**Neural Processes Reading Group** 

Andrew Foong, Sebastian Ober, Stratis Markou

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What are Neural Processes (NPs)?

- They are:
  - 1) a meta-learning framework.
  - **2** modelling stochastic processes.
  - **3** using neural networks.
- The hope: benefits of GPs and deep learning together.
- Introduced in Garnelo et al. [2018a].
- Many variants/extensions since proposed.

# Outline

This reading group in conceptual order.

- 1 Introduction: meta-learning stochastic processes. (Andrew)
- 2 Conditional Neural Processes. (Sebastian)
- 3 (Latent) Neural Processes. (Stratis)



Layout follows

https://yanndubs.github.io/Neural-Process-Family, made by Yann Dubois, Jonathan Gordon and Andrew Foong.

• Code for many NPs.

# **Problem Set-up**

Task: prediction under uncertainty in the small-data regime

- Examples:
  - Predicting time-series.
  - Image completion. View images as functions from the 2D plane  $\mathbb{R}^2 \to \mathbb{R}.$



 Could be difficult to design a GP kernel for this kind of data — can we learn this structure?

# **Meta-Learning**

Meta-learning is learning to learn.



- View learning as a map from data sets to predictives.
- Given observed context set  $D_{\mathcal{C}} = \{(x^{(c)}, y^{(c)})\}_{c=1}^{C}$ .
- Make predictions at a *target set*  $x_T = \{x^{(t)}\}_{t=1}^T$ .
- NPs use neural networks to directly parameterise map *D*<sub>C</sub> → *p*(y<sub>T</sub> |×<sub>T</sub>, *D*<sub>C</sub>).

# **General Challenges in Designing NPs**

#### Two challenges:

1 Standard NNs eat fixed-length vectors. NPs eat entire datasets:

- Datasets can be of varied sizes.
- The map  $D_{\mathcal{C}} \mapsto p(y_{\mathcal{T}} | x_{\mathcal{T}}, D_{\mathcal{C}})$  should be invariant to permutations of  $D_{\mathcal{C}}$ .
- **2** For any target set  $x_T$ , the NP must return  $p(y_T | x_T, D_C)$ .
  - Are these predictives be **consistent** for varying x<sub>T</sub>?
  - I.e. do NPs define a valid stochastic process?

We'll discuss challenge 1 first.

### First Challenge: Machine Learning on Sets

Deep learning on sets is well-studied, e.g. Zaheer et al. [2017].

Key result is a representation theorem:

**Theorem 1 (Zaheer et al. [2017], Wagstaff et al. [2019]).** Let  $M \in \mathbb{N}$ , and let  $f : [0,1]^M \to \mathbb{R}$  be a continuous, permutation-invariant function. Then there exist continuous maps  $\phi : [0,1] \to \mathbb{R}^M$  and  $\rho : \mathbb{R}^M \to \mathbb{R}$  such that for all  $X \in [0,1]^M$ ,

$$f(X) = \rho\left(\sum_{i=1}^{M} \phi(X_m)\right)$$

- Implement  $\phi$  and  $\rho$  as NNs.
- Think of X as a data set and  $\mathbb{R}^M$  as a representation space.
- Each data point  $X_m$  is mapped to  $\phi(X_m)$ , then summed.
- Known as a deep sets or sum decomposition.

# **Computational Graph**

Common NP computational graph:



- The encoder  $Enc_{\theta}$  maps each datapoint to a representation.
- Representations are **aggregated** to form *R*.
- The decoder  $\text{Dec}_{\theta}$  maps R along with target input  $x^{(t)}$  to predictions.

Many concrete instantiations during Seb and Stratis' talks.

## Second Challenge: Consistency of Predictives

NPs map  $D_{\mathcal{C}} \mapsto p(y_{\mathcal{T}} | x_{\mathcal{T}}, D_{\mathcal{C}})$  for any  $x_{\mathcal{T}}$ .

- What could go wrong with an arbitrary mapping?
- Consider 1D regression, with  $x_{\mathcal{T}} = \{1\}, x'_{\mathcal{T}} = \{1, 2\}$  for a fixed  $D_{\mathcal{C}}$ .
- We obtain  $p(y_1|\{1\}, D_C)$  and  $p(y_1, y_2|\{1, 2\}, D_C)$ .
- Must satisfy a consistency condition:

$$\int p(y_1, y_2 | \{1, 2\}, D_C) \, \mathrm{d}y_2 = p(y_1 | \{1\}, D_C).$$

• If not, predictions change arbitrarily depending on which points are in the target set!

