Inference for Generative Capsule Models

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Abstract

Capsule networks (see e.g. Hinton et al., 2018) aim to encode knowledge and reason about the relationship between an object and its parts. In this paper we specify a generative model for such data, and derive a variational algorithm for inferring the transformation of each object and the assignments of observed parts to the objects. We apply this model to (i) data generated from multiple geometric objects like squares and triangles (“constellations”), and (ii) data from a parts-based model of faces. Recent work by Kosiorek et al. [2019] has used amortized inference via stacked capsule autoencoders (SCAEs) to tackle this problem—our results show that we significantly outperform them where we can make comparisons (on the constellations data).

1 INTRODUCTION

An attractive way to set up the problem of object recognition is hierarchically, where an object is described in terms of its parts, and these parts are in turn composed of sub-parts, and so on. For example a face can be described in terms of the eyes, nose, mouth, hair, etc.; and a teapot can be described in terms of a body, handle, spout and lid parts. This approach has a long history in computer vision, see e.g. Recognition-by-Components by Biederman [1987]. Advantages of recognizing objects by first recognizing their constituent parts include tolerance to the occlusion of some parts, and that parts may vary less under a change of pose than the appearance of the whole object.

One big advantage of a parts-based setup is that if the pose of the object changes, this can have very complicated effects on the pixel intensities in an image, but the geometric transformation between the object and the parts can be described by a simple linear transformation (as used in computer graphics). Convolutional neural networks can allow a recognition system to handle 2D shifts of an object in the image plane, but attempts to generalize such equivariances across more general transformations lead to cumbersome constructions, and have not been very successful.

Recent work by Hinton and collaborators [Sabour et al., 2017; Hinton et al., 2018] has developed capsule networks. The key idea here is that a part in a lower level can vote for the pose of an object in the higher level, and an object’s presence is established by the agreement between votes for its pose. Hinton et al. [2018, p. 1] use an iterative process called “routing-by-agreement” which “updates the probability with which a part is assigned to a whole based on the proximity of the vote coming from that part to the votes coming from other parts that are assigned to that whole”. Subsequently Kosiorek et al. [2019] framed inference for a capsule network in terms of an autoencoder, the Stacked Capsule Autoencoder (SCAE). Here, instead of the iterative routing-by-agreement algorithm, a neural network $h_{\text{caps}}$ takes as input the set of input parts and outputs predictions for the object capsules’ instantiation parameters $(Y_k)_{k=1}^K$. Further networks $h_{\text{part}}^k$ are then used to predict part candidates from each $y_k$.

The objective function used in Hinton et al. [2018] (their eq. 4) is quite complex (involving four separate terms), and is not derived from first principles. In this paper we argue that the description in the paragraph above is backwards—it is more natural to describe the generative process by which an object gives rise to its parts, and that the appropriate routing-by-agreement inference algorithm then falls out naturally from this principled formulation. Below we focus on a single-layer of part-object relations, as we need to show
The contributions of this paper are to:

- Derive a variational inference algorithm for a generative model of object-part relationships, including a relaxation of the permutation-matrix formulation for matching object parts to observations;
- Obtain a principled and novel routing-by-agreement algorithm from this formulation;
- Demonstrate the effectiveness of our method on (i) “constellations” data generated from multiple geometric objects (e.g. triangles, squares) at arbitrary translations, rotations and scales; and (ii) data from a novel parts-based model of faces.
- Evaluate the performance of our model vs. competitors on the constellations data.
- Derive a variational inference algorithm for a generative model of object-part relationships, including a relaxation of the permutation-matrix formulation for matching object parts to observations;
- Obtain a principled and novel routing-by-agreement algorithm from this formulation;
- Demonstrate the effectiveness of our method on (i) “constellations” data generated from multiple geometric objects (e.g. triangles, squares) at arbitrary translations, rotations and scales; and (ii) data from a novel parts-based model of faces.
- Derive a variational inference algorithm for a generative model of object-part relationships, including a relaxation of the permutation-matrix formulation for matching object parts to observations;
- Obtain a principled and novel routing-by-agreement algorithm from this formulation;
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2 OVERVIEW

Our images consist of a set of objects in different poses. Examples include images of handwritten digits, faces, or geometric shapes in 2D or 3D. An object can be defined as an instantiation of a specific model object (or template) along with a particular pose (or geometric transformation). Furthermore, objects, and thus templates, are decomposed in parts, which are the basic elements that comprise the objects. For example, faces can be decomposed into parts (e.g. mouth, nose etc.), or a geometric shape can be decomposed into vertices. These parts can have internal variability, (e.g. eyes open or shut).

More formally, let \( T = \{T_k\}_{k=1}^K \) be the set of \( K \) templates that are used to generate a scene. Each template \( T_k = \{p_n\}_{n=1}^{N_k} \) is composed of \( N_k \) parts \( p_n \). We assume that scenes can only be generated using the available templates. Furthermore, every scene can present a different configuration of objects, with some objects missing from some scenes. For example, in scenes that could potentially contain all digits from 0 to 9 once, and if only the digits 2 and 5 are in the image, we consider that the other digits are missing. If all the templates were employed in the scene, then the number of observed parts \( M \) is equal to the sum of all the parts of all the templates \( N = \sum_{k=1}^K N_k \).

Each observed template \( T_k \) in a scene is then transformed by an independent transformation \( y_k \), different for each template, generating a transformed object \( X_k = \{x_n\}_{n=1}^{N_k} \) in a scene

\[
T_k \xrightarrow{y_k} X_k.
\]  

The transformation \( y_k \) includes a geometric transformation of the template, but also includes appearance variability in the parts.

Assume that we are given a scene \( X = \{x_m\}_{m=1}^M \) composed of \( M \) observed parts coming from multiple templates. The inference problem for \( X \) involves a number of different tasks. We need to determine which objects from the set of templates were employed to generate the scene. Also, we need to infer what transformation \( y_k \) was applied to each template to generate the objects. This allows us to infer the correspondences between the template parts and the scene parts.

We demonstrate our method on “constellations” data as shown in Fig. 1 and data from a parts-based model of faces illustrated in Fig. 2.

3 GENERATIVE MODEL FOR CAPSULES

We propose a generative model to describe the problem. Consider a template (or model) \( T_k \) for the \( k \)th object. \( T_k \) is composed of \( N_k \) parts \( \{p_n\}_{n=1}^{N_k} \). Each part \( p_n \) is described in its reference frame by its geometry \( p^g_n \) and its appearance \( p^a_n \). Each object also has associated latent variables \( y_k \) which transform from the reference frame to the image frame, so \( y_k \) is split into geometric variables \( y^g_k \) and appearance variables \( y^a_k \).

**Geometric transformations:** Here we consider 2D templates and a similarity transformation (translation, rotation and scaling) for each object, but this can be readily extended to allow 3D templates and a scene-to-viewer camera transformation. We assume that \( p^g_n \) contains the \( x \) and \( y \) locations of the part, and also its size \( s_n \) and orientation \( \phi_n \) relative to the reference frame\(^2\). The size and orientation are represented as the projected size of the part onto the \( x \) and \( y \) axes, as this allows us to use linear algebra to express the transformations (see below). Thus \( p^g_n = (p^g_{nx}, p^g_{ny}, s_n \cos \phi_n, s_n \sin \phi_n)^T \).

