On Contrastive Representations of Stochastic Processes

Emile Mathieu†∗, Adam Foster†∗, Yee Whye Teh†‡
{emile.mathieu, adam.foster, y.w.teh}@stats.ox.ac.uk
† Department of Statistics, University of Oxford, United Kingdom
‡ DeepMind, United Kingdom

Abstract

Learning representations of stochastic processes is an emerging problem in machine learning with applications from meta-learning to physical object models to time series. Typical methods rely on exact reconstruction of observations, but this approach breaks down as observations become high-dimensional or noise distributions become complex. To address this, we propose a unifying framework for learning contrastive representations of stochastic processes (CRESP) that does away with exact reconstruction. We dissect potential use cases for stochastic process representations, and propose methods that accommodate each. Empirically, we show that our methods are effective for learning representations of periodic functions, 3D objects and dynamical processes. Our methods tolerate noisy high-dimensional observations better than traditional approaches, and the learned representations transfer to a range of downstream tasks.

1 Introduction

The stochastic process (Doob, 1953; Parzen, 1999) is a powerful mathematical abstraction used in biology (Bressloff, 2014), chemistry (van Kampen, 1992), physics (Jacobs, 2010), finance (Steele, 2012) and other fields. The simplest incarnation of a stochastic process is a random function $\mathbb{R} \rightarrow \mathbb{R}$, such as a Gaussian Process (MacKay, 2003), that can be used to describe a real-valued signal indexed by time or space. Extending to random functions from $\mathbb{R}$ to another space, stochastic processes can model time-dependent phenomena like queuing (Grimmett and Stirzaker, 2020) and diffusion (Ito et al., 2012). In meta-learning, the stochastic process can be used to describe few-shot learning tasks—mappings from images to class labels (Vinyals et al., 2016)—and image completion tasks—mappings from pixel locations to RGB values (Garnelo et al., 2018a). In computer vision, 2D views of 3D objects can be seen as observations of a stochastic process indexed by the space of possible viewpoints (Eslami et al., 2018; Mildenhall et al., 2020). Videos can be seen as samples from a time-indexed stochastic process with 2D image observations (Zelnik-Manor and Irani, 2001).

Table 1: Example stochastic processes with covariate space $\mathcal{X}$ and observation space $\mathcal{Y}$.

| $\mathcal{X}$ | $\mathcal{Y}$ | Illustration |
|-------------|-------------|-------------|
| $\mathbb{R}$ | $\mathbb{R}$ |             |
| $\mathbb{Z}^2$ | $\mathbb{R}^3$ | ![Image](image1.png) |
| $SE(3)$ | Images | ![Image](image2.png) |
| $\mathbb{R}$ | Images | ![Image](image3.png) |

*Equal contribution. Author ordering determined by coin flip.
Machine learning algorithms that operate on data generated from stochastic processes are therefore in high demand. We assume that we have access to only a small set of covariate–observation pairs \( \{(x_i, y_i)\}_{i=1}^C \) from different realizations of the underlying stochastic process. This might correspond to a few views of a 3D object, or a few snapshots of a dynamical system evolving in time. Whilst conventional deep learning thrives when there is a large quantity of i.i.d. data available (Lake et al., 2017), allowing us to learn a fresh model for each realization of the stochastic process, when the context size is small it makes sense to use data from other realizations to build up prior knowledge about the domain which can aid learning on new realizations (Reed et al., 2018; Garnelo et al., 2018a).

Traditional methods for learning from stochastic processes, including the Gaussian Process family (MacKay, 2003; Rasmussen, 2003) and the Neural Process family (Garnelo et al., 2018a,b; Eslami et al., 2018), learn to reconstruct a realization of the process from a given context. That is, given a context set \( \{(x_i, y_i)\}_{i=1}^C \), these methods provide a predictive distribution \( q(y^*|x^*, (x_i, y_i)_{i=1}^C) \) for the observation that would be obtained from this realization of the process at any target covariate \( x^* \). These methods use an explicit likelihood for \( q \), typically a Gaussian distribution. Whilst this can work well when \( y^* \) is low-dimensional and unimodal, it is a restrictive assumption. For example, when \( p(y^*|x^*, (x_i, y_i)_{i=1}^C) \) samples a high-dimensional image with colour distortion, traditional methods must learn to perform conditional image generation, a notably challenging task (van den Oord et al., 2016; Chrysos and Panagakis, 2021).

In this paper, we do away with the explicit likelihood requirement for learning from stochastic processes. Our first insight is that, for a range of important downstream tasks, exact reconstruction is not necessary to obtain good performance. Indeed, whilst \( y \) may be high-dimensional, the downstream target label or feature \( \ell \) may be simpler. We consider two distinct settings for \( \ell \in L \). The first is a downstream task that depends on the covariate \( x \in \mathcal{X} \), formally a second process \( \mathcal{X} \rightarrow L \) that covaries with the first. For example, \( \ell(x) \) could represent a class label or annotation for each video frame. The second is a downstream task that depends on the entire process realization, such as a single label for a 3D object. In both cases, we assume that we have limited labelled data, so we are in a semi-supervised setting (Zhu, 2005).

To solve problems of this nature, we propose a general framework for Contrastive Representations of Stochastic Processes (CRESP). At its core, CRESP consists of a flexible encoder network architecture for contexts \( \{(x_i, y_i)\}_{i=1}^C \) that unifies transformer encoders of sets (Vaswani et al., 2017; Parmar et al., 2018) with convolutional encoders (LeCun et al., 1989) for observations that are images. To account for the two kinds of downstream task that may of interest, we propose a targeted variant of CRESP that learns a representations depending on the context and a target covariate \( x^* \), and an untargeted variant that learns one representation of the context. To train our encoder, we take our inspiration from recent advances in contrastive learning (Bachman et al., 2019; Chen et al., 2020) which have so far focused on representations of single observations, typically images. We define a variant of the InfoNCE objective (van den Oord et al., 2018) for contexts sampled from stochastic processes, allowing us to avoid training objectives that necessitate exact reconstruction. Rather than attempting pixel-perfect reconstruction, then, CRESP solves a self-supervised task in representation space.

The CRESP framework unifies and extends recent work, building on function contrastive learning (FCLR) (Gondal et al., 2021) by considering targeted as well as untargeted representations and using self-attention in place of mean-pool aggregation. We develop on noise contrastive meta-learning (Ton et al., 2021) by focusing on downstream tasks rather than multi-modal reconstruction, replacing conventional mean embeddings with neural representations and using a simpler training objective.

We evaluate CRESP on sinusoidal functions, 3D objects, and dynamical processes with high-dimensional observations. We empirically show that our methods can handle high-dimensional observations with naturalistic distortion, unlike explicit likelihood methods, and our representations lead to improved data efficiency compared to supervised learning. CRESP performs well on a range of downstream tasks, both targeted and untargeted, outperforming existing methods across the board. Our code is publicly available at github.com/ae-foster/creep.

2 Background

Stochastic Processes Stochastic Processes (SPs) are probabilistic objects defined as a family of random variables indexed by a covariate space \( \mathcal{X} \). For each \( x \in \mathcal{X} \), there is a corresponding random variable \( y|x \in \mathcal{Y} \) living in the observation space. For example, \( x \) might represent a pose and \( y \) a...
photograph of an underlying object take from pose $x$ (see Tab. 1). We assume that there is a realization $F$ sampled from a prior $p(F)$, and that the random variable $y|x$ is a sample from $p(y|F, x)$. Thus, for each $x \in \mathcal{X}$, $F$ defines a conditional distribution $p(y|F, x)$. We assume that observations are independent conditional on the realization $F$. Hence, the joint distribution of multiple observations at locations $x_{1:C}$ from one realization of the stochastic process with prior $p(F)$ is

$$p(y_{1:C}|x_{1:C}) = \int p(F) \prod_{i=1}^{C} p(y_i|F, x_i) \, dF. \quad (1)$$

Conversely, assuming exchangeability and consistency, the Kolmogorov Extension Theorem guarantees that the joint distribution takes the form (1) (Øksendal, 2003; Garnelo et al., 2018b).