Kolmogorov Extension Theorem guarantees that:

- If predictives consistent under marginalisation and permutation,
- they are indeed marginals of a stochastic process (random function).

Two main flavours:

**1** Conditional Neural Process Family assumes the predictive is factorised conditioned on the representation  $R(D_C)$ .

$$p(\mathbf{y}_{\mathcal{T}}|\mathbf{x}_{\mathcal{T}}, D_{\mathcal{C}}) = \prod_{t=1}^{T} p(\mathbf{y}_t|\mathbf{x}^{(t)}, R(D_{\mathcal{C}})).$$

- (Latent) Neural Process Family uses the representation R(D<sub>C</sub>) to define a latent variable z ~ p(z|R).
  - The predictive is factorised conditioned on z:

$$p(\mathbf{y}_{\mathcal{T}}|\mathbf{x}_{\mathcal{T}}, D_{\mathcal{C}}) = \int \prod_{t=1}^{T} p(\mathbf{y}_t|\mathbf{x}^{(t)}, \mathbf{z}) p(\mathbf{z}|R(D_{\mathcal{C}})) \, \mathrm{d}\mathbf{z}.$$

Allows for dependencies, unlike Conditional NPs!

# **Episodic Training**

How to train NPs?

- **1** Sample dataset *D* from a large collection  $\{D_i\}_{i=1}^{N_{\text{tasks}}}$ .
- **2** Randomly split into context and target sets:  $D = D_C \cup D_T$ .
- **3** Pass  $D_{\mathcal{C}}$  through the NP to obtain the predictive  $p(y_{\mathcal{T}}|x_{\mathcal{T}}, D_{\mathcal{C}})$ .
- Output objective L which measures predictive performance on the target set.
- **5** Compute  $\nabla_{\theta} \mathcal{L}$  to optimise parameters of the NP.

That's it! Now we'll take a closer look at the **Conditional** Neural Process family.

#### The Conditional Neural Processes Family

As we mentioned earlier, members of the Conditional Neural Process Family (CNPF) assume the following factorisation for the predictive:

$$p(\mathbf{y}_{\mathcal{T}}|\mathbf{x}_{\mathcal{T}}, D_{\mathcal{C}}) = \prod_{t=1}^{T} p(\mathbf{y}^{(t)}|\mathbf{x}^{(t)}, R(D_{\mathcal{C}})).$$



## The CNPF factorisation implies consistency

We briefly show how this factorisation implies the consistency required for stochastic processes:

**1** Permutation: Let  $\pi$  be any permutation of  $\{1, \ldots, T\}$ . Then

$$\prod_{t=1}^{T} p(y^{(t)}|x^{(t)}, R(D_{\mathcal{C}})) = \prod_{t=1}^{T} p(y^{\pi(t)}|x^{\pi(t)}, R(D_{\mathcal{C}}))$$
$$= p(y^{\pi(1)}, \dots, y^{\pi(T)}|x^{\pi(1)}, \dots, x^{\pi(T)}, D_{\mathcal{C}})$$

**2** Marginalisation: Let  $A \subset \{1, ..., T\}$  and  $A^c$  be its complement. Then

$$\int p(\mathbf{y}_{A}, \mathbf{y}_{A^{c}} | \mathbf{x}_{A}, \mathbf{x}_{A^{c}}, D_{\mathcal{C}}) d\mathbf{y}_{A^{c}} = \int p(\mathbf{y}_{A} | \mathbf{x}_{A}, D_{\mathcal{C}}) p(\mathbf{y}_{A^{c}} | \mathbf{x}_{A^{c}}, D_{\mathcal{C}}) d\mathbf{y}_{A^{c}}$$
$$= p(\mathbf{y}_{A} | \mathbf{x}_{A}, D_{\mathcal{C}})$$

Therefore, CNPF members do indeed satisfy both conditions necessary to be stochastic processes!

