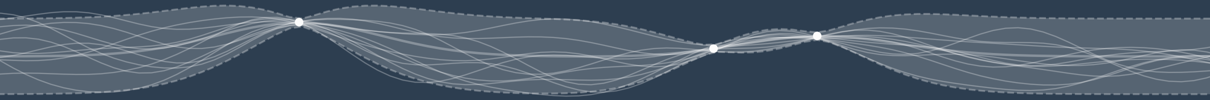


Autoregressive Conditional Neural Processes

Wessel Bruinsma

Microsoft Research AI4Science

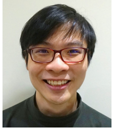
Research Talk
Center for Basic Machine Learning Research in Life Science (MLLS)
Copenhagen, 25 Jan 2024

Collaborators

Wessel Bruinsma[*,1,2]

Stratis Markou[*,2]

James Requeima[*,2]



Andrew Foong[*,1]

Tom Andersson[3]

Anna Vaughan[2]

Anthony Buonomo[2]

J. Scott Hosking[3,4]

Rich Turner[1,2]

[*]Equal contribution

[1]Microsoft Research AI4Science, [2]University of Cambridge, [3]British Antarctic Survey, [4]The Alan Turing Institute

Outline

- Autoregressive Conditional Neural Processes

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AUTOREGRESSIVE CONDITIONAL NEURAL PROCESSES

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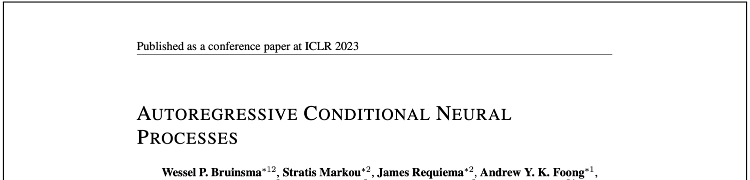
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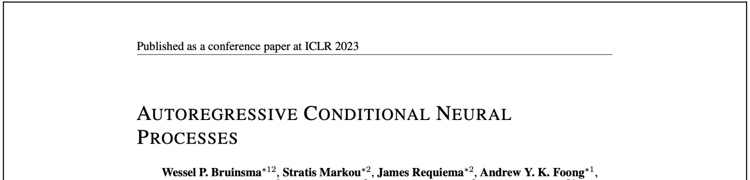

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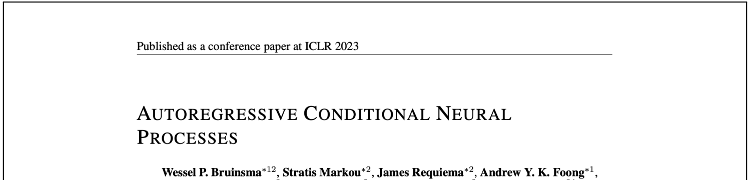

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AUTOREGRESSIVE CONDITIONAL NEURAL PROCESSES

Wessel P. Bruinsma[*12], **Stratis Markou**[*2], **James Requiema**[*2], **Andrew Y. K. Foong**[*1],

Today's Message

- ✗ A specific model
- ✗ Restricted to a meta-learning setting
- ✗ Very unique and new

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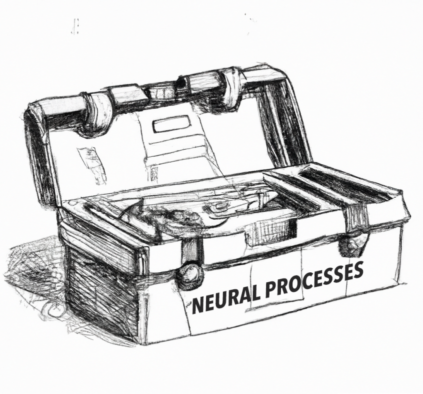

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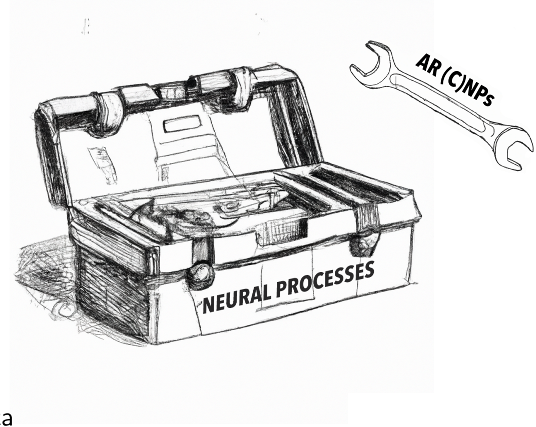
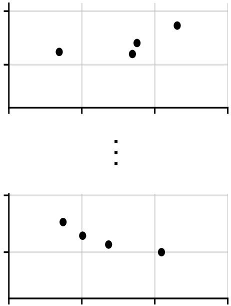