\(^2\)For simplicity of notation we suppress the dependence of \( p_n \) on \( k \) for now.

\(^3\)For the constellations data, the size and orientation information is not present, nor are there any appearance features.
Consider a template with parts \( p_k^a \) for \( n = 1, \ldots, N_k \) that we wish to scale by a factor \( s \) and covariance matrix \( \Sigma \). The dimensionality of the part is \( n \). The prior for \( \mu_0 \) is \( \mathcal{N}(0, I) \).

### Joint distribution

Let \( z_{mnk} \in \{0, 1\} \) indicate whether observed part \( x_m \) matches to part \( n \) of object \( k \). Every observation \( m \) belongs uniquely to a tuple \((k, n)\), or in other words, a point \( x_m \) belongs uniquely to the part defined by \( y_k \) acting on the template matrix \( F_{kn} \). The opposite is also partially true; every tuple \((k, n)\) belongs uniquely to a point \( m \) or it is unassigned if part \( n \) of template \( k \) is missing in the scene.

The joint distribution of the variables in the model is given by

\[
p(X, Y, Z) = p(X|Y,Z)p(Y)\prod_{k=1}^{K}N(x_m|F_{kn}y_k + m_{kn}, D_{kn})^{z_{mkn}},
\]

where \( D_{kn} \) consists of the diagonal matrices \( \lambda^{-1} I \) and \( D_{kn}^a \) and \( m_{kn} \) consists of a zero vector for the geometric features stacked on top of the mean for the appearance features \( m_{kn}^a \).

Note that \( F_{kn} \) has blocks of zeros so that \( x_m^a \) does not depend on \( y_k^a \), and \( x_m \) does not depend on \( y_k^a \). Note that such a model for a single object with geometric features only was developed by Revow et al. [1996].

### Annealing parameter

During the fitting of the model to data, it is useful to modify the covariance matrix \( D_{kn} \) to \( \beta^{-1} D_{kn} \), where \( \beta > 0 \). The effect of this is to inflate the variances in \( D_{kn} \), allowing greater uncertainty in the inferred matches early on in the fitting process, as used, e.g. in Revow et al. [1996]. \( \beta \) is increased according to an annealing schedule during the fitting.

### Match distribution \( p(Z) \)

In a standard Gaussian mixture model, the assignment matrix \( Z \) is characterized by a Categorical distribution, where each point \( x_m \) is assigned to one part

\[
p(Z) = \prod_{m=1}^{M} \text{Cat}(z_{m}|\pi),
\]

with \( z_{m} \) being a 0/1 vector with only one 1, and \( \pi \) being the probability vector for each tuple \((k, n)\). However, the optimal solution to our problem occurs when each part of a template belongs uniquely to one observed part in a scene. This means that \( Z \) should be a permutation matrix, where each point \( m \) is assigned to a tuple \((k, n)\) and vice versa. Notice that a permutation matrix is a square matrix, so if \( M \leq N \), we add dummy rows to \( Z \), which are assigned to missing points in the scene.
We propose to relax \( \rho \) variational inference for the above model can be derived with
\[
\sum_{i=1}^{N!} \pi_i I[Z = Z_i]
\] (9)
with \( \sum_{i=1}^{N!} \pi_i = 1 \) and \( I[Z = Z_i] \) the indicator function, being equal to 1 if \( Z = Z_i \) and 0 otherwise.

The number of possible permutation matrices increases as \( N! \), which makes exact inference over permutations intractable. An interesting property of \( p_{perm}(Z) \) is that its first moment \( \mathbb{E}_{p_{perm}}[Z] \) is a doubly-stochastic (DS) matrix, a matrix of elements in \([0,1]\) whose rows and columns sum to 1. We propose to relax \( p_{perm}(Z) \) to a distribution \( p_{DS}(Z) \) that is characterized by the doubly-stochastic matrix \( A \) with elements \( a_{mnk} \), such that \( \mathbb{E}_{p_{DS}}[Z] = A \):
\[
p_{DS}(Z) = \prod_{m=1}^{N} \prod_{k=1}^{K} \prod_{n=1}^{N_k} a_{mnk}^r
\] (10)

\( A \) is fully characterized by \((N-1)^2\) elements. In the absence of any prior knowledge of the affinities, a uniform prior over \( Z \) with \( a_{mnk} = \frac{1}{N^2} \) can be used. However, note that \( p_{DS} \) can also represent a particular permutation matrix \( Z \) by setting the appropriate entries of \( A \) to 0 or 1, and indeed we would expect this to occur during variational inference (see sec. 4) when the model converges to a correct solution.

\section{4 Variational Inference}

Variational inference for the above model can be derived similarly to the Gaussian Mixture model case [Bishop 2006 Chapter 10]. The variational distribution under the mean field assumption is given by \( q(Z,Y) = q(Z)q(Y) \), where the optimal solutions for \( \log q(Z) \) and \( \log q(Y) \) under the generative model can be expressed as
\[
\log q(Z) \propto \mathbb{E}_{q(Y)}[\log p(X,Y,Z)],
\] (11)
\[
\log q(Y) \propto \mathbb{E}_{q(Z)}[\log p(X,Y,Z)].
\] (12)

For \( q(Z) \) we obtain an expression with the same distribution model as the prior in (10)
\[
q(Z) \propto \prod_{m=1}^{N} \prod_{k=1}^{K} \prod_{n=1}^{N_k} \rho_{mnk}^r,
\] (13)

where \( \rho_{mnk}^r \) represents the unnormalized probability of point \( m \) being assigned to tuple \((k,n)\) and vice versa. These unnormalized probabilities have a different form depending on whether we are considering a point that appears in the scene \((m \leq M)\)
\[
\log \rho_{mnk} = \log a_{mnk} - \frac{1}{2} \log |\beta^{-1} D_{kn}| - \frac{d_{kn}}{2} \log 2\pi - \frac{\beta}{2} \mathbb{E}_{y_k}[(x_m - F_{kn}y_k - m_{kn})^T D_{kn}^{-1}(x_m - F_{kn}y_k - m_{kn})],
\] (14)

or whether we are considering a dummy row of the prior \((m > M)\),
\[
\log \rho_{mnk} = \log a_{mnk},
\] (15)

When a point is part of the scene \((14)\), and thus \( m \leq M \) the update of \( \rho_{mnk} \) is similar to the Gaussian mixture model case. However, if a point is not part of the scene \((15)\), and thus \( m > M \) then the matrix is not updated and the returned value is the prior \( a_{mnk} \). This specific choice of distribution for both \( p_{DS}(Z) \) and \( q(Z) \) leads naturally to the addition of dummy rows that are employed to make the matrix \( \rho \) square. Now, the normalized distribution \( q(Z) \) becomes:
\[
q(Z) = \prod_{m=1}^{N} \prod_{k=1}^{K} \prod_{n=1}^{N_k} r_{mnk}^s
\] (16)

where \( \mathbb{E}_{q(Z)}[r_{mnk}] = r_{mnk} \). The elements \( r_{mnk} \) of matrix \( R \) represent the posterior probability of each point \( m \) being uniquely assigned to the part-object tuple \((n,k)\) and vice-versa. This means that \( R \) needs to be a DS matrix. This can be achieved by employing the Sinkhorn-Knopp algorithm [Sinkhorn and Knopp 1967], which updates a square non-negative matrix by normalizing the rows and columns alternately, until the resulting matrix becomes doubly stochastic (see supp. mat. A for more details). The use of the Sinkhorn-Knopp algorithm for approximating matching problems has also been described by [Powell and Smith 2019] and [Mena et al. 2020], but note that in our case we also need to alternate with inference for \( q(Y) \). Furthermore, the optimal solution to the assignment problem occurs when \( R \) is a permutation matrix itself. When this happens we exactly recover a discrete posterior (with the same form as (2)) over permutation matrices where one of them has probability one, with the others being zero.

