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Topological Dynamic Bayesian Networks

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ABSTRACT

The objective of this research is to embed topology within the dynamic Bayesian network (DBN) formalism. This extension of a DBN (that encodes statistical or causal relationships) to a topological DBN (TDBN) allows continuous mappings (e.g., topological homeomorphisms), topological relations (e.g., homotopy equivalences) and invariance properties (e.g., surface genus, compactness) to be exploited. The mission of TDBN is not limited only to classify objects but to reveal how these objects are topologically related as well. Because TDBN formalism uses geometric constructors that project a discrete space onto a continuous space, it is well suited to identify objects that undergo smooth deformation. Experimental results in face identification across ages represent conclusive evidence that the fusion of statistics and topology embodied by the TDBN concept holds promise. The TDBN formalism outperformed the DBN approach in facial identification across ages.

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Topological Dynamic Bayesian Networks

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Abstract

The objective of this research is to embed topology within the dynamic Bayesian network (DBN) formalism. This extension of a DBN (that encodes statistical or causal relationships) to a topological DBN (TDBN) allows continuous mappings (e.g., topological homeomorphisms), topological relations (e.g., homotopy equivalences) and invariance properties (e.g., surface genus, compactness) to be exploited. The mission of TDBN is not limited only to classify objects but to reveal how these objects are topologically related as well. Because the TDBN formalism uses geometric constructors that project a discrete space onto a continuous space, it is well suited to identify objects that undergo smooth deformation. Experimental results in facial aging identification represent conclusive evidence that the fusion of statistics and topology embodied by the concept of TDBN holds promise. The TDBN formalism has outperformed the standard DBN approach.

1. Introduction

Dynamic Bayesian networks (DBNs) represent a powerful formalism for encoding probabilistic or causal relationships between random variables. Advances in theory and the availability of learning algorithms allowed DBNs to model a wide range of applications [1]. However, this graphical formalism does not serve as a panacea for all problems that one may encounter in the area of machine learning and pattern recognition. The DBN formalism has a major limitation; it is purely statistical: DBNs express solely probabilistic entailment via conditional probabilities and priors. Because of the lack of topology in their design, standard DBNs have difficulty to intrinsically manage continuous structures that vehicle the concepts of continuity, metrics, shapes and their deformations. Simple DBNs such as Kalman filters and HMM-based models [2,3,4,5] are not suitable to capture object change over time. For example, it is most likely that the face image of “Julie” at the age of fifteen, and her face image at the age of fifty-five will be assigned a different class during facial aging identification. Some of the HMM’s extensions such as “constrained” [6], and “situated space” [7] represent an attempt to capture structural information by assigning each hidden state a spatial region of a fictitious topology

space where a neighborhood between states is defined. However, the objective of these models is not to provide natural Euclidean space embeddings that allow examining topological relationships between objects. In other words, DBNs are not *ingrained with the power of merging topological properties (such as homeomorphy, homotopy or invariance) with probabilistic data*. The notion of “topological HMMs” (THMMs) that extends the HMM formalism will naturally unfold as an embedding of a simple DBN endowed with topological features. The branch of topology is fundamental to understanding the relationships between objects (e.g., “having the same roots”) as well as their evolution over time.

We propose a novel formalism whose goal is to: (i) embed the nodes of a DBN into a discrete set of a Euclidean space (section 2), (ii) map this set to a continuous set using geometric constructors such as the α -shapes, and (iii) extract topological features (section 3). Application in facial aging identification is depicted in section 4.

2. Topological DBN

The thrust is to embed data represented by a DBN into a low dimensional Euclidean space to form a topological DBN (TDBN). Let’s first define the word “embedding”: **Definition 1.** An embedding of a network $N=(V,E,d)$ on a Euclidean space Γ (or a surface: *compact, connected 2-manifold*) is a representation of N on Γ in which vertices of V are mapped to points of Γ and directed edges of E are mapped to simple arcs such that: (i) The endpoints of the arc mapped to a directed edge e are the points of Γ associated to the end vertices of e . (ii) No arcs contain points associated with other vertices. (iii) Two arcs never cross each other at a point which is interior to either of the arcs. The purpose of a DBN embedding is to represent each node of the DBN as a point in a low-dimensional Euclidean space that preserves similarities between the vertex pairs.