Introduction to Neural Processes

Meta-Learning and Neural Processes: Learning to Predict



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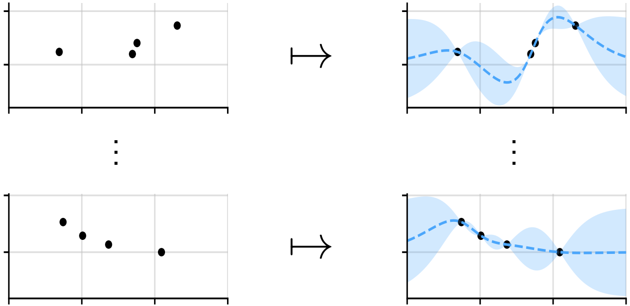

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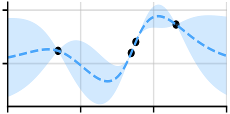

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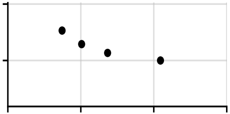

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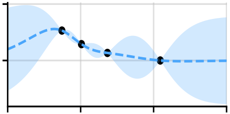

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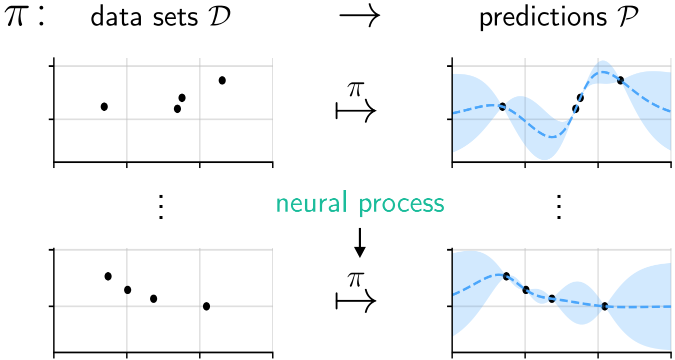

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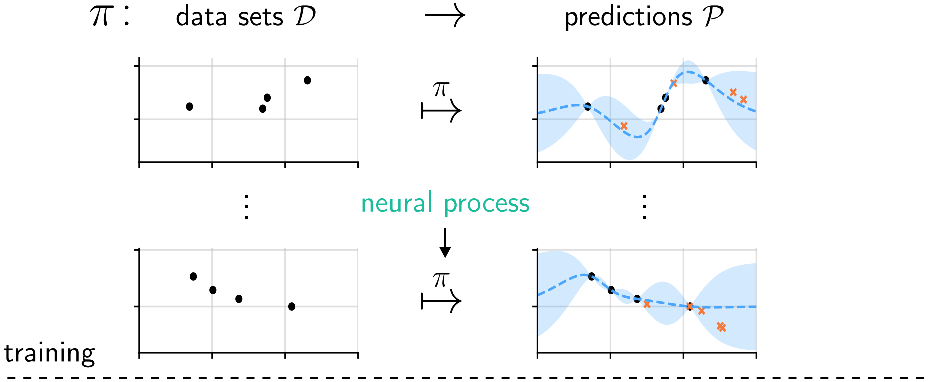

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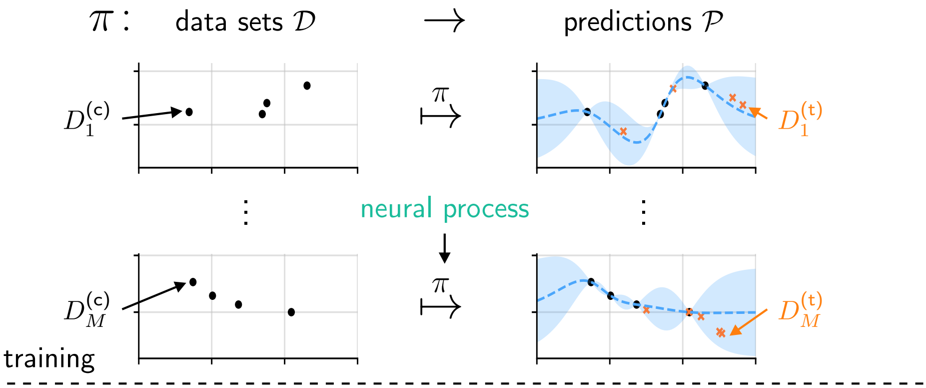

