Meta-Learning as Prediction Map Approximation

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Research Talk at CBL, 23 Feb 2022

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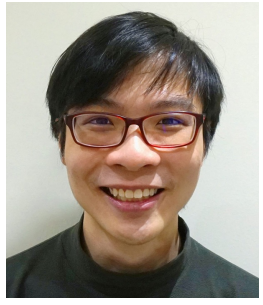

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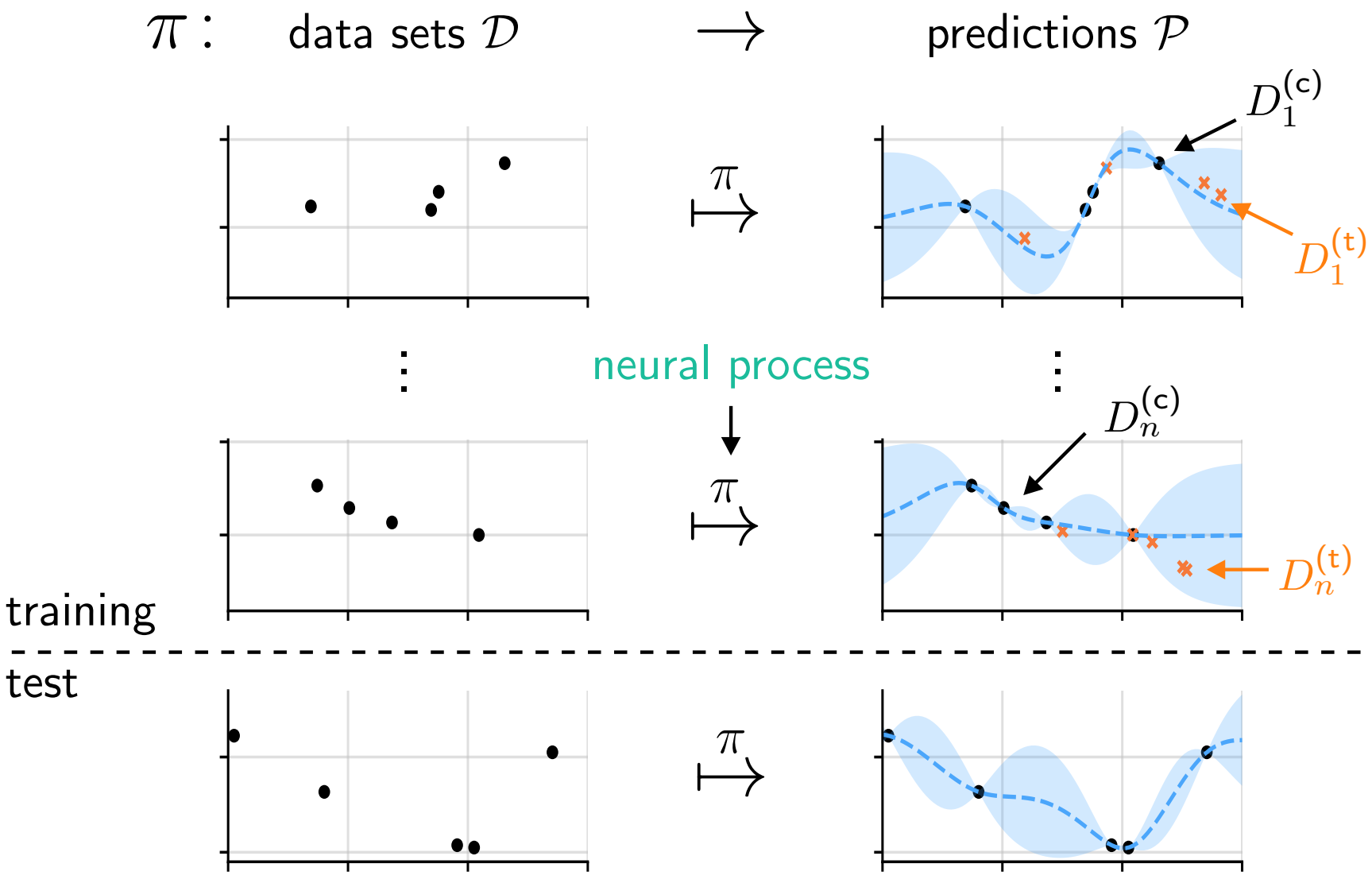
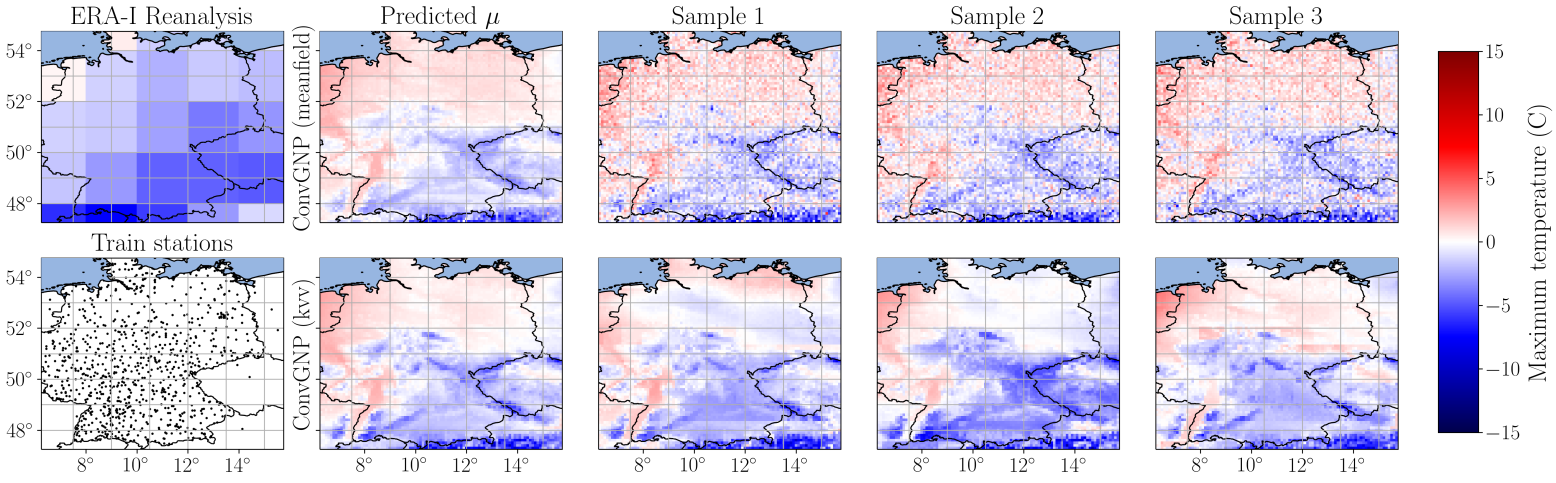
Meta-Learning and Neural Processes