The distribution for \( q(Y) \) is a Gaussian with
\[
q(Y) = \prod_{k=1}^{K} N(y_k | \mu_k, \Lambda_k^{-1}),
\] (17)
\[
\Lambda_k = D_0^{-1} + \beta \sum_{m}^{M} \sum_{n}^{N_k} r_{mnk} F_{kn}^T D_{kn}^{-1} F_{kn},
\] (18)
\[
\mu_k = \Lambda_k^{-1} \left[ D_0 \mu_0 + \beta \sum_{m}^{M} \sum_{n}^{N_k} r_{mnk} F_{kn}^T D_{kn}^{-1} (x_m - m_{kn}) \right],
\] (19)

where the updates for both \( \Lambda_k \) and \( \mu_k \) depend explicitly on the annealing parameter \( \beta \) and the templates employed.
Algorithm 1 Variational Inference

1: Initialize $β, β_{max}$ and $R \sim U[0,1]^{N \times N}$, $\forall m, n, k$
2: $R = \text{SinkhornKnopp}(R)$
3: while not converged do
   4: Update $Λ_k$ (18), $\forall k$
   5: Update $μ_k$ (19), $\forall k$
   6: Update $\log \rho_{mk}$ (14)-(15), $\forall m, n, k$
   7: Update $R = \text{SinkhornKnopp}(ρ)$
   8: if ELBO has converged then
      9: if $β < β_{max}$ then
         10: Anneal $β$
      else
         11: converged = True
   return $R, \{μ_k, Λ_k\}$

in the model. Note that the prediction from datapoint $m$ to the mean of $γ_k$ is given by $r_{mk} F_{k|n}^T(D_{kn})^{-1}(x_m - m_{kn})$, i.e. a weighted sum of the predictions of each part $n$ with weights $r_{mk}$. These expressions remain the same when considering a Gaussian mixture prior such as [9].

The expectation term in (14) under the model and evidence lower error bound (ELBO) are given in supp. mat. A. Algorithm 1 summarizes the inference procedure for this model; the alternating updates of $q(Y)$ and $q(Z)$ carry out routing-by-agreement.

4.1 COMPARISON WITH OTHER OBJECTIVE FUNCTIONS

In [Hinton et al. 2018] an objective function $cost^h_k$ is defined (their eq. 1) which considers inference for the pose of a higher-level capsule $k$ on pose dimension $h$. Translating to our notation, $cost^h_k$ combines the votes from each datapoint $m$ as $cost^h_k = \sum_m r_{mk} \ln p_{mk}^h$, where $p_{mk}^h$ is a Gaussian, and $r_{mk}$ is the “routing softmax assignment” between $m$ and $k$. It is interesting to compare this with our equation (19). Firstly, note that the vote of $x_m$ to part $n$ in object $k$ is given explicitly by $F_{k|n}^T x_m$, i.e. we do not require introduction of an independent voting mechanism, this falls out directly from the inference. Secondly, note that our $R$ must keep track not only of assignments to objects, but also to parts of the objects. In contrast to [Hinton et al. 2018], our inference scheme is derived from variational inference on the generative model, rather than introducing an ad hoc objective function.

The specialization of the SCAE method of [Kosiorek et al. 2019] to constellation data is called the “constellation capsule autoencoder (CCAЕ)” and discussed in their sec. 2.1.

Under their equation 5, we have that

$$p(x_{1:M}) = \prod_{m=1}^{M} \sum_{k=1}^{K} \sum_{n=1}^{N} a_k a_{k,n} \mu_k a_{k,n} \sum_{j=1}^{a_{ij}} N(x_m|\mu_{k,n}, \lambda_{k,n}),$$

(20)

where $a_k \in [0,1]$ is the presence probability of capsule $k$, $a_{k,n} \in [0,1]$ is the conditional probability that a given candidate part $n$ exists, and $\mu_{k,n}$ is the predicted location of part $k, n$. The $a_k$s are predicted by the network $h^{caps}$, while the $a_{k,n}s$ and $\mu_{k,n}s$ are produced by separate networks $h^{part}$ for each part $k$.

We note that (20) provides an autoencoder style reconstructive likelihood for $x_{1:M}$, as the $a$’s and $\mu$’s depend on the data. To handle the arbitrary number of datapoints $M$, the network $h^{caps}$ employs a Set Transformer architecture [Lee et al. 2019]. In comparison to our iterative variational inference, the CCAE is a “one shot” inference mechanism. This may be seen as an advantage, but in scenes with overlapping objects, humans may perform reasoning like “if that point is one of the vertices of a square, then this other point needs to be explained by a different object” etc, and it may be rather optimistic to believe this can be done in a simple forward pass. Also, CCAE cannot exploit prior knowledge of the geometry of the objects, as it relies on an opaque network $h^{caps}$ which requires extensive training.

4.2 RELATED WORK

Above we have discussed the work of [Sabour et al. 2017], [Hinton et al. 2018] and [Kosiorek et al. 2019]. There is some more recent work, for example [Li et al. 2020] present an undirected model, based on the capsule RBM of [Li and Zhu 2019]. Compared to our work, this is an undirected as opposed to directed generative model. Also [Smith et al. 2021] propose a layered directed generative model, where the children of higher level capsules inherit its pose (but transformed). Both [Li et al. 2020] and [Smith et al. 2021] consider tree-structured relationships between parents and children, similar to [Hinton et al. 2000] and [Storkey and Williams 2003]. However, most importantly, these recent capsule models do not properly handle the fact that the input to a capsule should be a set of parts; instead in their work the first layer capsules that interact with the input image model specific location-dependent features/templates in the image, and their second layer capsules have interactions with the specific first layer capsules (e.g. the fixed affinity $ρ_{ij}$ of [Smith et al. 2021] parent $i$ in layer $k$ for child $j$). But if we consider a second-layer capsule that is, for example, detecting the conjunction of the 3 strokes comprising a letter “A”, then at different translations, scales and rotations of the A it will need to connect to different image level stroke features, so these connection affinities must depend on transformation variables of the parent.
A radical alternative to “routing by agreement” inference is to make use of a “random sample consensus” approach (RANSAC, Fischler and Bolles [1981]), where a minimal number of parts are used in order to instantiate an object. The original RANSAC fitted just one object, but Sequential RANSAC (see, e.g., Tori [1998], Vincent and Lagnaïre [2001]) repeatedly removes the parts associated with a detected object and re-runs RANSAC, so as to detect all objects.