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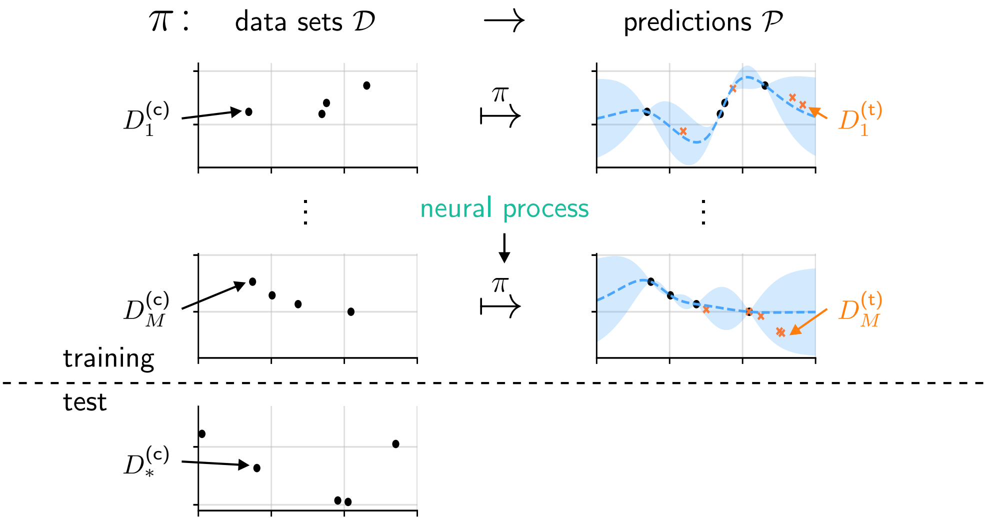

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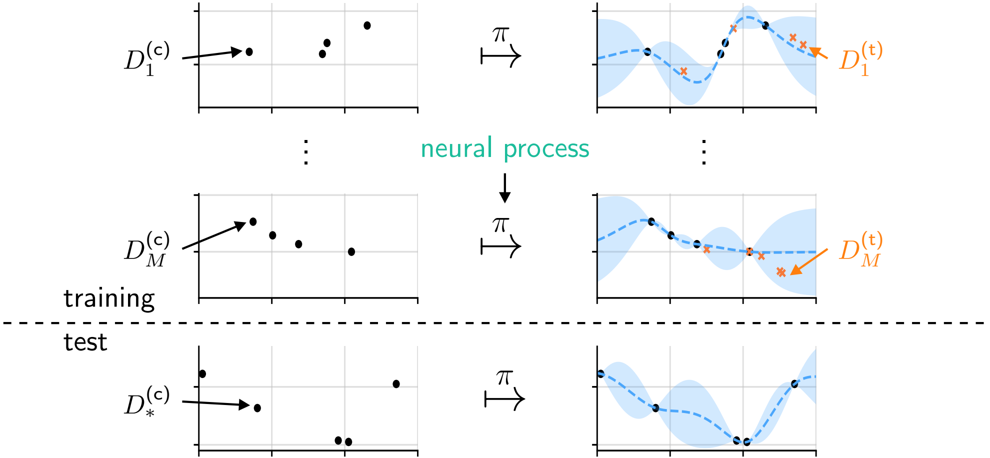

Definitions and Notation

- A neural process is a function $\pi_\theta \colon \mathcal{D} \to \mathcal{P}$ parametrised with neural networks.

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- NPs operate in setting of meta-learning, with meta–data sets:

$$(D_m)_{m=1}^{M} \quad \text{with} \quad D_m = D_m^{(\mathsf{c})} \cup D_m^{(\mathsf{t})}.$$

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will omit when clear from context

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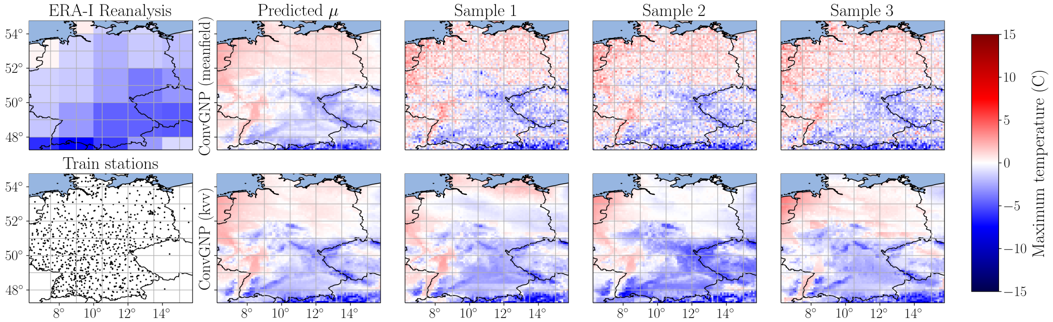
- Climate model downscaling (Markou et al., 2022):