2.1. Visible Observation Sequence: Its Model

We define a visible observation (VO) sequence as a flow of symbols which represents either: (i) temporal data (times series), generated by some causal process; and (ii) sequential data (such as bio-sequences), where the generating mechanism of this sequence is

unknown. Furthermore, it is often the case that the generating mechanism of the symbols forming a VO sequence is explained by different analytical models (made of the nodes of the entire VO sequence and some latent variables that explain the VO sequence). For example, the same VO sequence can be represented by an autoregressive model or a semi-HMM with mixtures or simply a standard HMM.

2.2. Determining the Pivot Nodes of a DBN

Because a VO sequence model is a network and therefore has no mathematical structure, our mission is to build a TDBN. There exist many algorithms in the literature that perform graph-embedding [8,9]; however, a very few have been dedicated to network embedding. We first convert every conditional probability value (between a variable and its parent) of the DBN into a *dissimilarity* value. Two nodes that are highly related probabilistically will be assigned a small dissimilarity value and conversely. Our approach consists of selecting a set P of m “pivot” nodes ($P = \{v_1, v_2, \dots, v_m\}$) that “best” represent the dimensions (basis) of the Euclidean vector space. The set P is constructed incrementally, first by randomly selecting the node v_1 ; then node v_2 , which is the one whose *shortest-distance* to v_1 is maximum, and then v_3 , which corresponds to the node whose shortest-distance to the set $\{v_1, v_2\}$ is maximum, etc. In general, a node v_j is chosen if its shortest-distance to the set $\{v_1, v_2, \dots, v_{j-1}\}$ is *maximum*. We denote by $d_N(u, v_i)$ the shortest-distance in the VO sequence model between node u and pivot node v_i . Each node u of the VO sequence model is mapped to a point $X_u = [x_1(u), x_2(u), \dots, x_m(u)]^t$, in a Euclidean space, where: $x_i(u) = d_N(u, v_i)$, ($i=1, \dots, m$). This drawing should exhibit the *distance preserving embedding* property: (i) two nodes u and v that are closely related in N ($d_N(u, v) \leq \epsilon$) should be mapped to two points x_u and x_v whose distance $d_\Gamma(x_u, x_v)$ is less than $d_N(u, v)$ in Γ . (ii) Conversely, two non-adjacent nodes in the network should be mapped to two points that are far apart in Γ . *The discrete set of points X_u that is formed through this embedding process constitutes the TDBN*. In practice, the dimension m is reduced to 3 using principal components analysis to avoid the curse of dimensionality and to visualize the DBN layout.

2.3. Topological Mapping

We first map the VO sequence to its analytical model (**function f**). We then embed the VO sequence model in a Euclidean space to obtain a TDBN (**function g**). The distances between TDBN points are computed on the basis of the conditional probability

values associated to the nodes of a DBN. We then map the TDBN to a continuous set via a shape constructor (**function h**), and finally extract topological features (signature vectors) from the TDBN shape representation (**function i**). A VO sequence O is then mapped to a signature vector S via a function composition as: $(i \circ h \circ g \circ f)(o_1, o_2, \dots, o_T) = S$.

3. Tasks Involved in a TDBN

These tasks are: (i) **Learning a TDBN**: The goal is to learn the positions of the points of the TDBN in the Euclidean space. This phase derives directly from the learning phase of a traditional DBN [1] but also from the choice of its pivot nodes. The refinement of the DBN structure and the local variable distributions given the data as well as a change of the dimension axes (pivot nodes) of the Euclidean space will decide on the positions of the TDBN points. (ii) **Shape of a TDBN**: Since a TDBN X is a discrete set of points, therefore the concept of continuity which represents the foundation of topology will not apply. *This is the reason why it is necessary to map a discrete set to a continuous set*. The most natural way to achieve this objective is via the notion of “shape”. An efficient means for creating shapes out of point sets is provided by *shape constructors* such as the “ α -shapes” formalism [10]. The α -shape concept represents a formalization of the intuitive notion of “shape” for spatial point set data. *An α -shape is a concrete geometric object that is uniquely defined for a particular set of points*. The “optimal” α -shape of a TDBN is produced by an optimal TDBN. The α -shapes define a hierarchy of shapes from a set of points that allows features multi-scale modeling that are very useful in macromolecule structure exploration or in facial aging identification. The α -shapes insert a ball of radius $\sqrt{\alpha}$ around each point and build a simplicial complex that respects the intersections among these balls. The simplicial space formed is the α -shapes. One can extract “signatures” of α -shapes such as *metric properties*: (volume, area and length), *combinatorial properties*: (number of tetrahedral, triangles, edges, vertices) and *topological properties*: (number of components, number of independent tunnels, and number of voids). These signatures are put into a *vector form* that characterizes an α -shape. (iii) **Topological Mappings**: Because shape constructors transform a TDBN into a continuous space, therefore other topological features such as homeomorphism and homotopy equivalence can now be applied. If $h(X) = A$ (A is a TDBN shape representation) then the pair (A, d) represents a metric space (d is a distance function). A homeomorphism