# Decoders and the Maximum Likelihood Objective

We have already discussed the encoder in neural processes, which encodes a context set  $D_{\mathcal{C}}$  into a global representation  $R(D_{\mathcal{C}})$ . We now discuss the **decoder** in the CNPF:

- **1** The decoder  $\text{Dec}_{\theta}$  takes the representation  $R(D_{\mathcal{C}})$  and a target input  $x^{(t)}$ , and maps them to parameters of the predictive distribution
- **2** For all the CNP types we consider, we assume a Gaussian predictive:

$$p(y^{(t)}|x^{(t)}, R(D_{\mathcal{C}})) = \mathcal{N}(y^{(t)}; \mu_t, \sigma_t^2)$$
$$(\mu_t, \sigma_t^2) = \text{Dec}_{\theta}(R(D_{\mathcal{C}}), x^{(t)})$$

In CNPs, there are no random variables we need to perform inference over - we can optimize using maximum likelihood!

$$\mathcal{L} = \log p(\mathbf{y}_{\mathcal{T}} | \mathbf{x}_{\mathcal{T}}, D_{\mathcal{C}})$$

#### **Conditional Neural Processes**

We start with the simplest member, known just as the CNP [Garnelo et al., 2018a].



- Encoder:  $R(D_C) = \operatorname{Enc}_{\theta}(D_C) = \frac{1}{C} \sum_{c=1}^{C} \operatorname{MLP}([x^{(c)}, y^{(c)}])$
- Decoder:  $(\mu_t, \sigma_t^2) = \text{Dec}_{\theta}(R(D_{\mathcal{C}}), x^{(t)}) = \text{MLP}([R(D_{\mathcal{C}}), x^{(t)}])$

For wide enough MLPs, this should be able to predict any mean  $\mu_t$  and variance  $\sigma_t^2$ !











CNP | CelebA32 | C=0 Context \_ Pred. Mean \_ Pred. Std I



CNP | MNIST | C=0



CNP | CelebA32 | C=1.0%

CNP | MNIST | C=1.0%



CNP | CelebA32 | C=5.0%



CNP | MNIST | C=5.0%



CNP | CelebA32 | C=10.0%

CNP | MNIST | C=10.0%

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CNP | CelebA32 | C=20.0%

CNP | MNIST | C=20.0%

CNP | CelebA32 | C=50.0%



CNP | MNIST | C=50.0%

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CNP | CelebA32 | C=Hhalf

CNP | MNIST | C=Hhalf



We've seen that even though the results are quite impressive, the standard CNP has a tendency to underfit.

- This may be due to the fact that the representation R(D<sub>C</sub>) is the same for each target input, x<sup>(t)</sup>
- Instead, we may want to focus on context points closer to the target input, and give less weight to those further away
- A great way of achieving this is attention: learn a weighting w<sub>θ</sub>(x<sup>(c)</sup>, x<sup>(t)</sup>) for each context-target point pair to be used in the encoding

$$R(D_{\mathcal{C}},\cdot) = \operatorname{Enc}_{\theta}(D_{\mathcal{C}}) = \sum_{c=1}^{C} w_{\theta}(x^{(c)},\cdot) \operatorname{MLP}([x^{(c)},y^{(c)}])$$

This motivates the Attentive CNP (AttnCNP) [Kim et al., 2019].



• Encoder:

 $R(D_{\mathcal{C}}, \cdot) = \operatorname{Enc}_{\theta}(D_{\mathcal{C}}) = \sum_{c=1}^{C} w_{\theta}(x^{(c)}, \cdot) \operatorname{MLP}([x^{(c)}, y^{(c)}])$ 

• Decoder:  $(\mu_t, \sigma_t^2) = \text{Dec}_{\theta}(R(D_{\mathcal{C}}), x^{(t)}) = \text{MLP}([R(D_{\mathcal{C}}, x^{(t)}), x^{(t)}])$ 











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AttnCNP | MNIST | C=1.0%




#### AttnCNP | CelebA32 | C=5.0%

AttnCNP | MNIST | C=5.0%



AttnCNP | CelebA32 | C=10.0%



AttnCNP | MNIST | C=10.0%



AttnCNP | CelebA32 | C=20.0% Context Context Pred. Mean Pred. Mean \_ Pred. Std Pred. Std \_ \_

AttnCNP | MNIST | C=20.0%

AttnCNP | CelebA32 | C=50.0%



AttnCNP | MNIST | C=50.0%

AttnCNP | CelebA32 | C=Hhalf



AttnCNP | MNIST | C=Hhalf



#### **Generalisation and Extrapolation**

We now look at the ability of CNPs to generalise outside of the region in which they were trained.











