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Predictive Coding with Topographic Variational Autoencoders

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Abstract

Predictive coding is a model of visual processing which suggests that the brain is a generative model of input, with prediction error serving as a signal for both learning and attention. In this work, we show how the equivariant capsules learned by a Topographic Variational Autoencoder can be extended to fit within the predictive coding framework by treating the slow rolling of capsule activations as the forward prediction operator. We demonstrate quantitatively that such an extension leads to improved sequence modeling compared with both topographic and non-topographic baselines, and that the resulting forward predictions are qualitatively more coherent with the provided partial input transformations.

1. Introduction

Topographic organization in the brain describes the observation that nearby neurons on the cortical surface tend to have more strongly correlated activations than spatially distant neurons. From the simple orientation of lines [22] to the complex semantics of natural language [23], organization of cortical activity is observed for a diversity of stimuli and across a range of species. Given such strong and ubiquitous observations, it seems only natural to wonder about the computational benefits of such organization, and if the machine learning community can take advantage of such design principles to develop better inductive priors for deep neural network architectures.

One inductive prior which has gained popularity in recent years is that of equivariance. At a high level, a representation is said to be equivariant if it transforms in a known predictable manner for a given transformation of the input. A fundamental method for constructing equivariant representations is through structured parameter sharing, constrained by the underlying desired transformation group [10, 41, 17, 18]. The most well known example of an equivariant map is the convolution operation, which is equivariant to translation. One can think of a convolutional layer as a function which shares the same feature extractor parameters over all elements of the translation group, i.e. all spatial locations. Similarly, a model which is equivariant to rotation is one which shares parameters across all rotations. Existing group equivariant neural networks [10] therefore propose to maintain ‘capsules’ of tied-parameters which are correlated by the action of the group. By reducing the number of trainable parameters while simultaneously increasing the information contained in the representation, equivariant neural networks have demonstrated significant improvements to generalization and data efficiency [10, 44, 53].

These sets of transformed weights, which we refer to as ‘equivariant capsules’, are reminiscent of a type of topographic organization observed in the primary visual cortex (V1), namely orientation columns [22]. This insight encouraged the development of the Topographic Variational Autoencoder (TVAE) [29], linking equivariance and topographic organization in a single framework. In the original work, the TVAE was introduced and demonstrated to learn topographic equivariant capsules in an entirely unsupervised manner from observed transformation sequences. Further, the inductive priors of equivariance and ‘slowness’ integrated into the TVAE were demonstrated to be beneficial for modeling sequence transformations, ultimately resulting in higher log-likelihood on held-out data when compared with VAE baselines.

In this work, we propose to extend the TVAE with an
additional inductive prior – that of predictive coding [19].
At a high level, predictive coding suggests that one signif-
ificant goal of the brain is to predict future input and use the
forward prediction error as a learning signal. In the context
of the TVAE, we observe that the existence of topographi-
cally organized capsules, combined with a slowness prior,
permit efficient forward prediction through simple forward
rolling of capsule activations. We demonstrate empirically
that such a model is able to more accurately predict the im-
mediate future, while simultaneously retaining the learned
equivariance properties afforded by the original TVAE.

2. Background

The Topographic VAE [29] relies on a combination of
fundamentally related inductive priors including Equivari-
ance, Topographic Organization, and Slowness. In this sec-
tion we will give a brief description of these concepts, and
further introduce predictive coding as it relates to this work.

2.1. Equivariance

Equivariance is the mathematical notion of symmetry
for functions. A function is said to be an equivariant map
if the result of transforming the input and then comput-
ing the function is the same as first computing the func-
tion and then transforming the output. In other words,
the function and the transformation commute. Formally,
\( f(\tau \rho(x)) = \Gamma_\rho[f(x)] \), where \( \tau \) and \( \Gamma \) denote the (potentially
different) operators on the domain and co-domain respect-
ively, but are indexed by the same element \( \rho \). The intro-
duction of the Group-convolution [10] and ensuing work [11,
53, 52, 18, 49] allowed for the development of analytically
equivariant neural network architectures to a broad range of
group transformations, demonstrating measurable benefits
in domains such as medical imaging [48, 2] and molecular
generation [43]. Recently, more work has begun to explore
the possibility of ‘learned’ equivariance guided by the data
itself [4, 14, 20]. The TVAE and the extension presented in
this paper are another promising step in this direction.

