds the Ising model manifold into an infinite dimensional Minkowski space, the length scales of adjacent principal components are well-separated.

IsKL embeds the Ising model manifold into \((2+2)\) dimensions. Not only is the curse of dimensionality broken, the Ising model manifold is embedded into finite dimensional Minkowski space. The expectation values of the sufficient statistics can be related directly to the Ising average energy \( E \) and magnetization \( M \) by

\[
(\langle \Phi_1 \rangle, \langle \Phi_2 \rangle) = (HM - E, M) \quad (39)
\]

The Ising model manifold is centered at the critical point \((\beta, h) = (\beta_c, 0)\) with the projection coordinates being

\[
T_{\beta}^\pm = \frac{1}{2} \left( \frac{1}{\lambda_\beta} (\beta - \beta_c) \pm \frac{1}{\lambda_\beta} (Mh/\beta - E + E_c) \right)
\]

\[
T_h^\pm = \frac{1}{2} \left( \frac{1}{\lambda_h} h \pm \frac{1}{\lambda_h} M \right) \quad (40)
\]

where \( E_c \) is the average energy at the critical point. Fig. 7 shows the isKL embedding of the 2D Ising manifold with \( E \) and \( M \) estimated from Monte Carlo simulations at \( n = 128 \times 128 \) spins using the Wolff algorithm in an external field \[38\]. The exact solution for the zero field is included in the embedding as well and is illustrated with a black line \[39, 40\]. For completeness we also show all the manifold projections. The first and third principal components are field like directions and the 2nd and the 4th components are temperature like directions. Reflection symmetry along \( H = 0 \) is depicted with a dotted line.

At the critical point there is an opening that corresponds to the growing spontaneous magnetization. This feature is important in resolving the following issue. For \( h = 0 \) in the low temperature phase, configurations of the Ising model with positive and negative spontaneous magnetizations are easily distinguishable and might be expected to be distant in distribution space. However, since the two systems have the same free energy, both the \( f \) divergence and the Rényi divergence give zero distance, suggesting they are distributionally identical. This embedding in Minkowski space suggests a resolution: the zero distributional distance manifests as a non-zero embedding distance, but along a line of light-like separation. This highlights the crucial role of timelike coordinates in
qualitatively differentiating unlike systems that have the same free energy. This is not the whole story of lightlike separations, however: the two arms highlighted at large $\beta$ in Fig. 7 are also light-like. These have a more conventional interpretation: for sufficiently high field the configuration with all spins in the direction of the field becomes the most probable, and the resulting distributions are difficult to distinguish. IsKL spreads these points out as well.

The connection between phase transitions and differential geometry has been widely investigated [41–44]. Researchers have argued that the scalar curvature $R$ can be viewed as a measurement of interactions and that the divergence of the scalar curvature signals a phase transition. The leading singularity in the scalar curvature of the 2D Ising model manifold as the critical point is approached can be computed from the metric above and the asymptotic scaling form

\[-\log Z \simeq t^2 \mathcal{F}(ht^{-15/8}) + t^2 \log t^2\]

for $t = \beta_c - \beta$ to be $R \sim -t^{-2}/\log(t^2)$. For small $\beta - \beta_c R$ diverges. Near the critical point one might expect to see a cusp as a result. Instead, there is an opening near the critical point in our embedding, and the surrounding manifold looks smooth. The identification of each point along the opening with an opposing point suggests that we may have disguised the cusp in our embedding by ‘cutting’ the manifold with lightlike displacements, the way one might remove the point of a cone by cutting up the side. The connection between the geometry of our manifold and the singularity of its scalar curvature will be further explored in future work.