We want predictions to depend on *relative* positions of context points, not *absolute* positions. This can be achieved with **translation equivariance**.



# Convolutional CNP (ConvCNP)

One model that encodes translation equivariance is the **convolutional CNP** (ConvCNP) [Gordon et al., 2019], using a special set operation called SetConv and a CNN, motivated by a ConvDeepSets result.



• Encoder:  $R(D_{\mathcal{C}}, \cdot) = \operatorname{Enc}_{\theta}(D_{\mathcal{C}}) =$ SetConv(CNN({SetConv( $D_{\mathcal{C}}$ )( $x^{(u)}$ )} $_{u=1}^{U}$ ))( $\cdot$ )

• Decoder:  $(\mu_t, \sigma_t^2) = \text{Dec}_{\theta}(R(D_{\mathcal{C}}), x^{(t)}) = \text{MLP}(R(D_{\mathcal{C}}, x^{(t)}))$ 

























#### Issues with the CNPF

One of the main issues in the CNPF is caused by the **factorisation** assumption on the predictive - we cannot draw coherent function samples, as could be done with a GP.



### Issues with the CNPF (cont'd)



Another issue is the **Gaussianity** assumption - this does not allow for multimodality in the predictive.

#### **Latent Neural Processes**

CNPs do not distinguish **noise** and uncertainty due to **finite**  $D_{\mathcal{C}}$ .





(a) CNP (b) What we would like to have CNPs push function uncertainty to the noise layer!

#### **1** Bayesian Optimisation (Thompson sampling)



Figure 2: Bayes. opt. with Thompson sampling [Garnelo et al., 2018b].

- **2 Reinforcement Learning** (Contextual bandits)
- **3** Sample plausible functions for downstream estimation



Figure 3: Precipitation over Europe, edited from Foong et al. [2020].

#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 0



Data: Periodic Kernel | Num. Context: 0



Data: Noisy Matern Kernel | Num. Context: 0



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 2



Data: Periodic Kernel | Num. Context: 2



Data: Noisy Matern Kernel | Num. Context: 2



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 4



Data: Periodic Kernel | Num. Context: 4



Data: Noisy Matern Kernel | Num. Context: 4



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 6



Data: Periodic Kernel | Num. Context: 6



Data: Noisy Matern Kernel | Num. Context: 6



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 8



Data: Periodic Kernel | Num. Context: 8



Data: Noisy Matern Kernel | Num. Context: 8



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 10



Data: Periodic Kernel | Num. Context: 10



Data: Noisy Matern Kernel | Num. Context: 10



#### **3** Sample plausible functions for downstream estimation

Data: RBF Kernel | Num. Context: 50



Data: Periodic Kernel | Num. Context: 50



Data: Noisy Matern Kernel | Num. Context: 50



#### The Latent Neural Process model



Garnelo et al. [2018b] introduce, this objective but do not use it.

Anecdotal evidence that it causes under-fitting. Instead they consider

$$p(D_{\mathcal{T}}|D_{\mathcal{C}}) \geq \mathbb{E}_{q(z|D_{\mathcal{C}\cup\mathcal{T}})} \Bigg[\log p(D_{\mathcal{T}}|z) + \log rac{p(z|D_{\mathcal{C}})}{q(z|D_{\mathcal{C}\cup\mathcal{T}})}\Bigg]$$

the marginal likelihood of the target conditioned on the context.
# The Latent Neural Process model

$$p(D_{\mathcal{T}}|D_{\mathcal{C}}) \geq \mathbb{E}_{q(z|D_{\mathcal{C}\cup\mathcal{T}})} \left[ \log p(D_{\mathcal{T}}|z) + \log \frac{p(z|D_{\mathcal{C}})}{q(z|D_{\mathcal{C}\cup\mathcal{T}})} \right]$$
  
But  $p(z|D_{\mathcal{C}})$  is intractable. Garnelo approximate  $p(z|D_{\mathcal{C}}) \approx q(z|D_{\mathcal{C}})$ 
$$\mathcal{L} = \mathbb{E}_{q(z|D_{\mathcal{C}\cup\mathcal{T}})} \left[ \log p(D_{\mathcal{T}}|z) + \log \frac{q(z|D_{\mathcal{C}})}{q(z|D_{\mathcal{C}\cup\mathcal{T}})} \right]$$

Not a lower bound anymore. Can be regarded as defining the model



### The Latent Neural Process model



**Defines** the conditional prior as  $q(z|D_C)$ .

**Chooses** the varational posterior  $q(z|D_{C\cup T})$ .

But this does not correspond to a single consistent Bayesian model.