2.2. Topographic Organization

Topographic generative models can be seen as a class of
generative models where the latent variables have an under-
lying topographic organization which determines their cor-
relation structure. As opposed to common generative
models such as Independent Component Analysis (ICA)
[3, 27] or VAEs [30, 42], the latent variables in a topo-
graphic generative model are not assumed to be entirely in-
dependent, but instead are more correlated when they are
spatially ‘close’ in a predetermined topology. Typically,
simple topologies such as 1 or 2 dimensional grids are used,
often with circular boundaries to avoid edge effects.

One way a topographic generative model can be de-
scribed, as in [25], is as a hierarchical generative model
where there exist a set of higher level independent ‘vari-
ance generating’ variables \( V \) which are combined locally
along the topology to generate the variances of the lower
level topographic variables \( T \). Formally, for an adjacency
matrix \( W \), and an appropriate non-linearity \( \phi \), the variances
are computed as \( \sigma = \phi(WV) \). In the second stage, the
lower level variables are sampled independently, but with
their scale determined by the now topographically orga-
nized variable \( \sigma \): \( T \sim \mathcal{N}(0, \sigma^2 I) \). In later work [26],
Hyvärinen 	extit{et al.} further showed this framework to be a gen-
eralization Independent Subspace Analysis (ISA) [24] and
some variants of Slow Feature Analysis (SFA) [45, 51, 46]
by careful choice of topography \( W \). The Topographic VAE
takes advantage of both this framework and these connec-
tions to construct slow-transforming capsules which learn to
become equivariant to observed sequence transformations.

2.3. Predictive Coding

In the machine learning literature, one of the most intu-
itive and common frameworks for unsupervised learning re-
lies on predicting unseen or missing contextual data from a
given input. This idea, informally called predictive coding,
has led to some of the most well known advances in the field
across a range of domains including: natural language pro-
cessing (word2vec [37], GPT3 [6], Bert [13]), vision (CPC
[47], SimCLR [7], GreedyInfoMax [35]), speech (APC [8]),
and more [21, 33]. In the theoretical neuroscience literature,
predictive coding denotes a framework by which the cortex
is a generative model of sensory inputs [16, 40, 19, 9], and
has been linked to probabilistic latent variable models such
as VAEs [36]. Substantial evidence has been gathered sup-
porting the existence of some form of predictive coding in
the brain [1, 12, 15], and numerous computational models
have been proposed which replicate empirical observations
[40, 34, 28]. Given these computational successes, and the
mounting support for such a mechanism underlying biolog-
ical intelligence, we strive to formalize the relationship be-
tween predictive coding and TVAEs in this work.

3. Predictive Coding with Topographic VAEs

In this section we introduce the generative model under-
lying the Predictive Coding Topographic VAE (PCTVAE)
and highlight the differences with the original model – in-
cluding making the conditional generative distribution for-
ward predictive, and limiting the temporal coherence win-
dow to only include past variables.

3.1. The Forward Predictive Generative Model

We assume that the observed sequence data is generated
from a joint distribution over observed and latent variables
\( x_t \) and \( t_t \) which factorizes over timesteps \( t \), and further fac-
torizes into the product of a forward predictive conditional
and the prior:

\[ p(x_{t+1}|T_i, t_0) = \prod_i p(x_{t+i}|x_{t+i-1}) p_T(t_i) \quad (1) \]

The prior distribution is assumed to be a Topographic Product of Student’s t (TPoT) distribution [50, 38], i.e. \( p_T(t_i) = \text{TPoT}(t_i; \nu) \), and we parameterize the conditional distribution with a flexible function approximator:

\[ p(x_{t+i}|T_i, x_{t+i-1}) = p_\theta(x_{t+i}|g_\theta(t_i)) \quad (2) \]

The goal of training is thus to learn the parameters \( \theta \) such that the marginal distribution of the model \( p_\theta(x_t) \) matches that of the observed data.