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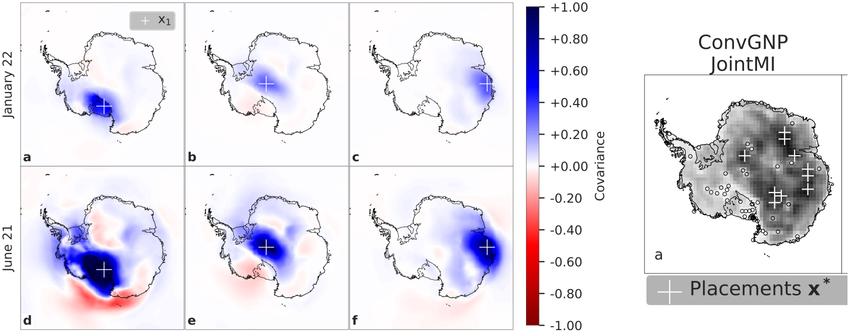
- Environmental sensor placement in Antarctica (Andersson et al., 2023):



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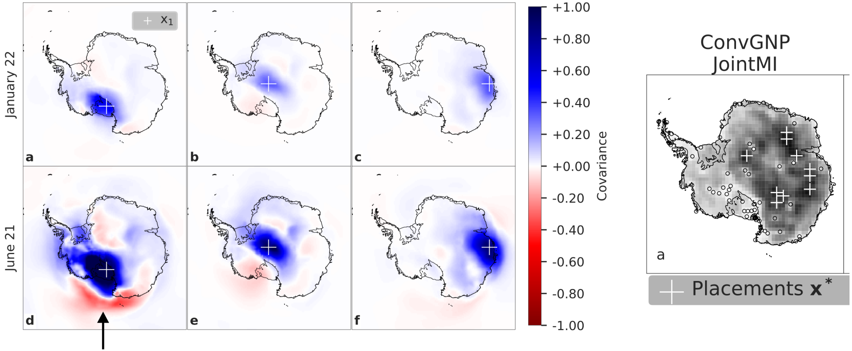

positive covariance extends to edge of Ross ice shelf when sea ice is present

Two Axes of Neural Process Design

- Starting point: want to parametrise $\pi_\theta : \mathcal{D} \to \mathcal{P}$.

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"prediction map"

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- How do we parametrise functions on $\mathcal{D}$?

First Axis: Form of Prediction

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- Non-Gaussian distributions, mixture distributions, normalising flows... much more!

Second Axis: Neural Network Architecture

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- Parametrise parameter functions of the form $f_\theta \colon \mathcal{X} \times \mathcal{D} \to Z$.

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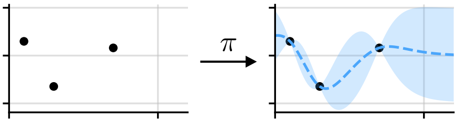

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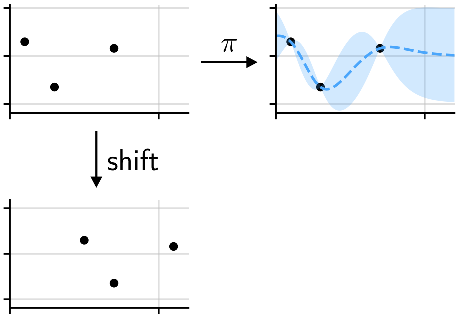

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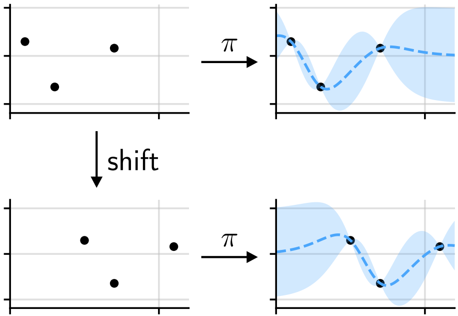

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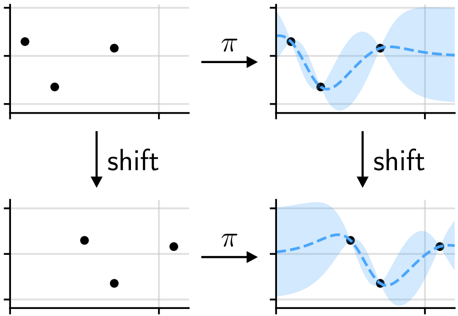

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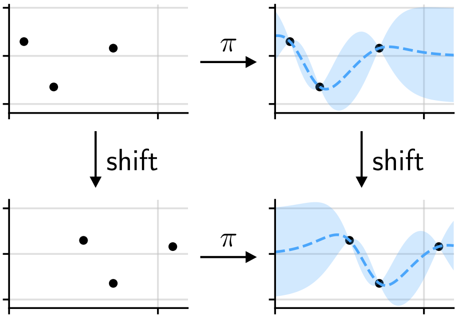

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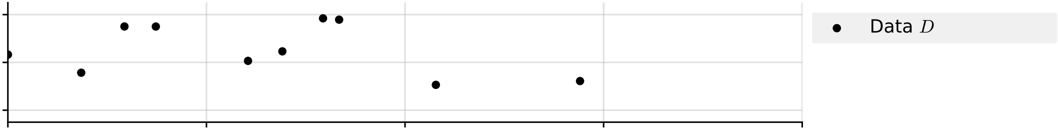
Autoregressive Neural Processes

Neural Processes Are Not Without Challenges...