**Neural Processes** The neural process (NP) and conditional neural process (CNP) are closely related models that learn representations of data generated by a stochastic process (SP)\(^1\). The training objective for the NP and CNP is inspired by the posterior predictive distribution for SPs: given a context $\{(x_i, y_i)\}_{i=1}^{C}$, the observation at the target covariate $x^*$ has the distribution

$$p(y^*|x^*, (x_i, y_i)_{i=1}^{C}) = \int p(F|(x_i, y_i)_{i=1}^{C}) p(y^*|F, x^*) \, dF. \quad (2)$$

The CNP learns a neural approximation $q(y^*|x^*, (x_i, y_i)_{i=1}^{C}) = p(y^*|c, x^*)$ to equation (2), where $c = \sum g_{\text{enc}}(x_i, y_i)$ is a permutation-invariant context representation and $p(\cdot|c, x)$ is an explicit likelihood. Conventionally, $p$ is a Gaussian with mean and variance given by a neural network applied to $c, x$. The CNP model is then trained by maximum likelihood. In the NP model, an additional latent variable $u$ is used to represent uncertainty in the process realization, more closely mimicking (2).

A significant limitation, common to the NP family, is the reliance on an explicit likelihood. Indeed, requiring $\log q(y^*|x^*, (x_i, y_i)_{i=1}^{C})$ to be large requires the model to successfully reconstruct $y^*$ based on the context, similarly to the reconstruction term in variational autoencoders (Kingma and Welling, 2014). Furthermore, the NP objective cannot be increased by extracting additional features from the context unless the predictive part of the model, the part mapping from $(c, x)$ to a mean and variance, is powerful enough to use them.

**Contrastive Learning and Likelihood-free Inference** Contrastive learning has enjoyed recent success in learning representations of high-dimensional data (van den Oord et al., 2018; Bachman et al., 2019; He et al., 2020; Chen et al., 2020), and is deeply connected to likelihood-free inference (Gutmann and Hyvärinen, 2010; van den Oord et al., 2018; Durkan et al., 2020). In its simplest form, suppose we have a distribution $p(y, y')$, for example $y$ and $y'$ could be differently augmented versions of the same image. Rather than fitting a model to predict $y'$ given $y$, which would necessitate high-dimensional reconstruction, contrastive learning methods can be seen as learning the likelihood-ratio $r(y'|y) = p(y'|y)/p(y')$. To achieve this, contrastive methods encode $y, y'$ to determinstic embeddings $z, z'$, and consider additional ‘negative’ samples $z'_1, \ldots, z'_{K-1}$ which are the embeddings of other independent samples of $p(y')$ (for example, taken from the same training batch as $y, y'$). The InfoNCE training loss (van den Oord et al., 2018) is then given by

$$L_{\text{InfoNCE}}^{\text{InfoNCE}} = -\mathbb{E} \left[ \log \frac{s(z, z')} {s(z, z') + \sum_k s(z, z'_k)} \right] - \log K. \quad (3)$$

for similarity score $s > 0$. Informally, InfoNCE is minimized when $z$ is more similar to $z'$—the ‘positive’ sample—than it is to the negative samples $z'_1, \ldots, z'_{K-1}$ that are independent of $z$. Formally, Eq. (3) is the multi-class cross-entropy loss arising from classifying the positive sample correctly. It can be shown that the optimal similarity score $s$ is proportional to the true likelihood ratio $r$ (van den Oord et al., 2018; Durkan et al., 2020). A key feature of InfoNCE is that learns about the predictive density $p(y'|y)$ indirectly, rather than by attempting direct reconstruction.

**3 Method**

Given data $\{(x_i, y_i)\}_{i=1}^{C}$ sampled from a realization of a stochastic process, one potential task is to make predictions about how observations will look at another $x^*$—this is the task that is solved

---

\(^1\)Note that neither the neural process (NP) nor the conditional neural process (CNP) is formally stochastic processes (SPs) as they do not satisfy the consistency property.
by the NP family. However, in practice the inference that we want to make from the context data could be different. For instance, rather than predicting a high-dimensional observation at a future time or another location, we could be interested in inferring some low-dimensional feature of that observation—whether two objects have collided at that point in time, or if an object can be seen from a given pose. Even more simply, we might be solely interested in classifying the context, deciding what object is being viewed, for example. Such downstream tasks provide a justification for learning representations of stochastic processes that are not designed to facilitate predictive reconstruction of the process at some \( x^* \). We break downstream tasks for stochastic processes into two categories.

**Targeted and untargeted tasks** A targeted task is one in which the label \( \ell \) depends on \( x \), as well as on the underlying realization of the process \( F \). This means that we augment the stochastic process of Sec. 2 by introducing a conditional distribution \( p(\ell | F, x) \). The goal is to infer the predictive density \( p \left( \ell^* | x^*, (x_i, y_i)_{i=1}^C \right) \). An untargeted task associates one label \( y \) with the entire realization \( F \) via a conditional distribution \( p(\ell | F) \). The aim is to infer the conditional distribution \( p \left( \ell | (x_i, y_i)_{i=1}^C \right) \).

**Representation learning** We assume a semi-supervised (Zhu, 2005) setting, with unlabelled contexts for a large number of realizations of the stochastic process, but few labelled realizations. To make best use of this unlabelled data, we learn representations of contexts, and then fit a downstream model on top of fixed representations. In the stochastic process context, we have the requirement for a representation learning approach that can transfer to both targeted and untargeted downstream tasks. We therefore propose a general framework to learn contrastive representations of stochastic processes (CR\(_E\)SP). Our framework consists of a flexible encoder architecture that processes the context \( \{(x_i, y_i)_{i=1}^C\} \) and a \( x^* \)-dependent head for targeted tasks. This means CR\(_E\)SP can encode data from stochastic processes in two ways: 1) a targeted representation that depends on the context \( \{(x_i, y_i)_{i=1}^C\} \) and some target location \( x^* \), being a predictive representation for the process at this covariate, suitable for targeted downstream tasks; or 2) a single untargeted representation of the context \( \{(x_i, y_i)_{i=1}^C\} \) that summarizes the entire realization \( F \), suitable for untargeted tasks.

### 3.1 Training

We have unlabelled data \( \{(x_i, y_i)_{i=1}^C\} \) that is generated from the stochastic process (1), but unlike the Neural Process family, we do not wish to place an explicit likelihood on the observation space \( \mathcal{Y} \). Instead, we adopt a contrastive self-supervised learning approach (van den Oord et al., 2018; Bachman et al., 2019; Chen et al., 2020) to training. Whilst we adopt subtly different training schemes for the targeted and untargeted cases, the broad strokes are the same. Given a mini-batch of contexts samples from different realizations of the underlying stochastic process, create predictive and ground truth representations from each. We then use representations from other observations in the same mini-batch as negative samples in an InfoNCE-style (van den Oord et al., 2018) training loss. This can be seen as learning an unnormalized likelihood ratio. Taking gradients through this loss function allows us to update our CR\(_E\)SP network by gradient descent (Robbins and Monro, 1951). We now describe the key differences between the targeted and untargeted cases.

**Targeted CR\(_E\)SP** This setting is closer in spirit to the CNP. Rather than making a direct estimate of the posterior predictive \( p(y^* | x^*, (x_i, y_i)_{i=1}^C) \) for each value of \( x^* \), we instead attempt to learn the following likelihood-ratio

\[
r(y^* | x^*, (x_i, y_i)_{i=1}^C) = \frac{p(y^* | x^*, (x_i, y_i)_{i=1}^C)}{p(y^*)}
\]

where \( p(y^*) \) is the marginal distribution of observations from different realizations of the process and different covariates. To estimate this ratio with contrastive learning, we first randomly separate the context \( \{(x_i, y_i)_{i=1}^C\} \) into a training context \( \{(x_i, y_i)_{i=1}^{C-1}\} \) and a target \( \{x^*, y^*\} \). We then process \( \{(x_i, y_i)_{i=1}^{C-1}, x^*\} \) and \( y^* \) separately with an encoder network, yielding respectively a predictive representation \( \hat{c} \) and a target representation \( c^* \). This encoder network is described in detail in the following Sec. 3.2. These representations are further projected into a low-dimensional space \( \mathcal{Z} \) using a shallow MLP, referred as Projection head on Fig. 1, giving \( \hat{z} \) and \( z^* \). We create negative samples \( z'_1, \ldots, z'_{K-1} \), defined as samples coming from other realisations of the stochastic process, from representations obtained from the other observations of the batch. This means that we are
We begin by applying separate networks to the covariate and observation preprocessing. For covariates that are angles, we use Random Fourier Features (Rahimi and Recht, 2008). For the untargeted version, we simply require a representation of each context; $x^*$ no longer plays a role. The key idea here is that, without estimating a likelihood ratio in $Y$ space, we can use contrastive methods to encourage two representations formed from the same realization of the stochastic process to be more similar than representations formed from different realizations. To achieve this, we randomly split the whole context $\{(x_i, y_i)\}_{i=1}^C$ into two training contexts $\{(x_i, y_i)\}_{i=1}^{C_1}$ and $\{(x_i', y_i')\}_{i=1}^{C_2}$, with an equal split $C_1 = C_2 = C/2$ being our standard approach. We encode both with an encoder network, giving two representations $c, c'$, further projected into lower-dimensional representations $z, z'$ as in the targeted case. We also take $K - 1$ negative samples $z_1', ..., z_K'$ using other representations in the same training mini-batch.