To allow for efficient training, we follow the construction outlined in [29], whereby we construct a TPoT random variable from simpler independent normal random variables \( Z_l \) and \( U_l \) which are amenable to variational inference:

\[ T_l = \frac{Z_l - \mu}{\sqrt{W U_l}} \quad Z_l, U_l \sim \mathcal{N}(0, I) \quad (3) \]

where \( W \) defines the chosen topology, and \( \mu \) is learned.

**Past Temporal Coherence**  As mentioned in the Section 2.2, the Topographic VAE takes advantage of the general- ized framework of topographic generative models to induce structured correlations of activations over time – thereby achieving equivariance. In this work, this is achieved by making \( T_l \) a function of a sequence \( \{U_{l-\delta}\}_\delta=0 \), and defining \( W \) to connect sequentially rolled copies of past \( U_l \):

\[ T_l = \frac{Z_l - \mu}{\sqrt{W [U_{l-\delta}; \cdots; U_{L-\delta}^2]}} \quad (4) \]

where \([U_{l-\delta}; \cdots; U_{L-\delta}^2]\) denotes vertical concatenation of the column vectors \( U_l \), and \( L \) can be seen as the past window size. Then, by careful definition of \( W \), we can achieve the “shifting temporal coherence”, defined in [29], yielding equivariant capsules. Explicitly, \( W \) is thus given by:

\[ W [U_{l-\delta}; \cdots; U_{L-\delta}^2] = \sum_{\delta=0}^L W_\delta \text{Roll}_\delta(U^2_{l-\delta}) \quad (5) \]

where \( W_\delta \) defines a set of disjoint ‘capsule’ topologies for each time-step, and \( \text{Roll}_\delta \) denotes a cyclic permutation of \( \delta \) steps along the capsule dimension (see [29] for exact implementation details).

### 3.2. The Predictive Coding TVAE

To train the parameters of the generative model \( \theta \), we use equation 4 to parameterize an approximate posterior for \( t_i \) in terms of a deterministic transformation of approximate posteriors over simpler Gaussian latent variables \( z_l \) and \( u_l \):

\[ q_\theta(z_l|x_l) = \mathcal{N}(z_l; \mu_\phi(x_l), \sigma_\phi(x_l)I) \quad (6) \]

\[ q_\gamma(u_l|x_l) = \mathcal{N}(u_l; \gamma_l, \sigma_l(x_l)I) \quad (7) \]

\[ t_l = \frac{z_l - \mu}{\sqrt{W [u_l^2; \cdots; u_{L-\delta}^2]}} \quad (8) \]

Additionally, to further encourage the capsule \( \text{Roll} \) as the forward prediction operator, we integrate a capsule \( \text{Roll} \) of \( t_i \) by one unit as the first step of the generative model, before decoding \( x_{t+i} \):

\[ p_\theta(x_{t+i}|g_\theta(t_i)) = p_\theta(x_{t+i}|g_\theta(\text{Roll}_1[t_i])) \quad (9) \]

We denote this model the Predictive Coding Topographic VAE (PCTVAE) and present an overview of forward prediction in Figure 1. We optimize the parameters \( \theta, \phi, \gamma \) (and \( \mu \)) through the ELBO, summed over the sequence length \( S \):

\[ \sum_{t=1}^S \mathbb{E}_{Q_{\phi, \gamma}, z_l, u_l|x_l} \left( \begin{array}{c} \log p_\theta(x_{t+1}|\text{Roll}_1[t_i]) \\ -D_{KL}(q_\phi(z_l|x_l)||p(z_l)) \\ -D_{KL}(q_\gamma(u_l|x_l)||p(u_l)) \end{array} \right) \quad (10) \]

where \( Q_{\phi, \gamma}(z_l, u_l|x_l) = q_\phi(z_l|x_l) \prod_{\delta=0}^L q_\gamma(u_{l-\delta}|x_{l-\delta}) \).

The fundamental differences of this model with the VAE are that this model is trained to maximize the likelihood of \( \text{future} \) inputs through the \( \text{Roll} \) operation present in the
ELBO, and that the construction of $t_\delta$ is now only a function of past inputs. As we will demonstrate in the next section, these extensions yield significant improvements to sequence modeling, while simultaneously increasing flexibility by allowing for online training and inference.