- Prediction by a Conditional Neural Process (CNP):



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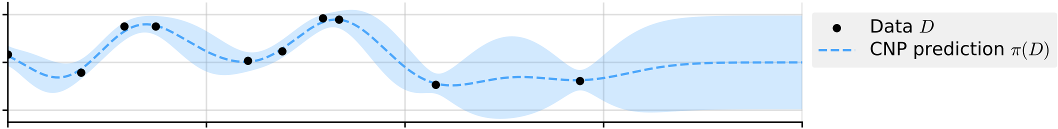

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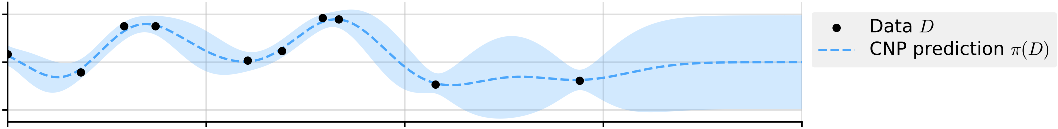

	Non-Gaussian predictions	Exact training
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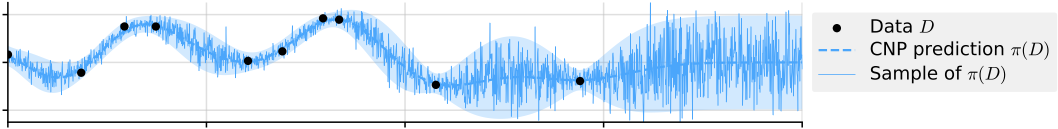

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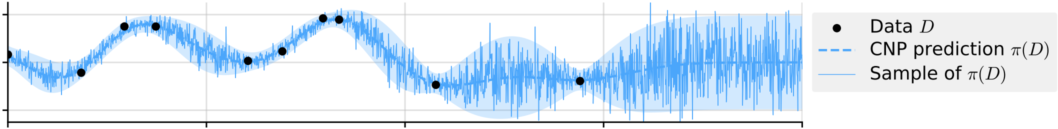

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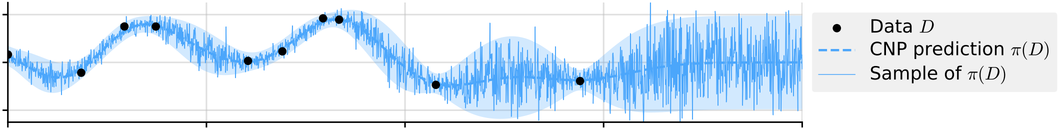

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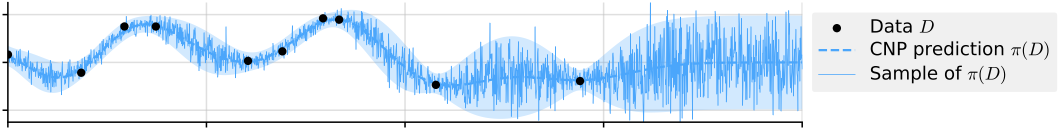

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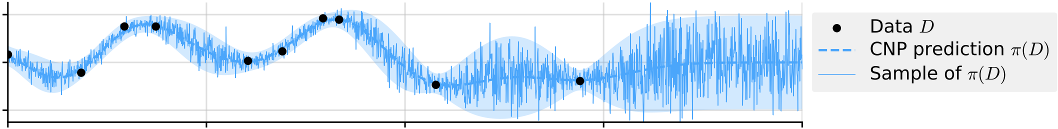

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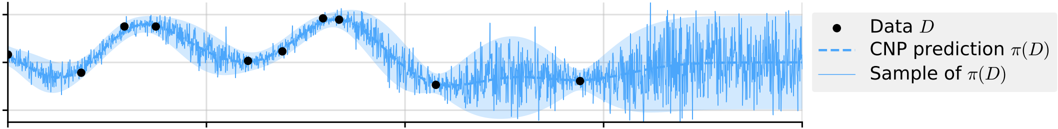

	Correlated predictions	Non-Gaussian predictions	Exact training	Consistent predictions
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- Idea: feed output of CNP back into the model in an autoregressive fashion:

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AR CNPs as a Neural Density Estimator

PixelCNN (Oord et al., 2016): the pixels of an image from top left to bottom right.