VII. NON-EXPONENTIAL FAMILIES: CAUCHY DISTRIBUTION

The success of the isKL embedding in obtaining an analytical expression for each coordinate is special to exponential family distributions. As an example of a non-exponential family, we consider the long tailed Cauchy distribution,

\[P(x|x_0, \gamma) = \frac{\gamma}{\pi(\gamma^2 + (x-x_0)^2)}. \tag{41}\]

Interestingly, its FIM, $(ds)^2 = (2\gamma^2)^{-1}((dx_0)^2 + (d\gamma)^2)$ has a constant negative scalar curvature just as the Gaussian fit in Sec. IV (b). In fact, there is a deeper connection between the Gaussian and Cauchy distributions: they both belong to the family of symmetric Lévy stable distributions

\[p(x|\alpha, \delta, c) = \frac{1}{\pi \alpha} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \Gamma \left( \frac{1 + 2n}{\alpha} \right) \left( \frac{x - \delta}{c} \right)^{2n} \tag{42}\]

where $0 < \alpha \leq 2$ is the shape parameter, $\delta$ is the location parameter, and $c$ is the scale parameter [45]. When $\alpha < 1$, Eq (42) diverges for all $x$ and converges otherwise. Both the Gaussian and Cauchy distributions can be recovered from Eq (42) by taking $\alpha = 2$ and $\alpha = 1$, respectively.
FIG. 8. **Cauchy distribution** is considered to exemplify the shortcoming of isKL embedding in visualizing non exponential family distributions. The first 5 manifold projections are shown in a descending order based on the manifold widths along the \((m,n)\) principal components. The embedding dimension is infinity with each projection components being spacelike as shown in (b).

Though not pursued in this paper, it is intriguing what subset of Levy distributions also have constant negative curvature. That the Gaussian and Cauchy distributions share this property but are distinct indicates that locally isometry is not enough to distinguish them. This demands the use of a global distance as an additional measure to characterize the model manifold. We embed the Cauchy distribution manifold using the isKL embedding with the distance measure \([46]\), which gives

\[
D^2_{sKL}(x_1, \gamma_1, x_2, \gamma_2) = 2\log \left( \frac{(\gamma_1 + \gamma_2)^2 + (x_1 - x_2)^2}{4\gamma_1\gamma_2} \right)
\]

(43)

The embedding dimension returned by isKL embedding appears to be infinity. Strikingly, not only this is also true for any symmetrized Rényi choices as shown in Fig. 8(b), the projections obtained from different symmetrized Rényi choices are almost the same. Thus \(D^2_{sKL}\) is not obviously better than other intensive Rényi divergences for models not in exponential families.

VIII. SUMMARY

In this paper, we demonstrate that any \(N\) parameter probabilistic model that takes the form of an exponential family can be embedded isometrically into a low dimensional \((N+N)\) Minkowskian space via the isKL embedding technique. This is done by using the symmetrized Kullback-Liebler divergence (sKL) as the pairwise distance between model predictions. To illustrate how the isKL
embedding technique can be used to visualize the exponential family probabilistic manifold in a simple and tractable way, we consider the coin toss problem, the ideal gas, the $n$ sided die, the nonlinear least square models, Gaussian fits to data, and the two dimensional Ising model. Additionally, we use the non-exponential Cauchy distribution to illustrate the importance of preserving both global and local structures in embeddings.

**Appendix A: Replica Zero Limit of $f$ Divergence**

To visualize the underlying geometry of probabilistic model data, a distance measure in probability space is needed. In this appendix, we will generalize the limit of zero data procedure in obtaining an intensive distance measure to a family of divergences, specifically from $f$ divergence to Rényi divergence. $f$ divergence measures the difference between two probability distribution $P$ and $Q$ with a convex function $f$ such that $f(1) = 0$ and takes the form

$$D_f(P, Q) = \int f\left(\frac{p(x)}{q(x)}\right) q(x) d\mu(x)$$  \hspace{1cm} (A1)