For the constellations problem, we can try matching any pair of points on one of the templates to every possible pair of \( M(M - 1) \) points in the scene. The key insight is that a pair of known points is sufficient to compute the 4-dimensional \( y_k \) vector in the case of similarity transformations. Using the transformation \( \hat{y}_k \), we can then predict the location of the remaining parts of the template, and check if these are actually present. If so, this provides evidence for the existence of \( T_k \) and \( \hat{y}_k \). After considering the \( M(M - 1) \) subsets, the algorithm then combines the identified instantiations to give an overall explanation of the scene. Details of RANSAC for the constellations problem are given in supp. mat. [B].

For the faces data, each part has location, scale and orientation information, so a single part is sufficient to instantiate the whole object geometrically. For the appearance, we follow the procedure for inference in a factor analysis model with missing data, as given in [Williams et al.] [2019], to predict \( y_k^* \) given the appearance of the single part.

5 EXPERIMENTAL DETAILS

Below we provide details of the data generators, inference methods and evaluation criteria for the constellations data in sec. 5.1 and the faces data in sec. 5.2.

5.1 CONSTELLATION DATA

In order to allow fair comparisons, we use the same dataset generator for geometric shapes employed by Kosiorek et al. [2019]. We create a dataset of scenes, where each scene consists of a set of 2D points, generated from different geometric shapes. The possible geometric shapes (templates) are a square and an isosceles triangle, with parts being represented by the 2D coordinates of the vertices. We use the same dimensions for the templates as used by Kosiorek et al. [2019], side 2 for the square, and base and height 2 for the triangle. All templates are centered at \((0, 0)\). In every scene there are at most two squares and one triangle. Each shape is transformed with a random transformation to create a scene of 2D points given by the object parts. To match the evaluation of Kosiorek et al. [2019], all scenes are normalized so as the points lie in \([-1, 1]\) on both dimensions. When creating the scene, we select randomly (with probability 0.5) whether an object is going to be present or not, but delete empty scenes. A test set used for evaluation is comprised of 450-460 non-empty scenes, based on 512 draws.

Additionally, we study how the methods compare when objects are created from noisy templates. We consider that the original templates used for the creation of the images are corrupted with Gaussian noise with standard deviation \( \sigma \). Once the templates are corrupted with noise, a random transformation \( y_k \) is applied to obtain the object \( X_k \) of the scene. As with the noise-free data, the objects are normalized to lie in \([-1,1]\) on both dimensions.

CCA is trained by creating random batches of 128 scenes as described above and optimizing the objective function in (20). The authors run CCA for 300,000 epochs, and when the parameters of the neural networks are trained, they use their model on the test dataset to generate an estimation of which points belong to which capsule, and where the estimated points are located in each scene.

The variational inference approach allows us to model scenes where the points are corrupted with some noise. The annealing parameter \( \beta \) controls the level of noise allowed in the model. We use an annealing strategy to fit \( \beta \), increasing it every time the ELBO has converged, up to a maximum value of \( \beta_{max} = 1 \). We set the hyperparameters of the model to \( \mu_0^2 = 0 \), \( D_0^2 = I_4 \), \( \lambda = 10^4 \) and \( a_{mnk} = \frac{1}{N} \). We run Algorithm 1 with 5 different random initializations of \( R \) and select the solution with the best ELBO. Similarly to Kosiorek et al. [2019], we incorporate a sparsity constraint in our model, that forces every object to explain at least two parts. Once our algorithm has converged, for a given \( k \) if any \( r_{mnk} > 0.9 \) and \( \sum_m \sum_n r_{mnk} < 2 \) it means that the model has converged to a solution where object \( k \) is assigned to less than 2 parts. In these cases, we re-run Algorithm 1 with a new initialization of \( R \). Notice that this is also related to the minimum basis size necessary in the RANSAC approach for the types of transformations that we are considering.

The implementation RANSAC (Algorithm 3) considers all matches between the predicted and the scene points where the distance between them is less than 0.1. Among them, it selects the matching with minimum distance between scene and predicted points. For both the variational inference algorithm and the RANSAC algorithm, a training dataset is not necessary. These algorithms are applied directly to each test scene and return a set of objects describing the points in the scene. Unfortunately we do not have access to the code employed by Hinton et al. [2018], so we have been unable to make comparisons with it.

Evaluation: Three metrics are used to evaluate the performance of the different methods: variation of information, adjusted Rand index and segmentation accuracy. They are based on partitions of the datapoints into those associated with each object, and those that are missing. Compared
to standard clustering evaluation metrics, some modifications are needed to handle the missing objects. Details are provided in supp. mat. We also use an average scene accuracy metric, where a scene is correct if the method returns the full original scene, and is incorrect otherwise.

5.2 PARTS-BASED FACE MODEL

We have developed a novel hierarchical parts-based model for face appearances. It is based on five parts, namely eyes, nose, mouth, hair and forehead, and jaw (see Fig. 2(a)). Each part has a specified mask, and we have cropped the hair region to exclude highly variable hairstyles. This decomposition is based on the “PhotoFit Me” work and data of Prof. Graham Pike, see https://www.open.edu/openlearn/PhotoFitMe. For each part we trained a probabilistic PCA (PPCA) model to reduce the dimensionality of the raw pixels; the dimensionality is chosen so as to explain 95% of the variance. This resulted in dimensionalities of 24, 11, 12, 16 and 28 for the eyes, nose, mouth, jaw and hair parts respectively. We then add a factor analysis (FA) model on top with latent variables $y_{kn}^a$ to model the correlations of the PPCA coefficients across parts. The dataset used (from PhotoFit Me) is balanced by gender (female/male) and by race (Black/Asian/Caucasian), hence the high-level factor analyser can model regularities across the parts, e.g. wrt skin tone. $x_{n}^a$ is predicted from $y_{kn}^a$ as $F_{kn}^o y_{kn}^a + m_{kn}^a$, as in 5. $y_{kn}^a$ would have an effect on the part appearance, e.g. by scaling and rotation, but this can be removed by running the PPCA part detectors on copies of the input image that have been rescaled and rotated.

The “PhotoFit Me” project utilizes 7 different part-images for each gender/race group, for each of the five part types. As a result, we generated $7^5$ synthetic faces for each group, by combining these face-parts, which lead to a total of 100,842 faces. All faces were centered on a $224 \times 224$ pixel canvas. For each synthetic face we created an appearance vector $x_{n}^a$, which consisted of the stacked vectors from the 5 different principal component subspaces. Finally, we created a balanced subset from the generated faces (18,000 images), which we used to train a FA model. We tuned the latent dimension of this model by training it multiple times with a different number of factors, and finally chose 12 factors, where a knee in the reconstruction loss on the face data was observed on a validation set.

Early work on PCA for faces—"eigenfaces" [Sirovich and Kirby 1987; Turk and Pentland 1991]—used a global basis as opposed to a parts-based representation. Rao and Ballard [1999] made use of a hierarchical factor analysis model, but used it to model extended edges in natural image patches rather than facial parts. Ross and Zemel [2006] developed a “multiple cause factor analysis” (MCFA) and applied it to faces; in contrast to our work this did not have a higher-level factor analyser to model correlations between parts, but it did allow variability in the masks of the parts.

Kosiorek et al. [2019] developed a Part Capsule Autoencoder (PCAE) to learn parts from images, and applied it to MNIST images. Each PCAE part is a template which can undergo an affine transformation, and it has "special features" that were used to encode the colour of the part. Thus the PCAE parts are less flexible than our facial parts—they only model global colour changes of the part, and not the rich variability that can be encoded with the PCA model. Also, we have found that the parts detected by PCAE are not equivariant to rotation. Figure 7 shows the PCAE part decompositions inferred for different angles of rotation of a 4 digit—notice e.g. in panel (a) how the part coloured white maps to different parts of the 4 for 45°-180° and 225°-0°.