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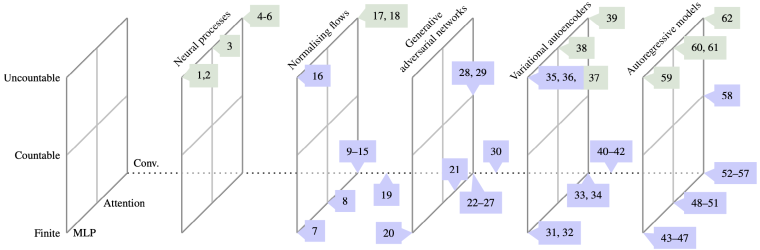
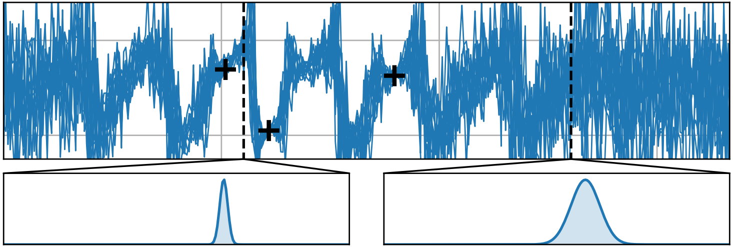
- A slightly insane diagram in the paper:



Example: ConvCNP (Gordon et al., 2020) on Sawtooth Data

ConvCNP:



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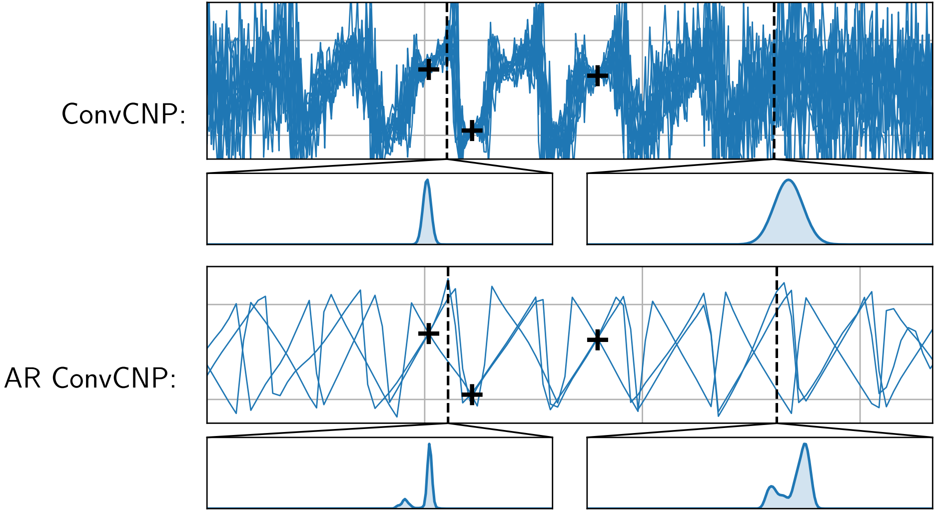

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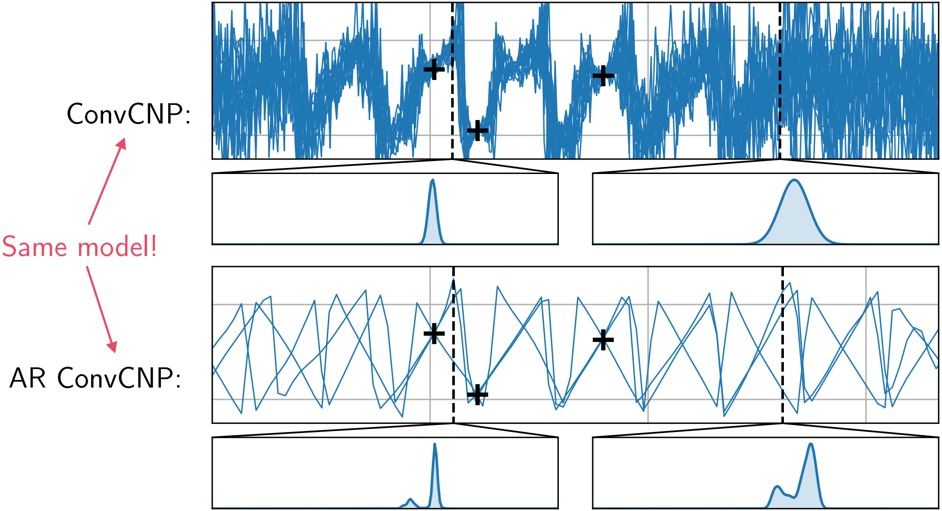