map (bijective, bicontinuous) between two metric spaces (A_1, d_1) and (A_2, d_2) is built. A_1 and A_2 are two topologically similar objects. Intuitively, *two spaces A_1 and A_2 are homotopy equivalent if they can be transformed into one another by bending, shrinking and expanding operations.* (iv) **Training:** Given a VO sequence, the first phase consists of selecting the DBN that explains the VO sequence. The second phase focuses on training the DBN from the data to obtain an optimal DBN. The third phase consists of assigning the optimal DBN to its corresponding optimal TDBN. The fourth phase consists of constructing the shapes

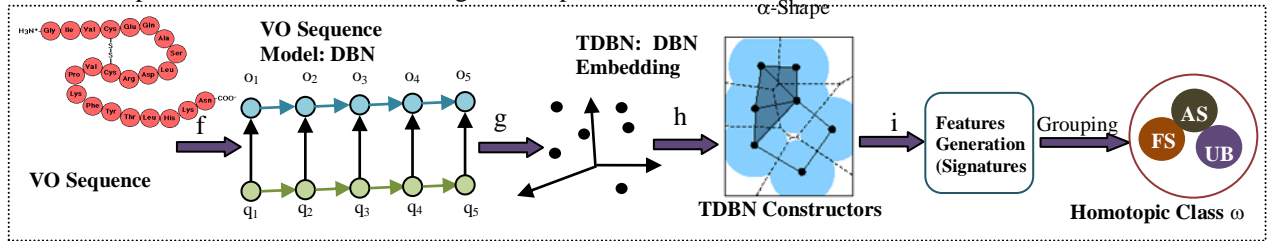


Figure 1. Embedding of an autoregressive HMM of an amino acid sequence in a Euclidean space.

(v) **Classification/Testing:** Given a VO sequence $O = o_1, o_2, \dots, o_T$, the classification problem is stated as follows: Determine the class ω^* among c target classes assigned to this VO sequence such that:

$$\omega^* = \underset{\omega_i}{\operatorname{argmax}} P[\omega_i | o_1, o_2, \dots, o_T], (i = 1, \dots, c).$$

Because (i) a VO sequence is viewed as a shape signature vector, and (ii) there are 3 homotopic equivalence constructors with different α values that generate a set of signature vectors represented by its mean vector \bar{S} ; therefore, the classification problem consists of determining the class ω^* , such that:

$$\omega^* = \underset{\omega_i}{\operatorname{argmax}} P[\omega_i | (i \ o \ h \ o \ g \ o \ f)(o_1, \dots, o_T) = \bar{S}].$$

Any continuous deformation of a shape is therefore captured. The classification problem is solved via Bayes' rule as: $P(\omega_i | \bar{S}) = \frac{P(\bar{S} | \omega_i) \cdot P(\omega_i)}{\sum_{i=1}^c P(\bar{S} | \omega_i) \cdot P(\omega_i)}$. We assume that each class ω_i is made of signature samples (by assigning different values of α in the constructors) originated from a known number of 3 (3 constructors) Gaussian mixtures whose probability.

$$P(\bar{S} | \omega_i) = \sum_{k=1}^{k=3} c_{ik} N(\bar{S}, \mu_{ik}, U_{ik}), \quad 1 \leq i \leq c,$$

where c_{ik} is the mixture coefficient for the k -th mixture in class ω_i . The function $N(\bar{S}, \mu_{ik}, U_{ik})$ is a Gaussian probability density function with mean vector μ_{ik} and covariance matrix U_{ik} .