To evaluate our inference algorithm we generated $224 \times 224$ pixel scenes of faces. These consisted of 2, 3, 4 or 5 randomly selected faces from a balanced test-set of 7,614 synthetic faces, which were transformed with random similarity transformations. The face-objects were randomly scaled down by a minimum of 50% and were also randomly translated and rotated, with the constraint that all the faces fit the scene and did not overlap each other. An example of such a scene is shown in Fig. 8(b), and further examples are shown in the supp. mat. Figure 8. Afterwards, these two constraints were dropped to test the ability of our model to perform inference with occluded parts, see Figure 8(e) for an example. In our experiments we assume that the face parts are detected accurately, i.e. as generated.

In the case of facial parts—and parts with both geometric and appearance features in general—it only makes sense to assign the observed parts $x_{n}$ to template parts $x_{kn}$ of the same type (e.g. an observed “nose” part should be assigned only to a template “nose” part). We assume that this information is known, since the size of the appearance vector of each part-type is unique. Thus it no longer makes sense to initialize the assignment matrix uniformly for all entries, but rather only for the entries that correspond to templates of the
Table 1: Comparison between the different methods. For SA, ARI and Scene Accuracy the higher the better. For VI the lower the better. Different levels of Gaussian noise with standard deviation $\sigma$ are considered.

| Metric     | Model     | $\sigma=0$ | $\sigma=0.1$ | $\sigma=0.25$ |
|------------|-----------|-------------|---------------|---------------|
|             | CCAE      | 0.828       | 0.754         | 0.623         |
|            | GCM-GMM   | 0.753       | 0.757         | 0.744         |
|            | GCM-DS    | 0.899       | 0.882         | 0.785         |
|            | RANSAC    | 1           | 0.992         | 0.965         |
|             | CCAE      | 0.599       | 0.484         | 0.248         |
|            | GCM-GMM   | 0.586       | 0.572         | 0.447         |
|            | GCM-DS    | 0.740       | 0.699         | 0.498         |
|            | RANSAC    | 1           | 0.979         | 0.914         |
|             | CCAE      | 0.481       | 0.689         | 0.988         |
|            | GCM-GMM   | 0.478       | 0.502         | 0.677         |
|            | GCM-DS    | 0.299       | 0.359         | 0.659         |
|            | RANSAC    | 0           | 0.034         | 0.135         |
|             | CCAE      | 0.365       | 0.138         | 0.033         |
|            | GCM-GMM   | 0.179       | 0.173         | 0.132         |
|            | GCM-DS    | 0.664       | 0.603         | 0.377         |
|            | RANSAC    | 1           | 0.961         | 0.843         |

observed part’s type. Consequently, \( \beta \) is only utilized for \( m, n \) pairs of the same type. Similarly to the constellation experiments, we initialized the assignment matrix 5 times and selected the solution with the largest ELBO.

In the experiments we evaluated the part assignment accuracy of the algorithms. In a given scene, the assignment is considered correct if all the observed parts have been correctly assigned to their corresponding template parts with the highest probability. In order to evaluate the prediction of the appearance features, we measured the root mean square error (RMSE) between the input and generated scenes.

### 6 RESULTS

We present results for the constellations and faces experiments in sections 6.1 and 6.2 respectively.

#### 6.1 CONSTELLATION EXPERIMENTS

In Table 1 we show a comparison between CCAE, the variational inference method with a Gaussian mixture prior (GCM-GMM), with a prior over permutation matrices (GCM-DS), and the RANSAC approach. For GCM-GMM and GCM-DS we show the results where the initial \( \beta = 0.05 \), relegating a comparison across different initializations of \( \beta \) to the supp. mat. \[4\] \[5\] \[6\] Scenes without noise and with noise levels of \( \sigma = 0.1, 0.25 \) are considered.

We see that GCM-DS improves over CCAE and GCM-

GMM in all of the metrics, with GCM-GMM being comparable to CCAE. Interestingly, for the noise-free scenarios, the RANSAC method achieves a perfect score for all of the metrics. Since there is no noise on the observations and the method searches over all possible solutions of \( y_k \), it can find the correct solution for any configuration of geometric shapes in a scene. For the noisy scenarios, all the methods degrade as \( \sigma \) increases. However, the relative performance between them remains the same, with RANSAC performing the best, followed by GCM-DS and then GCM-GMM. Example inferences are shown and discussed in supp. mat. \[7\] and \[8\]

#### 6.2 FACE EXPERIMENTS

Firstly, the VI algorithm was evaluated on scenes of multiple, randomly selected and transformed faces.\[4\] For scenes with 2, 3, 4 and 5 faces, the assignment accuracy was 100%, 100%, 99.2% and 93.7% respectively (based on 250 scenes per experiment). RANSAC gave 100% accurate assignments in all 4 cases. This is to be expected, since from each part the pose of the whole can be predicted accurately. However, RANSAC’s ability to infer the appearance of the faces proved to be limited. More specifically, in 250 instances uniformly distributed across scenes of 2, 3, 4 and 5 faces, the VI algorithm had RMSE of 0.036 ± 0.004, while RANSAC scored 0.052 ± 0.006, with consistently higher error on all scenes. This is illustrated in the examples of Figure 8 where it is clear that RANSAC is less accurate in capturing key facial characteristics. If inference for \( y_k \) is run as a post-processing step for RANSAC using all detected parts in an object, this difference disappears.

The supp. mat. contains a movie showing the fitting of the models to the data. It is not possible for us to compare results with the SCAE algorithm on the faces data, as the PCAE model used is not rich enough to model PCA subspaces.

Secondly, we evaluated the ability of our algorithm to perform inference in scenes where some parts have been occluded, either by overlapping with other faces or by extending out of the scene. In 250 scenes with 3 partially occluded faces, both the VI and RANSAC algorithms were fully successful in assigning the observed parts to the corresponding template accurately. See Figure 8(e) for an example.

### 7 DISCUSSION

Above we have described a principled generative capsules model. It leads directly to a variational inference algorithm which can handle either a mixture formulation or incorporation of the DS matrix constraint. We have also shown that this formulation outperforms the CCAE of Kosiorek et al. [2019] on the constellation data generator that they used.

\[4\] Code at: https://github.com/anazabal/GenerativeCapsules

\[5\] Code at: https://github.com/tsagkas/capsules
In our experiments RANSAC was shown to often be an effective alternative to variational inference (VI). This is particularly the case when the basis in RANSAC is highly informative about the object. RANSAC provides an interesting alternative to routing-by-agreement, although its sampling-based inference is less amenable to neural-network style parallel implementations than VI.

In this paper we have not discussed the learning of the geometric model (i.e. the $F_{kn}^q$ matrices), but in all such work, inference for $q(Z,Y)$ forms an inner loop, with model learning as an outer loop. Also, the interpretable nature of the model means that we can exploit knowledge where it is available; in contrast the SCAE’s opaque inference networks do not allow this.

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**Appendix A: Details for Variational Inference**

The Sinkhorn-Knopp algorithm is given in Algorithm A.2.