$$
L_K^{\text{untargeted}} = -\mathbb{E} \left[ \log \frac{s(z, z')} {s(z, z') + \sum_k s(z, z_k')} \right] - \log K.
$$

This training method is closer in spirit to SimCLR (Chen et al., 2020), but here we include attention and aggregation steps to combine the distinct elements of the context.

### 3.2 Representation

The core of our architecture is a flexible encoder of a context $\{(x_i, y_i)\}_{i=1}^C$, as illustrated in Fig. 1.

#### Covariate and observation preprocessing

We begin by applying separate networks to the covariate $g_{\text{cov}}(x)$ and observation $g_{\text{obs}}(y)$ of each pair $(x, y)$ of the context. When observations $y$ are high-dimensional, such as images, this step is crucial because we can use existing well-developed vision architectures such as CNNs (LeCun et al., 1989) and ResNets (He et al., 2016) to extract image features. For covariates that are angles, we use Random Fourier Features (Rahimi and Recht, 2008).

#### Pair encoding

We then combine separate encodings of $x, y$ into a single representation for the pair. We concatenate the individual representations and pass them through a simple neural network, i.e. $g_{\text{enc}}(x, y) := g_{\text{enc}}([g_{\text{cov}}(x), g_{\text{obs}}(y)])$. In practice, we found that a gated architecture works well.

---

**Figure 1:** CRReSP architecture with contrastive loss. [Left] Targeted, [Right] Untargeted.
Attention & Aggregation  We apply self-attention (Vaswani et al., 2017) over the $C$ different encodings of the context $\{g_{enc}(x_i, y_i)\}_{i=1}^C$. We found transformer attention (Parmar et al., 2018) to perform best. We then pool the $C$ reweighted representations to yield a single representation $c = \sum_i g_{enc}(x_i, y_i)$. For targeted representations, we concatenate $c$ and $x^\star$, then pass them through a target head yielding $\hat{c} = h(x^\star, c)$, the predictive representation at $x^\star$.

3.3 Transfer to downstream tasks

We have outlined the unsupervised part of CRE$\text{SP}$—a way to learn a representation of a context sampled from a stochastic process without explicit reconstruction. We now return to our core motivation for such representations, which is to use them to solve a downstream task, either targeted or untargeted. This will be particularly useful in a semi-supervised setting, in which labelled data for the downstream task is limited compared to the unlabelled data used for unsupervised training of the CRE$\text{SP}$ encoder. Our general approach to both targeted and untargeted downstream tasks is to fit linear models on the context representations of the labelled training set, and use these to predict labels on new, unseen realizations of the stochastic process, following the precedent in contrastive learning (Hjelm et al., 2019; Kolesnikov et al., 2019). We do not use fine-tuning.

For targeted tasks, we assume that we have labelled data from $n$ realizations of the stochastic process that takes the form of an unlabelled context $\{x_i, y_i\}_{i=1}^n$ along with a labelled pair $\{(x_i^\star, \ell_i^\star)\}$ for each $j = 1, \ldots, n$. Here, $\ell_i^\star$ is the label at location $x^\star$ for realization $j$. To fit a downstream classifier using CRESP representations with this labelled dataset, we first process each $\{x_{ij}, y_{ij}\}_{i=1}^C$ along with the covariate $x^\star$ through a targeted CRE$\text{SP}$ encoder to produce $\hat{c}_j$. This allows us to form a training dataset $\{(\hat{c}_j, \ell_j^\star)\}_{j=1}^n$ of representation, label pairs which we then use to train our downstream classifier. At test time, given a test context $\{x^\star_i, y^\star_i\}_{i=1}^C$, we can predict the unknown label at any $x^\star$ by forming the corresponding targeted representation with the CRE$\text{SP}$ network, and then feeding this into the linear classifier. This is akin to zero-shot learning (Xian et al., 2018).

For untargeted tasks, the downstream model is simpler. Given labelled data consisting of contexts $\{x_{ij}, y_{ij}\}_{i=1}^C$ with label $\ell_i^\star$ for $j = 1, \ldots, n$, we can use the untargeted CRE$\text{SP}$ encoder to produce a training dataset $\{(c_j, \ell_j)\}_{j=1}^n$ as before. Actually, targeted CRE$\text{SP}$ can also be used to obtain untargeted representations $c_j$—without applying the target head. We then use this to train the linear classifier. At test time, we predict labels for contexts from new, unseen realizations of the stochastic process.

4 Related work

Neural process family  Neural Processes (Garnelo et al., 2018b) and Conditional Neural Processes (Eslami et al., 2018; Garnelo et al., 2018a) are closely related methods that create a representation of an stochastic process realization by aggregating representations of a context. Unlike CRE$\text{SP}$, NPs are generative models that uses an explicit likelihood, generally a fully factorized Gaussian, to estimate the posterior predictive distribution. Attentive (Conditional) Neural Processes (Kim et al., 2019, (A)CNP) introduced both self-attention and cross-attention into the NP family. The primary distinction between this family and CRE$\text{SP}$ is the explicit likelihood that is used for reconstruction. As the most comparable method to CRE$\text{SP}$, we focus on the (A)CNP in the experiments.

SimCLR family  Recent popular methods in contrastive learning (van den Oord et al., 2018; Bachman et al., 2019; Tian et al., 2020; Chen et al., 2020) create neural representations of single objects, typically images, that are approximately invariant to a range of transformations such as random colour distortion. Like CRE$\text{SP}$, many of these approaches use the InfoNCE objective to train encoders. What distinguishes CRE$\text{SP}$ from conventional contrastive learning methods is that it provides representations of realizations of stochastic processes, rather than of individual images. Thus, standard contrastive learning solves a strictly less general problem than CRE$\text{SP}$ in which the covariate $x$ is absent. Standard contrastive encoders do not aggregate multiple covariate-observation pairs of a context, although simpler feature averaging (Foster et al., 2020) has been applied successfully.

Function contrastive learning  In their recent paper, Gondal et al. (2021) considered function contrastive learning (FCLR) which uses a self-supervised objective to learn representations of functions. FCLR fits naturally into the CRE$\text{SP}$ framework as an untargeted approach that uses
mean-pooling in place of our attention aggregation. Conceptually, then, FCLR does not take account of targeted tasks, nor does it propose a method for targeted representation learning.

**Noise contrastive meta-learning** Ton et al. (2021) proposed an approach for conditional density estimation in meta-learning, motivated by multi-modal reconstruction. Like targeted CRESP, their method targets the unnormalized likelihood ratio (4). They use a noise contrastive (Gutmann and Hyvärinen, 2010) training objective with an explicitly defined ‘fake’ distribution that is different from the CRESP training objective. Their primary method, MetaCDE, uses conditional mean embeddings to aggregate representations, unlike our attentive aggregation. This means that, when using it as a baseline within our framework, MetaCDE does not form a fixed-dimensional representation of contexts, and so cannot be applied to untargeted tasks. They also proposed MetaNN, a purely neural version of their main approach.