Big Surprise: AR ConvCNP Performs Really Well

	EQ Norm. KL to truth (↓ better)		Sawtooth Norm. log-lik. (↑ better)		Mixture Norm. log-lik. (↑ better)	
	$d_x, d_y = 1$	$d_x, d_y = 2$	$d_x, d_y = 1$	$d_x, d_y = 2$	$d_x, d_y = 1$	$d_x, d_y = 2$
ConvCNP	0.41 ±0.01	0.41 ±0.00	2.38±0.04	0.12 ±0.01	−0.23±0.04	−0.85 ±0.01
ConvCNP (AR)	0.01 ±0.00	**0.03** ±0.00	**3.60**±0.01	**0.38** ±0.00	**0.45**±0.04	**−0.62** ±0.01
ConvGNP	0.01 ±0.00	0.19 ±0.00	2.62±0.05	0.26 ±0.01	−0.24±0.02	−0.74 ±0.01
FullConvGNP	**0.00** ±0.00		2.16±0.04		−0.05±0.03	
ConvLNP (ML)	0.25 ±0.01	0.39 ±0.00	3.06±0.04	0.31 ±0.01	−0.06±0.03	−0.78 ±0.02
ConvLNP (ELBO)	0.06 ±0.00	0.79 ±0.00	3.51±0.02	0.04 ±0.00	0.12±0.04	−0.92 ±0.01
Diagonal GP	0.40 ±0.01	0.40 ±0.00				
Trivial	1.19 ±0.00	0.79 ±0.00	−0.18±0.00	−0.32 ±0.00	−1.32±0.00	−1.46 ±0.00

Some Intuition

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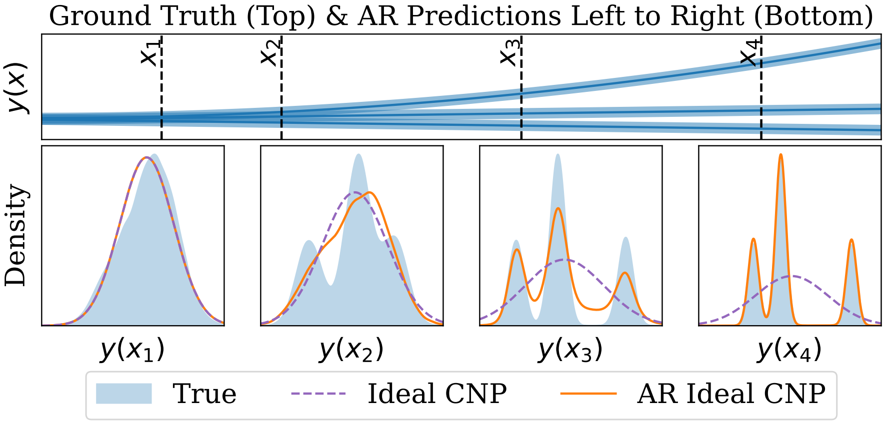
- First few AR steps poor, then become more accurate.
- Different random order for every sample: average out first few bad AR steps.

Some Intuition (2)



AR Sampling Design Space

Naively AR sampling 100 target points:

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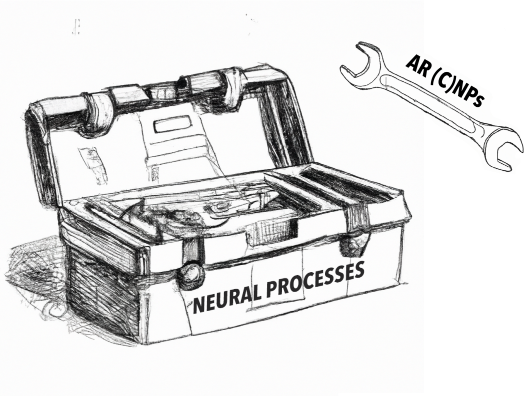
✓ Only 10 model forwards!

Today's Message



AR (C)NPs equip the NP toolbox with a new tool where modelling complexity and computational expense at training time can be traded for computational expense at test time.

Experiment: Cloud Cover Over Antarctica

- Cloud cover is in $[0,1]$, so use categorical–Beta mixture prediction:

$$q(\mathbf{y} \mid \mathbf{x}, D) = \prod_{i=1}^{|\mathbf{y}|} \begin{cases} p_{0,\theta} & \text{if } y_i = 0, \\ p_{1,\theta} & \text{if } y_i = 1, \\ (1 - p_{0,\theta} - p_{1,\theta}) \operatorname{Beta}(y_i; \alpha_\theta, \beta_\theta) & \text{if } y_i \in (0,1). \end{cases}$$