**Algorithm 2 Sinkhorn-Knopp algorithm**

1: procedure SINKHORNKNOPP(X)
2: while X not doubly stochastic do
3:  Normalize rows of X: \( x_{ij} = \frac{x_{ij}}{\sum_j x_{ij}}, \forall i \)
4:  Normalize columns of X: \( x_{ij} = \frac{x_{ij}}{\sum_i x_{ij}}, \forall j \)
5: return X

The evidence lower bound (ELBO) \( L(q) \) for this model is decomposed in three terms:

\[
L(q) = \mathbb{E}_q[\log p(X|Y, Z)] - KL(q(Y)||p(Y)) - KL(q(Z)||p(Z)),
\]

with \( KL(q||p) \) being the Kullback-Leibler divergence between distributions \( q \) and \( p \). The first term indicates how well the generative model \( p(X|Y, Z) \) fits the observations under our variational model \( q(Y, Z) \):

\[
\mathbb{E}_q[\log p(X|Y, Z)] = - \sum_{m=1}^{M} \sum_{k=1}^{K} \sum_{n=1}^{N_k} r_{mnk} \left[ \frac{d_{kn}}{2} \log 2\pi + \frac{1}{2} \log |\beta^{-1} D_{kn}| \right]
+ (x_m - F_k \mu_k - m_{kn})^T D_k^{-1} (x_m - F_k \mu_k - m_{kn})
+ \text{trace}(F_k^T D_k^{-1} F_k \Lambda_k^{-1})]. 
\]

The Kullback-Leibler divergence between the two Gaussian distributions \( q(Y) \) and \( p(Y) \) in our model has the following expression:

\[
KL(q(Y)||p(Y)) = \frac{1}{2} \sum_{k=1}^{K} \left( \text{trace}(D_0^{-1} \Lambda_k^{-1}) - d_k + (\mu_k - \mu_0)^T D_0^{-1} (\mu_k - \mu_0) + \log |D_0| + \log |\Lambda_k| \right),
\]

where \( d_k \) is the dimensionality of \( y_k \).

The expression for \( KL(q(Z)||p(Z)) \) is given by

\[
KL(q(Z)||p(Z)) = \sum_{m=1}^{N} \sum_{k=1}^{K} \sum_{n=1}^{N_k} r_{mnk} \log \frac{r_{mnk}}{a_{mnk}}.
\]

**Algorithm 3 RANSAC approach**

1: \( T: K \) templates of the scene
2: \( B_k: \) base matrix for template \( T_k \)
3: \( X: M \) points of the scene
4: \( \text{out} = [] \)
5: for \( x_i \in X \) do
6:  for \( x_j \in X \setminus x_i \) do
7:    \( x_{ij} = \text{Vectorize}(x_i, x_j) \)
8:  for \( k = 1: K \) do
9:    \( \hat{y}_k = B_k^{-1} x_{ij} \)
10:   \( T_k \hat{y}_k \rightarrow X_k \)
11:   if SubsetMatch(\( \hat{X}_k, X \)) then
12:     Add (\( T_k, \hat{y}_k, \hat{X}_k \)) to out
13: \)

The expectation term in [14] is:

\[
\mathbb{E}_{q_k}[(x_m - F_k \mu_k - m_{kn})^T D_k^{-1} (x_m - F_k \mu_k - m_{kn})] = (x_m - F_k \mu_k - m_{kn})^T D_k^{-1} (x_m - F_k \mu_k - m_{kn})
+ \text{trace}(F_k^T D_k^{-1} F_k \Lambda_k^{-1}).
\]

**B Details of RANSAC for the Constellations Data**

A summary of the algorithm is given in Algorithm B.3.

Assume we have chosen parts \( n_1 \) and \( n_2 \) as the basis for object \( k \), and that we have selected datapoints \( x_i \) and \( x_j \) as their hypothesized counterparts in the image. Let \( x_{ij} \) be the vector obtained by stacking \( x_i \) and \( x_j \), and \( B_k \) be the \( 4 \times 4 \) square matrix obtained by stacking \( F_{kn_1} \) and \( F_{kn_2} \). Then \( y_k = B_k^{-1} x_{ij} \). Finally, SubsetMatch(\( \hat{X}_k, X \)) selects those points in \( X_k \) that are close to \( X \) with a given tolerance and add them to the output. Among them, the solution is given by the one that minimizes \( \sum_{n=1}^{N_k} (\hat{x}_{nk} - x_{nk})^2 \).

The above algorithm chooses a specific basis for each object, but one can consider all possible bases for each object. It is then efficient to use a hash table to store the predictions for each part, as used in Geometric Hashing [Wolfson and Rigoutsos, 1997]. Geometric Hashing is traditionally employed in computer vision to match geometric features against previously defined models of such features. This technique works well with partially occluded objects, and is computationally efficient if the basis dimension is low.

**C Evaluation Metrics for the Constellations Data**

In a given scene \( X \) there are \( M \) points, but we know that there are \( N \geq M \) possible points that can be produced from all of the templates. Assume that \( K' \leq K \) templates are active in this scene. Then the points in the scene are
labelled with indices $1, \ldots, K'$, and we assign the missing points index 0. Denote the ground truth partition as $V = \{V_0, V_1, \ldots, V_{K'}\}$. An alternative partition output by one of the algorithms is denoted by $\hat{V} = \{\hat{V}_0, \hat{V}_1, \ldots, \hat{V}_{K'}\}$. The predicted partition $\hat{V}$ may instantiate objects or points that were in fact missing, thus it is important to handle the missing data properly.

In Information Theory, the variation of information (VI) [Meilă, 2003] is a measure of the distance between two partitions of elements (or clusterings). For a given set of elements, the variation of information between two partitions $V$ and $\hat{V}$, where $N = \sum_i |V_i| = \sum_j |\hat{V}_j|$ is defined as:

$$VI(V, \hat{V}) = - \sum_{i,j} r_{ij} \left[ \log \frac{r_{ij}}{p_i} + \log \frac{r_{ij}}{q_j} \right]$$

(26)

where $r_{ij} = \frac{|V_i \cap \hat{V}_j|}{N}$, $p_i = \frac{|V_i|}{N}$ and $q_j = \frac{|\hat{V}_j|}{N}$. In our experiments we report the average variation of information of the scenes in the dataset.

The Rand index [Rand, 1971] is another measure of similarity between two data clusterings. This metric takes pairs of elements and evaluates whether they do or do not belong to the same subsets in the partitions $V$ and $\hat{V}$

$$RI = \frac{TP + TN}{TP + TN + FP + FN},$$

(27)

where TP are the true positives, TN the true negatives, FP the false positives and FN the false negatives. The Rand index takes on values between 0 and 1. We use instead the adjusted Rand index (ARI) [Hubert and Arabie, 1985], the corrected-for-chance version of the Rand index. It uses the expected similarity of all pair-wise comparisons between clusterings specified by a random model as a baseline to correct for assignments produced by chance. Unlike the Rand index, the adjusted Rand index can return negative values if the index is less than the expected value. In our experiments, we compute the average adjusted Rand index of the scenes in our dataset.