## 5 Experiments

We consider three different stochastic processes and downstream tasks which possess high-dimensional observations or complex noise distributions: 1) inferring parameters of periodic functions, 2) classifying 3D objects and 3) predicting collisions in a dynamical process. We compare several models summarized in Tab. 2 to learn representations of these stochastic processes. All models share the same core encoder architecture. Please refer to Sec. D for full experimental details.

| Criteria        | CNP | ACNP | FCLR | MetaCDE | Targeted CRESP | Untargeted CRESP |
|-----------------|-----|------|------|---------|----------------|-------------------|
| Targeted        | No  | No   | No   | Yes     | Yes            | No                |
| Reconstruction  | Yes | Yes  | No   | No      | No             | No                |
| Attention       | No  | Yes  | No   | Yes     | Yes            | Yes               |

### 5.1 Sinusoids

We first aim to demonstrate that reconstruction-based methods like CNPs cannot cope well with a bi-modal noise process since their Gaussian likelihood assumption renders them misspecified. We focus on a synthetic dataset of sinusoidal functions with both the observations and the covariates living in \( \mathbb{R} \), i.e. \( \mathcal{X} = \mathbb{R} \) and \( \mathcal{Y} = \mathbb{R} \). We sample one dimensional functions \( F \sim p(F) \) such that \( F(x) = \alpha \sin(2\pi/T \cdot x + \phi) \) with random amplitude \( \alpha \sim \mathcal{U}([0.5, 2.0]) \), phase \( \phi \sim \mathcal{U}([0, \pi]) \) and period \( T = 8 \). We break the uni-modality by assuming a bi-modal likelihood: \( p(y|F, x) = 0.5 \delta_{F(x)}(y) + 0.5 \delta_{F(x)+\pi}(y) \) (see Fig. 2a). Context points \( x \in \mathcal{X} \) are uniformly sampled in \([-5, 5]\).

We consider the *untargeted* downstream task of recovering the functions parameters \( \ell = \{\alpha, \phi\} \), and consequently put to the test our untargeted CRESP model along with FCLR and ACNP. We train all models for 200 epochs, varying the distance between modes and the number of training context points. We observe from Fig. 2b that for high intermodal distance, the ACNP is unable to accurately

Figure 2: We use CRESP along with ACNP and FCLR to recover sinusoid parameters with a bi-modal likelihood. In each setting, we used 20 test views to form representations of the entire training set and fitted a linear classifier to predict the function parameters. Encoders and decoder are MLPs. (a) Visualization of conditional likelihood \( p(y|F, x) \). (b) Shaded areas represent 95% confidence interval calculated using 6 separately trained networks. We use the shorthand U = untargeted. In (b) we used 10 training views and in (c) the distance between the modes is set to 2.
Figure 4: We compare CRESP with various baseline methods. In each case, we use 10 test views to form representations of the entire training set and fitted a linear classifier to predict ShapeNet object labels. Encoder networks were lightweight CNNs. In (a) we used 3 training views, in (b) we used distortion strength 1. We present the test accuracy ±1 s.e. and we use the shorthand U = untargeted, T = targeted in figure legends.

recover the true parameters as opposed to CRESP, which is more robust to this bi-modal noise even for distant modes. Additionally, we see in Fig. 2c that self-attention is crucial to accurately recover the sinusoids parameters, as the MSE is several order of magnitude lower for CRESP than for FCLR. We also see that CRESP is able to utilize a larger context better than ACNP.

5.2 ShapeNet

We apply CRESP to ShapeNet (Chang et al., 2015), a standard dataset in the field of 3D object representations. Each 3D object can be seen as a realization of a stochastic process with covariates $x$ representing viewpoints. We sample random viewpoints involving both orientation and proximity to the object, with observations $y$ being $64 \times 64$ images taken from that point. We also apply randomized colour distortion as a noise process on the 2D images (see Fig. 3). As the likelihood of this noise process is not known in closed from, this should present a particular challenge to explicit likelihood driven models. The downstream task for ShapeNet is a 13-way object classification which associates a single label with each realization—an untargeted task.

CRESP outperforms reconstructive models Since the CNP learns by exact reconstruction of observations, we would expect it to struggle with high-dimensional image observations, and particularly suffer as we introduce colour distortion, which is a highly non-Gaussian noise process. To verify this, we trained CNP and ACNP models, along with an attentive untargeted CRESP model which we would expect to perform well on this task. We used the same CNN observation processing network for each method, and an additional CNN decoder for the CNP and ACNP. Fig. 4a shows that CRESP significantly outperforms both the CNP and ACNP, with reconstructive methods faring worse as the level of colour distortion is increased; CRESP actually benefits from mild distortion.

CRESP outperforms previous contrastive methods We next compare different contrastive approaches along two axes: targeted vs untargeted, and attentive vs pool aggregation. This allows a comparison with FCLR (Gondal et al., 2021), which is an untargeted pool-based method. Fig. 4b shows that no contrastive approach performs as badly as the reconstructive methods. Untargeted CRESP performs best, while the targeted method does less well on this untargeted downstream task. With our CNN encoders and a matched architecture for a fair comparison, FCLR does about as well as attentive targeted CRESP and worse than the untargeted counterpart. To further examine the benefits of the attention mechanism used in CRESP, we vary the number of views used during training, focusing on untargeted methods. Fig. 4c shows that as we increase the number of training views, the attentive method outperforms the non-attentive FCLR by an increasing margin. This indicates that careful aggregation and weighting of different views of each object is essential for learning the best representations. The degradation in the performance of FCLR as more training
views are used is likely due to a weaker training signal for the encoder as the self-supervised task becomes easier, this phenomenon also explains why CRESP slightly decreases in performance from 6 to 12 training views.

**CRESP benefits from improved label efficiency**  We compare CRESP with semi-supervised learning that does not use any pre-training, but instead trains the entire architecture on the labelled dataset. In Fig. 5a we see that pre-training with CRESP can outperform supervised learning on the same fixed dataset at every label fraction including 100%. Another axis of variation in the stochastic process setting is the number C of views aggregated at test time. In Fig. 5b, we see that performance increases across the board as we make more views available to form test representations, but that CRESP performs best in all cases.

Figure 5: CRESP for semi-supervised learning. We re-trained the final linear classifiers with different quantities of labelled data and number of test views, supervised learning trained the entire encoder architecture on the same labelled datasets. (a) We used 10 test views, (b) We used 100% of labels. Other settings were as in Fig. 4.

### 5.3 Snooker dynamical process over images

We now focus on the setting where downstream tasks depend on the covariate \( x^* \), i.e. targeted downstream tasks. In particular, we consider a dynamical system that renders 2D images of two objects with constant velocities and evolving through time as illustrated in Fig. 6a. The objects are constrained in a 1 \( \times \) 1 box and collisions are assumed to result in a perfect reflection. The observation space \( \mathcal{Y} \) is consequently the space of \( 28 \times 28 \) RGB images, whilst the covariate space is \( \mathbb{R} \), representing time. We consider the downstream task of predicting whether the two objects are overlapping at a given time \( x^* = t \) or not. This experiment aims to reproduce, in a stripped-down manner, the real world problem of collision detection. Even though the object’s position can be expressed in closed-form, it is non trivial to predict the 2D image at a specific time given a collection of snapshots. We expect targeted CRESP to be particularly well-suited for such a task since the model is learning to form and match a targeted representation to the representation of the ground truth observation thorough the unsupervised task.

CRESP outperforms reconstructive and previous contrastive methods  Alongside targeted CRESP, we consider the CNP, FCLR and MetaCDE models. They are trained for 200 epochs, with contexts of 5 randomly sampled pairs \( \{y_i = F(x_i), x_i \sim U([0, 1])\} \). The encoder is a ResNet18 (He et al., 2016). We found that self-attention did not seem to help any method for this task, so we report un-attentive models. Both CNP and FCLR learn untargeted representations during the unsupervised task. We thus feed the downstream linear classifier with the concatenation \( \{c, x^*\} \).

Conversely, targeted CRESP and MetaCDE directly produce a targeted representation \( \hat{c} = h(x^*, c) \) (see Sec. 3.1). The downstream classifier can simply rely on \( \hat{c} \) to predict the overlap label \( \ell^* \). We
consequently expect such a targeted representation \( \hat{c} \) to be better correlated with the downstream label than untargeted representations \( c \).