Performs VI over a family of models (one for each possible dataset).

### Not a single consistent Bayesian model

Given context data  $\mathcal{D}_{\mathcal{C}}$ , conditional prior defined as

 $p(z|\mathcal{D}_{\mathcal{C}}) := q(z|\mathcal{D}_{\mathcal{C}})$ 

New datum  $x^{(n+1)}, y^{(n+1)}$  arrives

$$\mathcal{D}_{\mathcal{C}'} = \mathcal{D}_{\mathcal{C}} \cup \{(x^{(n+1)}, y^{(n+1)})\}$$

Should update the prior by Bayes

$$p(z|\mathcal{D}_{\mathcal{C}'}) = \frac{p(y^{(n+1)}|x^{(n+1)}, z)q(z|\mathcal{D}_{\mathcal{C}})}{Z}$$

Instead LNP defines a separate model for  $\mathcal{D}_{\mathcal{C}'}$ 

$$p(z|\mathcal{D}_{\mathcal{C}'}) := q(z|\mathcal{D}_{\mathcal{C}'})$$













LNP fitted to data, from Dubois et al. [2020].



Computational graphs (left) Latent NP (right) Attentive LNP [Dubois et al., 2020].



LNP with/without attention from Dubois et al. [2020].



LNP with/without attention from Dubois et al. [2020].



LNP with/without attention from Dubois et al. [2020].



LNP with/without attention from Dubois et al. [2020].



LNP with/without attention from Dubois et al. [2020].



LNP with/without attention from Dubois et al. [2020].



Computational graphs (left) ConvCNP (right) Latent ConvNP [Dubois et al., 2020].













# Conclusions

- NPs do meta-learning on functions.
- Family splits into **conditional** and **latent** models.

Strong points:

- Fast inference at test time.
- Well calibrated uncertainty (if enough D's available).
- Data driven, more flexible than hand-picked priors.
- Can bake in (some) required properties translation equivariance.

Weak points:

- Need a large collection of meta-learning datasets.
- Underfitting and smoothness issues.

# **References** I

- Y. Dubois, J. Gordon, and A. Y. Foong. Neural process family. http://yanndubs.github.io/Neural-Process-Family/, September 2020.
- A. Foong, W. Bruinsma, J. Gordon, Y. Dubois, J. Requeima, and R. Turner. Meta-learning stationary stochastic process prediction with convolutional neural processes. *Advances in Neural Information Processing Systems*, 33, 2020.
- M. Garnelo, D. Rosenbaum, C. Maddison, T. Ramalho, D. Saxton, M. Shanahan, Y. W. Teh, D. Rezende, and S. A. Eslami. Conditional neural processes. In *International Conference on Machine Learning*, pages 1704–1713, 2018a.
- M. Garnelo, J. Schwarz, D. Rosenbaum, F. Viola, D. J. Rezende, S. Eslami, and Y. W. Teh. Neural processes. arXiv preprint arXiv:1807.01622, 2018b.

# **References II**

- J. Gordon, W. P. Bruinsma, A. Y. Foong, J. Requeima, Y. Dubois, and R. E. Turner. Convolutional conditional neural processes. *arXiv* preprint arXiv:1910.13556, 2019.
- H. Kim, A. Mnih, J. Schwarz, M. Garnelo, A. Eslami, D. Rosenbaum, O. Vinyals, and Y. W. Teh. Attentive neural processes. arXiv preprint arXiv:1901.05761, 2019.
- E. Wagstaff, F. Fuchs, M. Engelcke, I. Posner, and M. A. Osborne. On the limitations of representing functions on sets. In *International Conference on Machine Learning*, pages 6487–6494, 2019.
- M. Zaheer, S. Kottur, S. Ravanbakhsh, B. Poczos, R. R. Salakhutdinov, and A. J. Smola. Deep sets. *Advances in Neural Information Processing Systems*, 30:3391–3401, 2017.