The segmentation accuracy (SA) is based on obtaining the maximum bipartite matching between $V$ and $\hat{V}$, and was used by Kosiorek et al. [2019] to evaluate the performance of CCAE. For each set $V_i$ in $V$ and set $\hat{V}_j$ in $\hat{V}$, there is an edge $w_{ij}$ with the weight being the number of common elements in both sets. Let $W(V, \hat{V})$ be the overall weight of the maximum matching between $V$ and $\hat{V}$. Then we define the average segmentation accuracy as:

$$SA = \frac{1}{N} \sum_{i=1}^{l} \frac{W(V_i, \hat{V}_i)}{W(V_i, \hat{V})},$$

(28)

where $l$ is the number of scenes. Notice that $W(V_i, \hat{V}_i)$ represents a perfect assignment of the ground truth, both the observed and missing subsets, and thus $W(V_i, \hat{V}_i) = N$.

There are some differences on how we compute the SA metric compared to Kosiorek et al. [2019]. First, they do not consider the missing points as part of their ground truth, but as we argued above this is necessary. They evaluate the segmentation accuracy in terms of the observed points in the ground truth, disregarding possible points that were missing in the ground truth but predicted as observed in $V$. Second, they average the segmentation accuracy across scenes as

$$SA = \frac{\sum_{i=1}^{l} W(V_i, \hat{V}_i)}{\sum_{i=1}^{l} W(V_i, \hat{V})}$$

(29)

For them, $W(V_i, \hat{V}_i) = M_i$, where $M_i$ is the number of points present in a scene. In our case, both averaging formulae are equivalent since our $W(V_i, \hat{V}_i)$ is the same across scenes.

**D  FAILURES OF ROTATION EQUIVARIANCE FOR SCAE**

We trained the SCAE model with digit “4” images from the training set of the MNIST dataset[^1] after they had been uniformly rotated by up to 360° and uniformly translated by up to 6 pixels on the x and y axes. Since we used a single class in the dataset we altered SCAE’s architecture to use only a single object capsule.

We repeated the training of SCAE multiple times for 8k epochs, and collected distinct sets of learned 11×11 parts that the digit “4” can be composed into (see Fig. 3). After wards, we evaluated PCAE’s ability to detect these parts in MNIST digit “4” images that had been rotated by multiples of $45^\circ$. Then, we measured the average inferred pose of each part at each of the different angles of rotations. Our results indicate that the PCAE model is not equivariant to rotations. This is apparent from Fig. 7, where the learned parts from part-sets 2 and 3 of Fig. 3 are inconsistently assigned to the regions of the digit-object, depending on the angle of rotation. We hypothesize that this phenomenon stems from the fact that PCAE seems to generate either parts that are characterized by an intrinsic symmetry –and thus their pose is ambiguous– (e.g. template 3 of column (a) in Fig. 3) or pairs of parts that are transformed versions of themselves, and thus can be used interchangeably (e.g. templates 1 and 3 of part-set 3 in Fig. 3). This leads to identifiability issues, where the object can be decomposed into its parts in numerous ways.

**E  DIFFERENT INITIALIZATIONS OF $\beta$**

In this section, we show the effect of varying the initial value of $\beta$ for the variational inference method with a Gaussian mixture prior [8] (GCM-GMM) and with a prior over

[^1]: http://yann.lecun.com/exdb/mnist
Figure 3: Each column corresponds to a part-set of learned templates parts of size 3, 4, 4 and 6 respectively.

permutation matrices (GCM-DS). We have tested 6 different values of $\beta$: 0.005, 0.01, 0.05, 0.1, 0.2, 0.5. In Tables 2, 3 and 4 we show the results for all metrics, methods and initial values of $\beta$ for $\sigma = 0$, $\sigma = 0.1$, and $\sigma = 0.25$ resp.

We can observe that no matter the initialization of $\beta$, GCM-DS is always better than CCAE and GCM-GMM. As we increase the initial $\beta$, GCM-DS performs better across all the metrics. We have found that the performance of GCM-DS and GCM-GMM degrades with $\beta > 0.1$.

We have conducted paired t-tests between CCAE and GCM-GMM, GCM-DS and RANSAC on the three clustering metrics for $\sigma = 0$ and initial $\beta = 0.05$. The differences between CCAE and GCM-DS are statistically significant with p-values less than $10^{-7}$, and between CCAE and RANSAC with p-values less than $10^{-28}$. For CCAE and GCM-GMM the differences are not statistically significant.

### Table 2: Different initializations of $\beta$. For SA, ARI and Scene Accuracy the higher the better. For VI the lower the better. Noise-free case.

| Model       | SA ↑ | ARI ↑ | VI ↓ | Sc. Acc. ↑ |
|-------------|------|-------|------|------------|
| CCAE        | 0.828 | 0.599 | 0.481 | 0.365      |
| GCM-DS $\beta = 0.005$ | 0.869 | 0.667 | 0.350 | 0.581      |
| GCM-DS $\beta = 0.01$ | 0.876 | 0.678 | 0.328 | 0.624      |
| GCM-DS $\beta = 0.05$ | 0.899 | 0.740 | 0.299 | 0.664      |
| GCM-DS $\beta = 0.1$ | **0.904** | **0.752** | 0.302 | 0.653      |
| GCM-DS $\beta = 0.2$ | 0.899 | 0.728 | 0.332 | 0.622      |
| GCM-DS $\beta = 0.5$ | 0.886 | 0.679 | 0.402 | 0.576      |
| GCM-GMM $\beta = 0.005$ | 0.823 | 0.449 | 0.592 | 0.402      |
| GCM-GMM $\beta = 0.01$ | 0.823 | 0.487 | 0.555 | 0.362      |
| GCM-GMM $\beta = 0.05$ | 0.753 | 0.586 | 0.478 | 0.179      |
| GCM-GMM $\beta = 0.1$ | 0.771 | 0.550 | 0.543 | 0.214      |
| GCM-GMM $\beta = 0.2$ | 0.764 | 0.513 | 0.613 | 0.199      |
| GCM-GMM $\beta = 0.5$ | 0.762 | 0.488 | 0.650 | 0.194      |

### Table 3: Different initializations of $\beta$. For SA, ARI and Scene Accuracy the higher the better. For VI the lower the better. Gaussian noise with $\sigma = 0.1$.

| Model       | SA ↑ | ARI ↑ | VI ↓ | Sc. Acc. ↑ |
|-------------|------|-------|------|------------|
| CCAE        | 0.754 | 0.484 | 0.689 | 0.138      |
| GCM-DS $\beta = 0.005$ | 0.840 | 0.608 | 0.451 | 0.518      |
| GCM-DS $\beta = 0.01$ | 0.859 | 0.644 | 0.389 | 0.559      |
| GCM-DS $\beta = 0.05$ | 0.883 | 0.699 | 0.359 | **0.603** |
| GCM-DS $\beta = 0.1$ | **0.888** | **0.715** | **0.352** | 0.601      |
| GCM-DS $\beta = 0.2$ | 0.874 | 0.682 | 0.406 | 0.544      |
| GCM-DS $\beta = 0.5$ | 0.872 | 0.659 | 0.443 | 0.515      |
| GCM-GMM $\beta = 0.005$ | 0.793 | 0.468 | 0.566 | 0.322      |
| GCM-GMM $\beta = 0.01$ | 0.800 | 0.497 | 0.547 | 0.318      |
| GCM-GMM $\beta = 0.05$ | 0.757 | 0.573 | 0.502 | 0.173      |
| GCM-GMM $\beta = 0.1$ | 0.768 | 0.521 | 0.595 | 0.204      |
| GCM-GMM $\beta = 0.2$ | 0.765 | 0.460 | 0.684 | 0.178      |
| GCM-GMM $\beta = 0.5$ | 0.753 | 0.403 | 0.780 | 0.140      |