We observe from Tab. 3 that targeted CRE:SP significantly outperforms both likelihood-based and previous contrastive methods, though MetaCDE outperforms both untargeted methods (CNP and FCLR). This highlights the need for the targeted contrastive loss from Eq. (5) along with a flexible target head \( h \) to learn targeted representations. Additionally, we observe that in the absence of a noise process, CNP performs as well as FCLR. We further investigate the quality of the learned targeted representations. To do so, given a fixed context we make an overlap prediction at different points in time as shown in Fig. 6b. We observe that targeted CRE:SP has successfully learned to smoothly predict the overlap label, but also to be uncertain when the overlap is ambiguous. Thus CRE:SP can successfully interpolate and extrapolate the semantic feature of interest (overlap) without reconstruction.

Table 3: We examine how well learned representations can predict whether the two snooker balls overlap at randomly sampled test times. 95% confidence intervals were computed over 6 runs.

| Method     | Accuracy (%) |
|------------|--------------|
| CNP        | 85.3±0.5     |
| FCLR       | 85.6±0.3     |
| Targeted CRE:SP | 96.8±0.1   |
| MetaCDE    | 87.7±0.3     |

6 Discussion

Limitations Our method directly learns representations from stochastic processes, without performing reconstruction on the observations, thus if one requires prediction in the observation space \( \mathcal{Y} \) then our method cannot be directly applied. Whilst our method is tailor made for a setting of limited labelled data, we require access to a large quantity of unlabelled data to train our encoder network.

In this work, we do not place uncertainty over context representations. Learning stochastic embeddings would have the primary benefit of producing correlated predictions at two or more covariates, similarly to NPs. As there is no trivial nor unique way to extend the InfoNCE loss to deal with distributions (e.g. Wu and Goodman, 2020), we leave such an extension of our method to future work.

Future applications One potential use of CRE:SP is to generate representations that can be used for reinforcement learning, following the approach of Eslami et al. (2018). One of the key differences between real environments and toy environments is the presence of high-dimensional observations with naturalistic noise. This is a case where the contrastive approach can bring an edge because naturalistic noise significantly damages explicit likelihood methods, but CRE:SP continues to perform well with more distortion.

Conclusion In this work, we introduced a framework for learning contrastive representation of stochastic processes (CRE:SP). We proposed two variants of our method specifically designed to effectively tackle targeted and untargeted downstream tasks. By doing away with exact reconstruction, CRE:SP directly works in the representation space, bypassing any challenge due to high dimensional and multimodal data reconstruction. We empirically demonstrated that our methods are effective for dealing with multi-modal and naturalistic noise processes, and outperform previous contrastive methods for this domain on a range of downstream tasks.

Acknowledgments

We would like to thank Yann Dubois and Jef Ton for valuable discussions. We also thank Hyunjik Kim, Neil Band and Lewis Smith for providing feedback on earlier versions of the paper. EM research leading to these results received funding from the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007- 2013) ERC grant agreement no. 617071 and he acknowledges Microsoft Research and EPSRC for funding EM’s studentship. AF gratefully acknowledges funding from EPSRC grant no. EP/N509711/1.


References

Ba, J. L., Kiros, J. R., and Hinton, G. E. (2016). Layer normalization. arXiv preprint arXiv:1607.06450.

Bachman, P., Hjelm, R. D., and Buchwalter, W. (2019). Learning representations by maximizing mutual information across views. In Advances in Neural Information Processing Systems, pages 15535–15545.

Bressloff, P. C. (2014). Stochastic processes in cell biology, volume 41. Springer.

Chang, A. X., Funkhouser, T., Guibas, L., Hanrahan, P., Huang, Q., Li, Z., Savarese, S., Savva, M., Song, S., Su, H., Xiao, J., Yi, L., and Yu, F. (2015). ShapeNet: An Information-Rich 3D Model Repository. arXiv:1512.03012 [cs].

Chen, T., Kornblith, S., Norouzi, M., and Hinton, G. (2020). A simple framework for contrastive learning of visual representations. In III, H. D. and Singh, A., editors, Proceedings of the 37th International Conference on Machine Learning, volume 119 of Proceedings of Machine Learning Research, pages 1597–1607. PMLR.

Cho, K., van Merrienboer, B., Gülçehre, Ç., Bahdanau, D., Bougares, F., Schwenk, H., and Bengio, Y. (2014). Learning phrase representations using RNN encoder-decoder for statistical machine translation. In Moschitti, A., Pang, B., and Daelemans, W., editors, Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing, EMNLP 2014, October 25-29, 2014, Doha, Qatar, A meeting of SIGDAT, a Special Interest Group of the ACL, pages 1724–1734. ACL.

Choy, C. B., Xu, D., Gwak, J., Chen, K., and Savarese, S. (2016). 3d-r2n2: A unified approach for single and multi-view 3d object reconstruction. In Proceedings of the European Conference on Computer Vision (ECCV).

Chrysos, G. G. and Panagakis, Y. (2021). Cope: Conditional image generation using polynomial expansions. arXiv preprint arXiv:2104.05077.

Doob, J. L. (1953). Stochastic processes, volume 10. John Wiley & Sons, New York. MR 15,445b. Zbl 0053.26802.

Durkan, C., Murray, I., and Papamakarios, G. (2020). On contrastive learning for likelihood-free inference. In Proceedings of the 37th International Conference on Machine Learning, ICML 2020, 13-18 July 2020, Virtual Event, volume 119 of Proceedings of Machine Learning Research, pages 2771–2781. PMLR.

Eslami, S. M. A., Jimenez Rezende, D., Besse, F., Viola, F., Morcos, A. S., Garnelo, M., Ruderman, A., Rusu, A. A., Danilhelka, I., Gregor, K., Reichert, D. P., Buesing, L., Weber, T., Vinyals, O., Rosenbaum, D., Rabinowitz, N., King, H., Hillier, C., Botvinick, M., Wierstra, D., Kavukcuoglu, K., and Hassabis, D. (2018). Neural scene representation and rendering. Science, 360(6394):1204–1210.

Foster, A., Pukdee, R., and Rainforth, T. (2020). Improving transformation invariance in contrastive representation learning. arXiv preprint arXiv:2010.09515.

Garnelo, M., Rosenbaum, D., Maddison, C., Ramalho, T., Saxton, D., Shanahan, M., Teh, Y. W., Rezende, D., and Eslami, S. M. A. (2018a). Conditional neural processes. In Dy, J. and Krause, A., editors, Proceedings of the 35th International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pages 1704–1713. PMLR.

Garnelo, M., Schwarz, J., Rosenbaum, D., Viola, F., Rezende, D. J., Eslami, S., and Teh, Y. W. (2018b). Neural processes. arXiv preprint arXiv:1807.01622.

Gondal, M. W., Joshi, S., Rahaman, N., Bauer, S., Wuthrich, M., and Schölkopf, B. (2021). Function contrastive learning of transferable meta-representations. In Meila, M. and Zhang, T., editors, Proceedings of the 38th International Conference on Machine Learning, volume 139 of Proceedings of Machine Learning Research, pages 3755–3765. PMLR.
Grimmett, G. and Stirzaker, D. (2020). *Probability and random processes*. Oxford university press.

Gutmann, M. and Hyvärinen, A. (2010). Noise-contrastive estimation: A new estimation principle for unnormalized statistical models. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pages 297–304.

He, K., Fan, H., Wu, Y., Xie, S., and Girshick, R. (2020). Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 9729–9738.

He, K., Zhang, X., Ren, S., and Sun, J. (2016). Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 770–778.

Hjelm, R. D., Fedorov, A., Lavio-Marchildon, S., Grewal, K., Bachman, P., Trischler, A., and Bengio, Y. (2019). Learning deep representations by mutual information estimation and maximization. In *International Conference on Learning Representations*.

Hochreiter, S. and Schmidhuber, J. (1997). Long short-term memory. *Neural computation*, 9(8):1735–1780.

Itô, K., Henry Jr, P., et al. (2012). *Diffusion processes and their sample paths*. Springer Science & Business Media.

Jacobs, K. (2010). *Stochastic processes for physicists: understanding noisy systems*. Cambridge University Press.

Kim, H., Mnih, A., Schwarz, J., Garnelo, M., Eslami, A., Rosenbaum, D., Vinyals, O., and Teh, Y. W. (2019). Attentive neural processes. In *International Conference on Learning Representations*.

Kingma, D. P. and Welling, M. (2014). Auto-Encoding Variational Bayes. In *2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings*.

Kolesnikov, A., Zhai, X., and Beyer, L. (2019). Revisiting self-supervised visual representation learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 1920–1929.