4. Experiments

In this section we measure the performance of our model, compared with non-predictive coding baselines, on the transforming color MNIST dataset from [29]. The dataset is composed of MNIST digits [32] sequentially transformed by one of three randomly chosen transformations: spatial rotation, rotation in color (hue) space, or scaling. For each training example, the starting pose (color, angle, scale) is randomly set, and a cyclic sequence of 18 examples is generated according to the chosen transformation. The same model architecture as [29] (a 3-layer MLP with ReLU activations) is used for all encoders and decoders of all models presented. For topographic models, the latent space is structured as 18 1-dimensional circular capsules, each of 18 dimensions. Further training details can be found at https://github.com/akandykeller/PCTVAE.

4.1. Forward Prediction Likelihood

To quantitatively measure the ability of the PCTVAE to predictively model sequences, we train the model to maximize Equation 10 with stochastic gradient descent, and measure the likelihood of held-out test sequences, with only partial sequences as input. Explicitly, for both the TVAE and PCTVAE, a window size of 9 observations are provided as input and used to generate a capsule representation $t_0$. The likelihood of the remaining 9 sequence elements is then measured by sequentially rolling the capsule activations forward, and measuring $p_\theta(x_\delta|g_\theta(\text{Roll}_\delta(t_0)))$ for $\delta \in \{0, ..., 9\}$. The final reported likelihood values are computed by importance sampling with 10 samples. In Table 4.1 we report the average log-likelihood over this forward predicted sequence for both the original TVAE and PCTVAE, in addition to the log-likelihood at $\delta_t = 0$ (no forward prediction) with a standard VAE. We see the PCTVAE achieves a significantly lower average negative likelihood for a non-topographic VAE, TVAE, and PCTVAE. The PCTVAE achieves the lowest average NLL over the forward predicted sequence while also maintaining low equivariance error. Mean ± std. over 3 random initializations.

Table 1. Neg. log-likelihood (NLL in nats) without forward prediction ($\delta_t = 0$), NLL averaged over the forward predicted sequence, and equivariance error $\mathcal{E}_{eq}$ for a non-topographic VAE, TVAE, and PCTVAE. The PCTVAE achieves the lowest average NLL over the forward predicted sequence while also maintaining low equivariance error. Mean ± std. over 3 random initializations.

<table>
<thead>
<tr>
<th>Model</th>
<th>NLL @ $\delta_t = 0$</th>
<th>NLL Avg. Seq.</th>
<th>$\mathcal{E}_{eq}$ Avg. Seq.</th>
</tr>
</thead>
<tbody>
<tr>
<td>VAE</td>
<td>190 ± 1</td>
<td>N/A</td>
<td>13274 ± 0</td>
</tr>
<tr>
<td>TVAE</td>
<td>187 ± 1</td>
<td>452 ± 16</td>
<td>2122 ± 21</td>
</tr>
<tr>
<td>PCTVAE</td>
<td>207 ± 1</td>
<td>232 ± 1</td>
<td>2201 ± 9</td>
</tr>
</tbody>
</table>

Figure 3. Forward prediction log-likelihood vs. future time offset $\delta_t$. We see that the PCTVAE has consistently high likelihood for sequence elements into the future whereas the likelihood of the TVAE model drops off rapidly. Shading denotes ± 1 std.

4.2. Sequence Generation

As a qualitative evaluation of the PCTVAE’s sequence modeling capacity, we show forward predicted sequences generated by both models in Figure 2. The top row shows the input sequence with grey images held out, and the lower row shows the forward predicted sequence, generated by sequentially rolling the representation $t_0$ forward, and decoding at each step. As can be seen, the PCTVAE (left) appears to generate sequences which are more coherent with the provided input sequence, while the TVAE (right) is observed to quickly diverge from the true transformation, in agreement with likelihood values of Figure 3.

5. Discussion

In this paper we have proposed an extension of the Topographic VAE to the framework of predictive coding, and have demonstrated an improved ability to model the imme-
diate future both qualitatively and quantitatively. This work is inherently preliminary and limited by the fact that the model is only tested on a single artificial dataset. In future work, we intend to explore the ability of such a model to learn more realistic transformations from natural data, such as from the Natural Sprites dataset [31], and additionally further investigate the downstream computational benefits gained from the learned equivariant capsule representation.

References


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