4. Application: Facial Aging Identification

Given a face sample of an individual at age a_0 ; one determines if this face sample is associated with any of a large number of enrolled faces of individuals.

assigned to the TDBN by applying different geometric constructors (e.g., α -shapes (AS), flow-shapes (FS) and union of balls (UB)) using state-of-the-art shape constructor algorithms [10,11]. Because it has been proven that the AS, the FS, and the UB constructors are homotopy equivalent [11], therefore they provide “similar” continuous shapes when applied to the same TDBN. Finally, signature vectors of these similar shapes are computed and grouped together to form a *homotopic equivalence class ω* (Figure 1).

However, several face images of the same individual at ages ($a_1 \geq a_0 + 15$ years) are *among the enrollees*. In other words, given two faces, can one infer that they represent the same individual at different ages?

A human face is viewed as an ordered VO sequence $O = o_1, \dots, o_T$. Each o_i is a vector that captures a facial region (e.g., “hair”, “forehead”, “eyes”). These vectors are obtained by scanning the image from left to right and top to bottom using a 2D window. Each block image undergoes discrete wavelet transform (DWT) decomposition, producing an average image and a sequence of detail images. The sub-image is then decomposed to a certain level and the sub-band energies are chosen to form the vector o_i . The facial regions are hidden variables and the o_i are the observables; all these variables represent nodes of a DBN (autoregressive HMM). The DBN is embedded in a Euclidean space to form the TDBN subspace of a face. We apply shape constructors to the TDBN to extract the face *signature vectors*. Since we are considering 3 equivalent shape constructors with different α values, therefore several signature vectors are extracted and grouped to form a face image homotopic equivalence class ω (Figure 2).

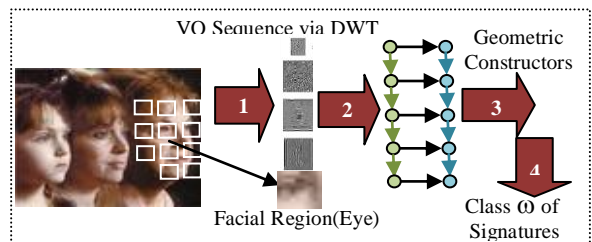


Figure 2. A homotopic class of a face image.

We have conducted the same task with 3 face images of different ages of the same individual. 2 of these 3 faces are left for training whereas 1 face of the same individual is left for testing. The homotopic classes assigned to the 2 training faces of the same individual are merged together to form a “*super homotopic class*”. We collected $50 \times 3 = 150$ face images *from family members and friends*; but since it is difficult to obtain a large number of faces of same individuals at different ages that would provide a statistical significance, we have used $100 \times 3 = 300$ simulated faces using dedicated software. We have therefore built a database of 450 faces in total. In order to measure the power of generalization of the TDBN classifier, we used a 5-fold cross-validation estimation technique. We divided the 450 face images into 5 sets. We then selected 1 set for testing and the other 4 sets for training ensuring that only 1 face of an individual is part of testing and the 2 other faces of this individual are part of training. We repeated this procedure 5 times with each time selecting a different set for a validation data. The 5 results from the folds are then averaged to produce a single estimation. We extracted the mean vector signature \bar{S} of the input face and computed the class ω^* that maximizes the posterior probability $P(\omega_i | \bar{S})$. The highest precision (in %) of **94.7** is achieved by TDBN via the Coiflet(3) DWT kernel (Table 1).

Table 1. Comparison between DBN and TDBN.

Cross Validation	DWT Kernels	Average Precisions	
		DBN	TDBN
5-fold	Haar	84.2	92.2
5-fold	Biorh9/7	78.0	89.8
5-fold	Coiflet(3)	85.6	94.7
5-fold	Gabor	85.9	91.3

The precision is defined as the ratio of correctly identified face images to the number of tested images.

5. Conclusion

We have embedded the DBN formalism in a Euclidean vector space where topological features abound. This fusion of statistics and topology embodied by the

TDBNs is a preliminary endeavor to connect discrete and continuous structures together. Experimental results demonstrate the need for such formalism that goes beyond pure statistical pattern recognition. Our future work consists of analyzing faces images that were misidentified in order to help gain an insight into how fat is compartmentalized within a human face; (ii) deform a damaged face into a healthy one in order to identify the location and the causes of a face injury. This investigation is crucial for medical researchers working on facial rejuvenation and plastic surgery.

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