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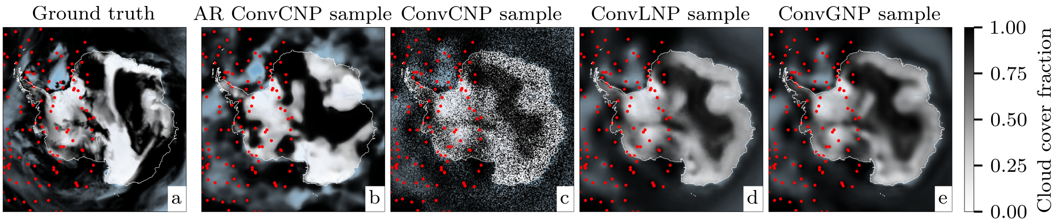

Prediction Map Approximation: A Theoretical Analysis

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Sketch of Theoretical Analysis

e.g., CNPs choose all GPs with independent predictions

- Prediction map: $\pi\colon \mathcal{D} \to \mathcal{Q}$.

- Posit a ground truth stochastic process f, possibly non-Gaussian.
- Posterior prediction map: $\pi_f\colon \mathcal{D} \to \mathcal{P}$, $\pi_f(D) = p(f \mid D)$.
- Approximate π_f with a neural process $\pi_\theta\colon \mathcal{D} \to \mathcal{Q}$.
- Do this by minimising the neural process objective $\mathcal{L}_{\mathsf{NP}}$:

$f(\mathbf{x}) + \boldsymbol{\varepsilon} \sim P^\sigma_{\mathbf{x}}\mu$

with $f \sim \mu$ and $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$

$$\hat{\theta} \in \arg\min \mathcal{L}_{\mathsf{NP}}(\pi_f, \pi_\theta), \quad \mathcal{L}_{\mathsf{NP}}(\pi_f, \pi_\theta) = \mathbb{E}_{p(\mathbf{x})p(D)}[\mathrm{KL}(P^{\sigma_f}_{\mathbf{x}}\pi_f(D), P^{\sigma}_{\mathbf{x}}\pi_\theta(D))].$$

- Study minimisers for CNPs and GNPs.

convergence to minimiser (consistency); compare minimisers for CNPs and GNPs

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Many results obvious...

But exciting that all can be established in one unifying theoretical framework!

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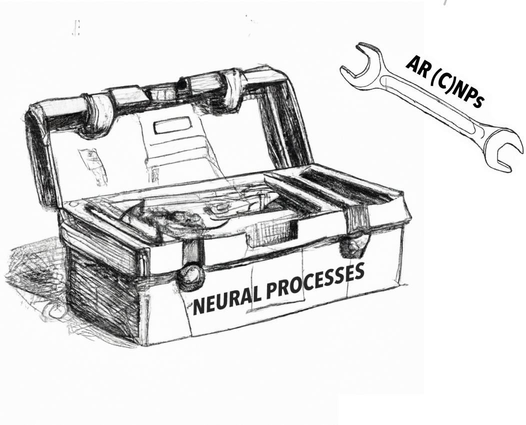
- Approximate equivariances? Got some preliminary results!

Conclusion

Wrapping Up

Neural processes:

- a flexible collection of architectural neural network techniques
- for general supervised learning problems.



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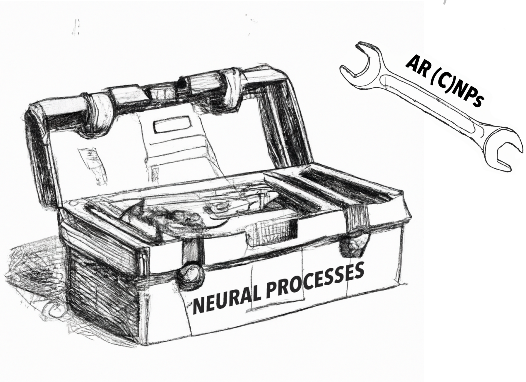
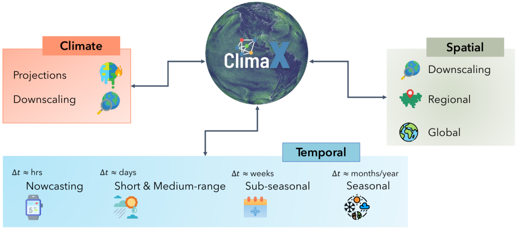


Paper:	This presentation:	Code:
`wessel.ai/pdf/arcnps`	`wessel.ai/pdf/arcnps-mlls`	`github.com/wesselb/neuralprocesses`

Would you like to collaborate? Reach out at `hi@wessel.ai`

Microsoft Research

- Member of the PDE Team within the AI4Science initiative at Microsoft Research
- We're building a foundation model for weather and climate prediction:



Nguyen, Brandstetter, et al. (2023)

Interested? Reach out at `wbruinsma@microsoft.com`

Appendix

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