By assuming $f$ is analytic \[47\], we can Taylor expand it about $x = 1$, $f(x) = \sum_{m=0}^{\infty} \frac{1}{m!} f^{(m)}(1)(x - 1)^m$. Thus, $f$ divergence takes the form

$$D_f(P, Q) = \int f\left(\frac{p(x)}{q(x)}\right) q(x) dx$$

$$= \sum_{m=0}^{\infty} \int \frac{1}{m!} f^{(m)}(1) \left(\frac{p(x)}{q(x)} - 1\right)^m q(x) dx$$  \hspace{1cm} (A2)

$$= \sum_{m=0}^{\infty} \frac{1}{m!} f^{(m)}(1) \chi_{1,q}^m(P, Q)$$

where

$$\chi_{1,q}^m(P, Q) = \int \frac{(p(x) - q(x))^m}{q^{m-1}(x)} dx$$  \hspace{1cm} (A3)

is the $\chi^k$-divergence with parameter 1. Expanding the polynomial and simplifying,

$$\chi_{1,q}^m(P, Q) = \int \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} q^{1-k}(x) p^k(x) dx$$

$$= \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \int q^{1-k}(x) p^k(x) dx$$  \hspace{1cm} (A4)
Suppose we increase the number of data sample by $N$ which amounts to having $N$-replicated system,

$$\chi^m_{1,q}(P_N, Q_N) = \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \left( \int \cdots \int q^{1-k}(x_1, \ldots x_N) p^k(x_1, \ldots, x_N) dx_1 \ldots dx_N \right)$$

Since $p(x_1, \ldots, x_N) = \prod_{i=1}^{N} p(x_i)$ and $q(x_1, \ldots, x_N) = \prod_{i=1}^{N} q(x_i)$

$$= \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \left( \int q^{1-k}(x)p^k(x) dx \right)^N$$

$$= \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \left[ \left( \int q^{1-k}(x)p^k(x) dx \right)^N - 1 \right] + \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k}$$

Note that $(1 - x)^n = \sum_{n=0}^{\infty} \binom{n}{k} (-x)^n$ so

$$\sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} = 0 \quad \text{(A6)}$$

Thus

$$\chi^m_{1,q}(P_N, Q_N) = \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \left[ \left( \int q^{1-k}(x)p^k(x) dx \right)^N - 1 \right] \quad \text{(A7)}$$

Upon closer inspection, each $\chi^m$ term contains partition function like terms $\left( \int q^{1-k}dx \right)^N$ that is known as Hellinger divergence of order $k$ that increase geometrically with $N$. Upon sending $N$ continuously to zero, we have

$$\lim_{N \to 0} \chi^m_{1,q}(P_N, Q_N) = \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \frac{\log \left( \int q^{1-k}p^k dx \right)}{N} \quad \text{(A8)}$$

As $D_\alpha(P, Q) = \frac{1}{\alpha-1} \log \left( \int p^\alpha q^{1-\alpha} dx \right)$ is the Rényi divergence,

$$\lim_{N \to 0} \chi^m_{1,q}(P_N, Q_N) = \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k}(k-1)D_k(P, Q) \quad \text{(A9)}$$

Thus for any $f$ divergences,

$$\lim_{N \to 0} \frac{D_f(P_N, Q_N)}{N} = \sum_{m=1}^{\infty} \sum_{k=0}^{m} \frac{f^{(m)}(1)}{m!} \binom{m}{k} (-1)^{m-k}(k-1)D_k(P, Q) \quad \text{(A10)}$$

Appendix B: Coin Toss and inPCA: The Bernoulli Problem model manifold embedded with the Bhattacharyya distance

In the Bernoulli problem, the inPCA embedding is given by the following pairwise distance

$$d^2(\theta_1, \theta_2) = \log(\cos(\theta_1 - \theta_2)) \quad \text{(B1)}$$
To find the embedding, we need to solve the eigenvalue problem discussed in Sec. \[\text{V}\] As the double mean centering matrix \( P \) gives rotation and boost transformation to the coordinates, for simplicity we proceed our calculation for each projection with just our distance function as an infinite matrix, acting on continuous variables \( \phi \) and \( \theta \): \( \log \cos(\phi - \theta) \). This implies the evaluation of the following eigenvalue problem:

\[
\int_0^{\pi/2} \log \cos(\phi - \theta) v_\alpha(\theta) d\theta = \lambda_\alpha v_\alpha(\phi) \quad (B2)
\]