Lacoste, A., Luccioni, A., Schmidt, V., and Dandres, T. (2019). Quantifying the carbon emissions of machine learning. *arXiv preprint arXiv:1910.09700*.

Lake, B. M., Ullman, T. D., Tenenbaum, J. B., and Gershman, S. J. (2017). Building machines that learn and think like people. *Behavioral and brain sciences*, 40.

LeCun, Y., Boser, B., Denker, J. S., Henderson, D., Howard, R. E., Hubbard, W., and Jackel, L. D. (1989). Backpropagation applied to handwritten zip code recognition. *Neural computation*, 1(4):541–551.

Liu, D. C. and Nocedal, J. (1989). On the limited memory bfgs method for large scale optimization. *Math. Program.*, 45(1-3):503–528.

MacKay, D. J. (2003). *Information theory, inference and learning algorithms*. Cambridge university press.

Mildenhall, B., Srinivasan, P. P., Tancik, M., Barron, J. T., Ramamoorthi, R., and Ng, R. (2020). Nerf: Representing scenes as neural radiance fields for view synthesis. In *European Conference on Computer Vision*, pages 405–421. Springer.

Øksendal, B. (2003). Stochastic differential equations. In *Stochastic differential equations*, pages 65–84. Springer.

Parmar, N., Vaswani, A., Uszkoreit, J., Kaiser, L., Shazeer, N., Ku, A., and Tran, D. (2018). Image transformer. In *International Conference on Machine Learning*, pages 4055–4064. PMLR.

Parzen, E. (1999). *Stochastic processes*. SIAM.
Paszke, A., Gross, S., Chintala, S., Chanan, G., Yang, E., DeVito, Z., Lin, Z., Desmaison, A., Antiga, L., and Lerer, A. (2017). Automatic differentiation in PyTorch. In *NIPS-W*.

Radford, A., Metz, L., and Chintala, S. (2016). Unsupervised representation learning with deep convolutional generative adversarial networks. In Bengio, Y. and LeCun, Y., editors, *4th International Conference on Learning Representations, ICLR 2016, San Juan, Puerto Rico, May 2-4, 2016, Conference Track Proceedings*.

Rahimi, A. and Recht, B. (2008). Random features for large-scale kernel machines. In Platt, J., Koller, D., Singer, Y., and Roweis, S., editors, *Advances in Neural Information Processing Systems*, volume 20. Curran Associates, Inc.

Rasmussen, C. E. (2003). Gaussian processes in machine learning. In *Summer school on machine learning*, pages 63–71. Springer.

Reed, S., Chen, Y., Paine, T., van den Oord, A., Eslami, S. M. A., Rezende, D., Vinyals, O., and de Freitas, N. (2018). Few-shot autoregressive density estimation: Towards learning to learn distributions. In *International Conference on Learning Representations*.

Robbins, H. and Monro, S. (1951). A stochastic approximation method. *The annals of mathematical statistics*, pages 400–407.

Steele, J. M. (2012). *Stochastic calculus and financial applications*, volume 45. Springer Science & Business Media.

Tian, Y., Krishnan, D., and Isola, P. (2020). Contrastive Multiview Coding. *arXiv:1906.05849 [cs]*.

Ton, J.-F., CHAN, L., Whye Teh, Y., and Sejdinovic, D. (2021). Noise contrastive meta-learning for conditional density estimation using kernel mean embeddings. In Banerjee, A. and Fukumizu, K., editors, *Proceedings of The 24th International Conference on Artificial Intelligence and Statistics*, volume 130 of *Proceedings of Machine Learning Research*, pages 1099–1107. PMLR.

van den Oord, A., Kalchbrenner, N., Espeholt, L., kavukcuoglu, k., Vinyals, O., and Graves, A. (2016). Conditional image generation with PixelCNN decoders. In Lee, D., Sugiyama, M., Luxburg, U., Guyon, I., and Garnett, R., editors, *Advances in Neural Information Processing Systems*, volume 29. Curran Associates, Inc.

van den Oord, A., Li, Y., and Vinyals, O. (2018). Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*.

van Kampen, N. G. (1992). *Stochastic processes in physics and chemistry*, volume 1. Elsevier.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, Ł., and Polosukhin, I. (2017). Attention is all you need. In Guyon, I., Luxburg, U. V., Bengio, S., Wallach, H., Fergus, R., Vishwanathan, S., and Garnett, R., editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc.

Vinyals, O., Blundell, C., Lillicrap, T., kavukcuoglu, k., and Wierstra, D. (2016). Matching networks for one shot learning. In Lee, D., Sugiyama, M., Luxburg, U., Guyon, I., and Garnett, R., editors, *Advances in Neural Information Processing Systems*, volume 29. Curran Associates, Inc.

Wu, M. and Goodman, N. (2020). A simple framework for uncertainty in contrastive learning. *arXiv preprint arXiv:2010.02038*.

Xian, Y., Lampert, C. H., Schiele, B., and Akata, Z. (2018). Zero-shot learning—a comprehensive evaluation of the good, the bad and the ugly. *IEEE transactions on pattern analysis and machine intelligence*, 41(9):2251–2265.

Zelnik-Manor, L. and Irani, M. (2001). Event-based analysis of video. In *Proceedings of the 2001 IEEE Computer Society Conference on Computer Vision and Pattern Recognition. CVPR 2001*, volume 2, pages II–II. IEEE.

Zhu, X. (2005). Semi-supervised learning literature survey. Technical Report 1530, Computer Sciences, University of Wisconsin-Madison.
Appendix A  Broader impact

The work presented in this paper focuses on the learning of representations for stochastic processes. Applications in the field of computer vision could lead to better understanding of 3D scenes. Such applications could in turns lead to improved safety in products such as self-driving cars, as well as improved performance in areas such as medical imaging. Nonetheless, as with any computer vision technique, it might also be used in a way that carries societal risk. As a foundational method, our work inherits the broader ethical aspects and future societal consequences of machine learning in general.

Appendix B  Additional background

Neural Processes  Neural processes (NPs) learn a neural approximation \( q(y^*|x^*, (x_i, y_i))_{i=1}^C \) to the posterior predictive distributions for stochastic processes given in Eq. (2). To create an efficient neural network architecture, the NP family use the fact that the posterior predictive distribution is unchanged under a permutation of the order \( 1, \ldots, C \) of the context points. The CNP combines representations of the observed data \( x_{1:C}, y_{1:C} \) into a context representation \( c \). To respect the permutation-invariance property, the CNP representation is of the form \( c = \sum_c g_{enc}(x_c, y_c) \) where \( g_{enc}: X \times Y \to C \) is an encoder. The CNP predictions are then given by

\[
q(y^*|x^*, (x_i, y_i))_{i=1}^C = p_\theta(y^*|c, x^*)
\]

where \( p_\theta(y^*|c, x) \) is an explicit likelihood, conventionally a Gaussian with mean and variance given by a neural network applied to \( c, x \). The CNP model is then trained by maximum likelihood, i.e. by minimizing the following condition log probability

\[
\mathcal{L}_{\text{CNP}} = -E_{F} \left[ E_{x,y} \left[ \log q(y^*|(x_i, y_i))_{i=1}^C, x^*) \right] \right].
\]

Recall that the NP, unlike the CNP, includes an additional random variable \( u \). We can in fact view \( u \) as a finite dimensional approximation to \( F \) in (2). In NPs, the random variable \( u \) is sampled from an approximate posterior \( q(u|(x_i, y_i))_{i=1}^C \). The NP constructs the approximate posterior so that it is invariant to the order of the context, by using a sum pooling approach to aggregate the context. In order to learn this distribution, the NP introduces a modified training objective. Considering a context set \( (x_i, y_i)_{i=1}^C \) and target set \( (x_i^*, y_i^*)_{i=1}^T \), the NP training loss (Garnelo et al., 2018b) is

\[
- \mathbb{E} \left[ \sum_{i=1}^T \log q(y_i^*|x_i^*, u) + \log \frac{q(y_i|u((x_i, y_i))_{i=1}^C)}{q(u|(x_i, y_i))_{i=1}^C, (x_i^*, y_i^*)_{i=1}^T) \right]
\]

where \( q(y^*|x^*, u) \) is the explicit likelihood model, typically a Gaussian, as in the CNP. The outer expectation is with respect to the data \( F, x, y \).