### F COMPARISON ACROSS METHODS USING THE GROUND TRUTH MISSING INDICATORS

The results above include the missing objects in the creation of $V$, as described in supp. mat. C. Failing to recognize exactly which points in a scene are missing leads to a decrease in performance for all the metrics. However, Kosiorek et al. [2019] instead used the ground truth missing indicators for the objects in order to compute the segmentation accuracy of their method (see equation 29). If we use this strategy to all the models and metrics, we obtain Tables 5, 6 and 7. When we compare these results with the tables in the previous section we can see that this alternative leads to a clear improvement in the scores of all the methods, but with GCM-DS still performing better than CCAE or GCM-GMM.
Table 4: Different initializations of $\beta$. For SA, ARI and Scene Accuracy the higher the better. For VI the lower the better. Gaussian noise with $\sigma = 0.25$.

| Model     | SA up | ARI up | VI down | Sc. Acc. up |
|------------|-------|--------|---------|-------------|
| CCAE       | 0.623 | 0.248  | 0.988   | 0.033       |
| GCM-DS $\beta = 0.005$ | 0.771 | 0.475  | 0.669   | 0.338       |
| GCM-DS $\beta = 0.01$  | 0.781 | 0.486  | 0.652   | 0.362       |
| GCM-DS $\beta = 0.05$  | 0.785 | 0.498  | 0.659   | 0.377       |
| GCM-DS $\beta = 0.1$   | 0.779 | 0.476  | 0.699   | 0.351       |
| GCM-DS $\beta = 0.2$   | 0.768 | 0.470  | 0.708   | 0.291       |
| GCM-DS $\beta = 0.5$   | 0.766 | 0.435  | 0.752   | 0.272       |
| GCM-GMM $\beta = 0.005$ | 0.736 | 0.469  | 0.564   | 0.265       |
| GCM-GMM $\beta = 0.01$  | 0.730 | 0.467  | 0.581   | 0.221       |
| GCM-GMM $\beta = 0.05$  | 0.744 | 0.447  | 0.677   | 0.132       |
| GCM-GMM $\beta = 0.1$   | 0.735 | 0.387  | 0.801   | 0.102       |
| GCM-GMM $\beta = 0.2$   | 0.727 | 0.310  | 0.921   | 0.088       |
| GCM-GMM $\beta = 0.5$   | 0.717 | 0.242  | 1.036   | 0.064       |

Table 5: Different initializations of $\beta$ using the ground truth missing mask. For SA, ARI and Scene Accuracy the higher the better. For VI the lower the better. Noise-free case.

| Model     | SA up | ARI up | VI down | Sc. Acc. up |
|------------|-------|--------|---------|-------------|
| CCAE       | 0.950 | 0.897  | 0.157   | 0.736       |
| GCM-DS $\beta = 0.005$ | 0.985 | 0.967  | 0.052   | 0.915       |
| GCM-DS $\beta = 0.01$  | 0.989 | 0.973  | 0.042   | 0.941       |
| GCM-DS $\beta = 0.05$  | 0.971 | 0.938  | 0.095   | 0.886       |
| GCM-DS $\beta = 0.1$   | 0.966 | 0.929  | 0.108   | 0.860       |
| GCM-DS $\beta = 0.2$   | 0.966 | 0.930  | 0.104   | 0.854       |
| GCM-DS $\beta = 0.5$   | 0.958 | 0.912  | 0.132   | 0.825       |
| GCM-GMM $\beta = 0.005$ | 0.886 | 0.805  | 0.209   | 0.646       |
| GCM-GMM $\beta = 0.01$  | 0.905 | 0.830  | 0.191   | 0.683       |
| GCM-GMM $\beta = 0.05$  | 0.942 | 0.884  | 0.160   | 0.718       |
| GCM-GMM $\beta = 0.1$   | 0.937 | 0.879  | 0.179   | 0.657       |
| GCM-GMM $\beta = 0.2$   | 0.927 | 0.861  | 0.213   | 0.603       |
| GCM-GMM $\beta = 0.5$   | 0.925 | 0.858  | 0.216   | 0.585       |

G EXAMPLES OF CCAE AND GCM-DS INFERENCE FOR THE CONSTELLATIONS DATA

Figure [1] shows some reconstruction examples from CCAE and GCM-DS for the noise-free scenario. We show additional examples for the noisy cases in the supp. mat. [2] In columns (a) and (b) we can see that CCAE recovers the correct parts assignments but the object reconstruction is amiss. In (a) one of the squares is reconstructed as a triangle, while in (b) the assignment between the reconstruction and the ground truth is not exact. For GCM-DS, if the parts are assigned to the ground truth properly, and there is no noise, then the reconstruction of the object is perfect. In column (c) all methods work well. In column (d), CCAE fits the square correctly (green), but adds an additional red point. In this case GCM-DS actually overlays two squares on top of each other. Both methods fail badly on column (e). Note that CCAE is not guaranteed to reconstruct an existing object correctly (square or triangle in this case). In column (f) we can see that CCAE fits an irregular quadrilateral (blue) to the assigned points, while GCM-DS obtains the correct fit.

H NOISY CASES EXAMPLES

In Figures [5] and [6] we show several examples of objects generated from noisy templates with corruption levels of $\sigma = 0.1$ and $\sigma = 0.25$ resp. GCM-DS and RANSAC does not allow for deformable objects to try to fit the points exactly, contrary to CCAE. Both methods try to find the closest reconstruction of the noisy points in the image by selecting the geometrical shapes that are a best fit to those points. Nonetheless, both methods can determine that which parts belong together to form a given object, even when the matching is not perfect.
Figure 4: Reconstruction examples from CCAE and GCM-DS for noise-free data. The upper figures show the ground truth of the test images. The middle figures show the reconstruction and the capsule assignments (by colours) of CCAE. The lower figures show the reconstruction and the parts assignment of GCM-DS. Datapoints shown with a given colour are predicted to belong to the reconstructed object with the corresponding colour.

Figure 5: Reconstruction examples from CCAE, GCM-DS and RANSAC with Gaussian noise $\sigma = 0.1$. 
Figure 6: Reconstruction examples from CCAE, GCM-DS and RANSAC with Gaussian noise $\sigma = 0.25$.

| Ground truth | CCAE       | GCM-DS     | RANSAC        |
|--------------|------------|------------|---------------|
| (a)          | (b)        | (c)        | (d)           |
| 0°           | 45°        | 90°        | 135°          |
| 180°         | 225°       | 270°       | 315°          |

Figure 7: Average part-based reconstruction for different angles of rotation of the input scenes. Row (a) corresponds to reconstructions with the learned part-sets 2 and row (b) reconstructions with the learned part-sets 3 of Fig. 3.
Figure 8: Reconstruction examples with our Variational Inference (VI) algorithm and the RANSAC-type algorithm: (a) scene with 2 faces, (b) scene with 3 faces, (c) scene with 4 faces, (d) scene with 5 faces, and (e) 3 faces with partially occluded faces. All faces have been randomly selected and transformed.