where \( v_\alpha(\phi) \) are the eigenfunctions with the corresponding eigenvalues \( \lambda_\alpha \). We solve this numerically by expanding the pairwise distance function in terms of Chebyshev polynomials: \( d^2(\theta, \phi) = -\log(2) + \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \cos(2k(\theta - \phi)) \) and assuming that the eigenfunction \( v_\alpha(\theta) \) is odd with respect to \( \theta = \pi/4 \) and can be expanded as Fourier series: \( \sum_{k=1}^{\infty} b_k \sin(k(\theta - \pi/4)) \). Thus we have

\[
\sum_{k,m=1}^{\infty} (-1)^{k+1} \frac{b_m}{k} F(\phi) = \lambda_\alpha \sum_{k=1}^{\infty} b_k \sin(k(\theta - \pi/4)) \quad (B3)
\]

with \( F(\phi) = \int_0^{\pi/2} d\theta \cos(2k(\theta - \phi)) \sin(m(\theta - \pi/4)) \), where as \( F(\phi) \) only produces terms containing \( \sin(2k(\phi - \pi/4)) \) and \( \cos(2k(\phi - \pi/4)) \) for all values of \( m \in \mathbb{Z}^+ \), it is thus natural to conjecture that the Fourier series expansion must have its coefficient \( b_{2k+1} = 0 \). Hence,

\[
v_\alpha(\theta) = \sum_{k=1}^{\infty} b_{2k} \sin(2k(\theta - \pi/4)) \quad (B4)
\]

With this assumption, the eigenvalue equation simplifies into matching the coefficient of each Fourier mode \( \sin(2k(\phi - \pi/4)) \):

\[
\sum_{m=1}^{\infty} \xi(k, m) b_{2m} = \lambda_\alpha b_{2k} \quad (B5)
\]

or more succinctly, \( \xi \vec{b} = \lambda_\alpha \vec{b} \) where \( \vec{b} = (b_2, b_4, ..., b_{2N}, ...) \). The matrix \( \xi(k, m) \) is computed via \( F(\phi) \) to be

\[
\xi(k, m) = \begin{cases} 
\frac{(-1)^{k+1}}{k} \pi/4 & (m = k) \\
\frac{(-1)^{k+1}}{k} \frac{1}{m^2 - k^2} (k \cos(k \pi/2) \sin(m \pi/2) - m \cos(m \pi/2) \sin(k \pi/2)) & (m \neq k)
\end{cases} 
\]

\[\text{(B6)}\]

For even eigenfunctions \( v_\alpha(\theta) = \sum_{k=0}^{\infty} c_k \cos(k(\theta - \pi/4)) \), the argument is almost identical, except we now have an extra contribution from the constant \( c_0 \) term which needs to be handled separately.

Going through the same derivation, we again have the matrix eigenvalue equation, i.e. \( \eta \vec{c} = \lambda_\alpha \vec{c} \), where \( \vec{c} = (c_0, c_2, ..., c_{2N}) \) and we have
FIG. 9. A-F. Normalized projection of coin toss manifold onto the first 6 principal axes. The dashed line is the numerical approximation of the analytical expressions given in Eq. A6 and Eq. A7 with $N = 2000$

\[
\eta(k, n) = \begin{cases} 
-\frac{\pi}{2}\log(2) & (n = k = 0) \\
-\log(2)\sin\left(\frac{n\pi}{2}\right) & (k = 0, n \geq 1) \\
\frac{(-1)^{k+1}}{k}\sin\left(\frac{kn\pi}{2}\right) & (k \geq 1, n = 0) \\
\frac{(-1)^{k+1}}{k}\pi & (k = n \geq 1) \\
\frac{(-1)^{k+1}}{k}\left(\frac{1}{n^2-k^2}(n\cos\left(\frac{k\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right) - k\cos\left(\frac{n\pi}{2}\right)\sin\left(\frac{k\pi}{2}\right))\right) & (n \geq 1, k \geq 1, n \neq k)
\end{cases} 
\]

One could get numerical approximation for the analytical calculation above by taking $\eta$ and $\xi$ to be finite-dimensional matrix $N \times N$, where $N \gg 1$ as shown in Fig. 9.

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