Attentive Neural Processes  The ANP (Kim et al., 2019) introduced attention into the NP family in two different ways: self-attention applies to the context to create context-aware representations of each context pair \( (x_i, y_i) \); cross-attention allows the ANP to attend to different components of the context depending on the target covariate \( x^* \). These result in a representation \( \hat{c}(x_{1:C}, y_{1:C}, x_i^*) \) that depends on \( x^* \). As with the NP, the ANP can include a latent variable \( u \) to be sampled under a distribution that depends on \( (x_i, y_i)_{i=1}^C \), self-attention can be used to generate the approximate posterior for \( u \) in this case. The overall training loss for the ANP is

\[
\mathcal{L}_{\text{ANP}} = -E_{F,x,y} \left[ \sum_{i=1}^T \log q(y_i^*|x_i^*, u, \hat{c}(x_{1:C}, y_{1:C}, x_i^*)) \right]
\]

where \( q(y^*|x^*, u, \hat{c}(x_{1:C}, y_{1:C}, x_i^*)) \) is the explicit likelihood model in this case. We refer to the ANP model without the latent \( u \) as the ACNP, for which the training loss is simply

\[
\mathcal{L}_{\text{ACNP}} = -E_{F,x,y} \left[ \sum_{i=1}^T \log q(y_i^*|x_i^*, \hat{c}(x_{1:C}, y_{1:C}, x_i^*)) \right].
\]
We provide below all necessary details to understand and reproduce the empirical results obtain in Sec. 5. Hyperparameters are summarized in Tab. 4. Models were implemented in PyTorch (Paszke et al., 2017). For downstream tasks we fit linear models with L-BFGS (Liu and Nocedal, 1989), we applied L2 regularization to the weights. Our code is available at [github.com/ae-foster/cresp](http://github.com/ae-foster/cresp).

**Appendix C Method details**

**C.1 Downstream Tasks for Stochastic Processes**

We provide some additional details on targeted and untargeted tasks. For a targeted task, we extend the stochastic process of Section 2 by introducing a second conditional distribution \( p(\ell | F, x) \). We assume that the joint distribution over observations \( y_{1:C} \) and labels \( \ell_{1:C} \) is given by

\[
p(y_{1:C}, \ell_{1:C} | x_{1:C}) = \int p(F) \prod_{i=1}^{C} p(y_i | F, x_i) p(\ell_i | F, x) \, dF, \tag{14}
\]

implying that the predictive density of the label \( \ell^* \) at \( x^* \) given the context \( \{(x_i, y_i)_{i=1}^{C}\} \) is

\[
p(\ell^* | x^*, (x_i, y_i)_{i=1}^{C}) = \frac{\int p(F)p(\ell^* | F, x^*) \prod_{i=1}^{C} p(y_i | F, x_i) \, dF}{\int p(F)p(\ell^* | F, x^*) \, dF}. \tag{15}
\]

In CR\(E\)SP, we estimate this by forming a targeted representation \( \hat{c} \) of \( (x_i, y_i)_{i=1}^{C} \) and \( x^* \), and fitting a linear model \( q(\ell | \hat{c}) \).

For untargeted tasks, there is one \( \ell \) sampled along with the entire realization \( F \) via a conditional distribution \( p(\ell | F) \), giving the joint distribution

\[
p(y_{1:C}, \ell | x_{1:C}) = \int p(F)p(\ell | F) \prod_{i=1}^{C} p(y_i | F, x_i) \, dF. \tag{16}
\]

This means that we can predict \( \ell \) using the context \( \{(x_i, y_i)_{i=1}^{C}\} \) using the predictive distribution

\[
p(\ell | (x_i, y_i)_{i=1}^{C}) = \frac{\int p(F)p(\ell | F) \prod_{i=1}^{C} p(y_i | F, x_i) \, dF}{\int p(F)p(\ell | F) \, dF}. \tag{17}
\]

In CR\(E\)SP, we estimate this using a representation \( c \) of \( (x_i, y_i)_{i=1}^{C} \); we fit a linear model \( q(\ell | c) \).

**Appendix D Experimental details**

We provide below all necessary details to understand and reproduce the empirical results obtain in Sec. 5. Hyperparameters are summarized in Tab. 4. Models were implemented in PyTorch (Paszke et al., 2017). For downstream tasks we fit linear models with L-BFGS (Liu and Nocedal, 1989), we applied L2 regularization to the weights. Our code is available at [github.com/ae-foster/cresp](http://github.com/ae-foster/cresp).
Table 4: Hyperparameters used for the different experiments.

| Parameter                          | Sinusoids | ShapeNet | Snooker |
|-----------------------------------|-----------|----------|---------|
| Covariate space $\mathcal{X}$     | $\mathcal{R}$       | $\mathcal{R}^{15}$  | $\mathcal{R}$ |
| Observation space $\mathcal{Y}$   | $\mathcal{R}$       | RBG 64x64 images | RBG 28x28 images |
| Dataset sizes                     | 17.6k/2.2k/2.2k    | 26270/8756/8756 | 15k/3k/20k |
| Observation Net                   | Id          | CNN      | ResNet18 |
| Covariate Net                     | Id          | Id       | Id      |
| Encoder Net                       | MLP         | Gated    | Gated   |
| Decoder model                     | MLP         | CNN      | DCGAN   |
| Attention                         | 2 transformer layers | 2 transformer layers | MLP |
| Target network                    |             | Gated    |         |
| Training views                    | 10          | 3        | 5       |
| Test views                        | 20          | 10       | 9       |
| Representation dim                | 512         | 512      | 512     |
| Projection dim                    | 128         | 128      | 128     |
| Training batch size               | 256         | 512      | 256     |
| Training epochs                   | 200         | 10       | 200     |
| Optimizer                         | Adam        | LARS     | Adam    |
| Scheduler                         | Cosine      | Cosine + Ramp | Cosine + Ramp |
| Scheduler Ramp length             |             |          | 10      |
| Learning rate                     | 3e-4        | 2e-1     | 2e-3    |
| Momentum                          | 0.9         | 0.9      | 0.9     |
| Weight decay                      | 1e-6        | 1e-6     | 1e-6    |
| Temperature $\tau$                | 0.5         | 0.5      | 0.5     |
| Downstream L2 regularization      | 1e-6        | 1e-3     | 1e-3    |

D.1 CO₂ emissions

Experiments were conducted using a private infrastructure, which has an estimated carbon efficiency of 0.188 kgCO₂eq/kWh². An estimated cumulative 1000 hours of computation was performed on hardware of type RTX 2080 Ti (TDP of 250W), or similar such as RTX 1080 Ti. Total emissions are estimated to be 47 kgCO₂eq. Estimations were conducted using the Machine Learning Impact calculator presented in Lacoste et al. (2019).

D.2 Sinusoids dataset

**Data** We sample unidimensional functions $F \sim p(F)$ such that $F(x) = \alpha \sin(2\pi/T \cdot x + \varphi)$ with random amplitude $\alpha \sim \mathcal{U}([0.5, 2.0])$, phase $\varphi \sim \mathcal{U}([0, \pi])$ and period $T = 8$. We assume a bimodal likelihood: $p(y|F, x) = 0.5 \delta_{F(x)}(y) + 0.5 \delta_{F'(x)}(y)$. Context points $x \in \mathcal{X}$ are uniformly sampled in $[-5, 5]$.

**Architectures** Since both the covariate and observation variables are unidimensional, we do not preprocess them, i.e. $g_{\text{cov}} = \text{Id}$ and $g_{\text{obs}} = \text{Id}$. For the encoder–processing $g_{\text{enc}}(g_{\text{cov}}(x), g_{\text{obs}}(y))$–we rely on an multilayer perceptron (MLP) with 3 hidden layer of 512 hidden units. For reconstructive methods (CNP and ACNP), the decoder is also parametrized by an MLP with 512 hidden units and 3 hidden layers.

D.3 Shapenet dataset

**Data** We utilize the renderings of ShapeNet objects provided in 3D-R²N² (Choy et al., 2016). These renderings are constructed from different orientations. We also apply a random crop to each image to simulate a random proximity to the object. Specifically, we choose a random area from $\mathcal{U}(0.08, 1)$ and then a random crop of that area. This process is summarized by the PyTorch snippet

²Average carbon intensity in March, April and June in the Great Britain. Source https://electricityinfo.org/carbon-intensity-archive.
This means that the covariate $x$ representing the view consists of the angles describing the orientation of the render, and the bounding box. We apply additional featurization to $x$ described in the next section. We also apply random colour distortion of strength $s$ as a noise process on the images $y$. Inspired by the colour distortion of Chen et al. (2020) we apply randomized brightness, contrast, saturation, hue and gamma adjustment (see our code for the exact implementation).

**Feature processing** We process the covariate $x$ as follows. For the azimuthal angle $\theta$, we use $\sin(n\theta), \cos(n\theta)$ for $n = 1, 2, 3$ and the original angle (7 features). We include the elevation and distance of the $R^2N^2$ render without additional features (2 features): in practice these vary little in this dataset. We include the bounding box mid-point and area as additional features, along with the four corners of the bounding box (6 features). All told, this gives a covariate of dimension 15. We finally apply normalization to the covariate so that each component has mean 0 and variance 1 over the entire dataset. To images $y$ we apply a linear rescaling that means each channel has mean 0 over the dataset.

**Learning set-up and downstream tasks** For unsupervised learning, we resample the view and distortion randomly each time an object is encountered. For learning on downstream tasks, we fix a dataset of covariates, observations and labels, and learn exclusively from this fixed dataset without resampling views, providing a more realistic semi-supervised test case. The labels are included in the dataset, but only utilized by our algorithm when we train downstream linear classifiers (except for the supervised baseline). The following 13 categories are represented in our dataset: display (1095), watercraft (1939), bench (1816), telephone (1052), cabinet (1572), sofa (3173), rifle (2373), loudspeaker (1618), airplane (4045), table (8509), chair (6778), car (7496), lamp (2318).

**Architectures** For the observation network, we use a CNN described by the following PyTorch snippet

```python
nn.Sequential(
    nn.Conv2d(num_channels, ngf // 8, 3, stride=2, padding=1, bias=False),
    nn.BatchNorm2d(ngf // 8),
    nn.LeakyReLU(),
    nn.Conv2d(ngf // 8, ngf // 4, 3, stride=2, padding=1, bias=False),
    nn.BatchNorm2d(ngf // 4),
    nn.LeakyReLU(),
    nn.Conv2d(ngf // 4, ngf // 2, 3, stride=4, padding=1, bias=False),
    nn.BatchNorm2d(ngf // 2),
    nn.LeakyReLU(),
    nn.Conv2d(ngf // 2, ngf, 3, stride=4, padding=1),
    nn.BatchNorm2d(ngf),
    nn.LeakyReLU(),
)
```

and we set $ngf = 512$. For reconstructive methods (CNP and ACNP), we use a convolutional decoder of the following form

```python
nn.Sequential(
    nn.UpsamplingNearest2d(scale_factor=2),
    nn.ConvTranspose2d(nz, ngf // 2, 2, stride=2, padding=0, bias=False),
    nn.BatchNorm2d(ngf // 2),
    nn.LeakyReLU(),
    nn.UpsamplingNearest2d(scale_factor=2),
    nn.ConvTranspose2d(ngf // 2, ngf // 4, 2, stride=2, padding=0, bias=False),
    nn.BatchNorm2d(ngf // 4),
)```

17
nn.LeakyReLU(),
nn.ConvTranspose2d(ngf // 4, ngf // 8, 2, stride=2, padding=0, bias=False),
nn.BatchNorm2d(ngf // 8),
nn.LeakyReLU(),
nnn.ConvTranspose2d(ngf // 8, nc, 2, stride=2, padding=0),
)
where nz= 512 + 15, ngf= 512, nc= 6. Finally, we extract three means and three standard deviations from the output at each pixel location for three colour channels, applying a sigmoid to the means (to put them in the correct range for image data) and a softplus transform to the standard deviations.

The gated unit that we use is as follows

class Gated(nn.Module):

    def __init__(self, in_dim, representation_dim):
        super(Gated, self).__init__()
        self.fc1 = nn.Linear(in_dim, representation_dim)
        self.fc2 = nn.Linear(in_dim, representation_dim)
        self.activation = nn.Sigmoid()

    def forward(self, x):
        representation = self.fc1(x)
        multiplicative = self.activation(self.fc2(x))
        return multiplicative * representation

inspired by gated units that appear in Hochreiter and Schmidhuber (1997); Cho et al. (2014). The gated unit is utilized in two places: as the pair encoding (Sec. 3.2) that processes the covariate and observation features after concatenation, and as the target network for our targeted CRESP implementation on ShapeNet. We found that it slightly outperformed an MLP with a similar number of parameters.

D.4 Snooker dataset

Data This synthetic dataset simulates a dynamical system with two objects evolving through time with constant velocities. Formally, let’s consider two objects at positions $s_i$ at time $t$. A free object moving at velocity $v_i$ has position $s_i(t) = s_i(0) + v_i t$. We now consider both objects constrained so that $0 \leq s_i \leq 1$ and assume that collisions with the boundaries result in a perfect reflection. The position of the particle can be expressed by the following formula

$$\tilde{s}_i(t) = s_i(0) + v_i t, \quad (18)$$
$$s_i(t) = (\lfloor \tilde{s}_i(t) \rfloor \mod 2)(1 - \tilde{s}_i(t) + \lfloor \tilde{s}_i(t) \rfloor) + (1 - \lfloor \tilde{s}_i(t) \rfloor \mod 2)(\tilde{s}_i(t) - \lfloor \tilde{s}_i(t) \rfloor) \quad (19)$$

for $i = 1, 2$.

We then assume that we only have access to a 2D image $y$ of the state at time $x = t$ for a given realization $F$. We sample realizations $F \sim p(F)$ such that $s_i(0) \sim U([0, 1]^2)$, and $v_i = v_0 \alpha$ with $\alpha \sim U(S^1)$ and $v_0 = 0.4$. The objects are assumed to be non-interacting discs of radius 0.15.

The downstream task is to predict whether the two objects are overloading at a given time, i.e. $E_{\ell \sim p(t | F, x = t)}[\ell]$ with $\ell = 1$ if there is an overlap. The objects position can be expressed at any time in closed-form (cf Eq. (18)), yet it is quite challenging to predict the 2D image at a specific time given a collection of snapshots.

Architectures For the observation network, we use a CNN described by the following PyTorch snippet

```python
nn.Sequential(
    nn.Conv2d(nc, ngf, kernel_size=2, stride=2, bias=False),
    nn.BatchNorm2d(ngf),
    nn.ReLU(True),
```
nn.Conv2d(ngf, 2 * ngf, kernel_size=2, stride=2, bias=False),
nn.BatchNorm2d(2 * ngf),
nn.ReLU(True),
nn.Conv2d(2 * ngf, 4 * ngf, kernel_size=2, stride=2, bias=False),
nn.BatchNorm2d(4 * ngf),
nn.ReLU(True),
nn.Conv2d(4 * ngf, nz, kernel_size=2, stride=2),
)

where \( ngf = 64 \) and \( nc = 3 \). For reconstructive methods (CNP and ACNP), we use a convolutional decoder inspired by DCGAN (Radford et al., 2016), of the form

nn.Sequential(
    nn.ConvTranspose2d(nz, ngf * 4, 4, 1, 0, bias=False),
nnn.BatchNorm2d(ngf * 4),
nnn.ReLU(True),
nn.ConvTranspose2d(ngf * 4, ngf * 2, 3, 2, 1, bias=False),
nnn.BatchNorm2d(ngf * 2),
nnn.ReLU(True),
nn.ConvTranspose2d(ngf * 2, ngf, 4, 2, 1, bias=False),
nnn.BatchNorm2d(ngf),
nnn.ReLU(True),
nn.ConvTranspose2d(ngf, 2 * nc, 4, 2, 1),
)

where \( nz = 512 + 1, ngf = 64 \) and \( nc = 2 \times 3 \). Similarly to Sec. D.3, we extract three means and three standard deviations from the output at each pixel location.

For the encoder–processing \( g_{enc}(g_{cov}(x), g_{obs}(y)) \)–we rely on the gated architecture described above in Sec. D.3. For the target network \( h \), which outputs the predictive representation \( \hat{c} = h([x^*, c]) \), we rely on an MLP with 3 hidden layers of 512 units each.