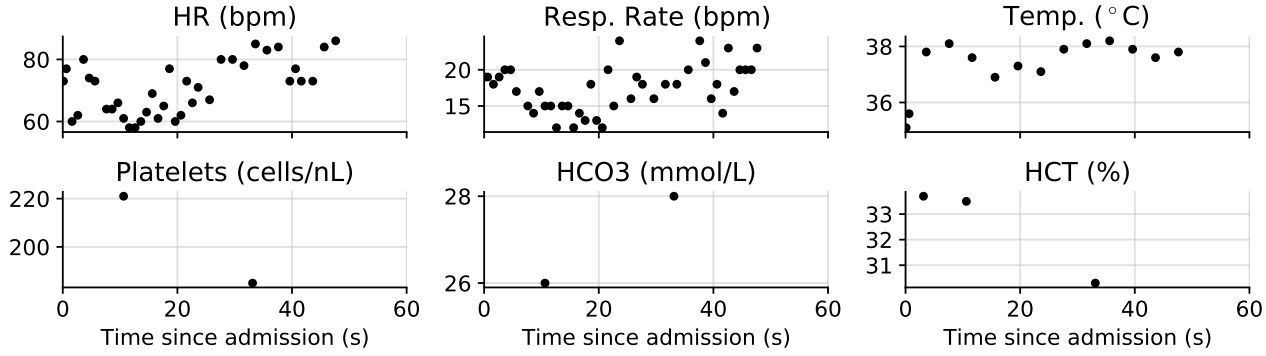


Applications of Neural Processes

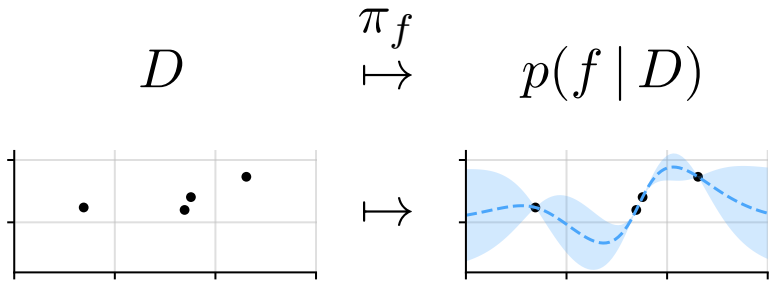
- Climate model downscaling (Markou et al., 2022):

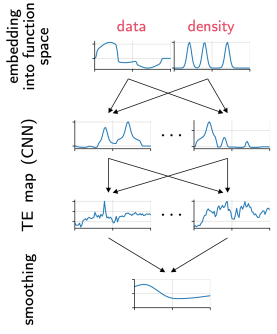


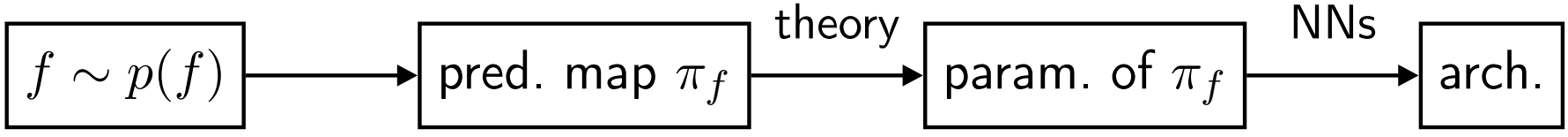
- ICU monitoring (Silva et al., 2012; Shysheya, 2020):

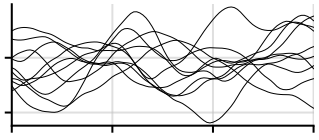


Today: Prediction Map Approximation









$$m(D) = \rho\big(\textstyle\sum_{(x,y)\in D} \phi(x,y)\big)$$

- ✓ Theoretical framework
- ✓ Architectures with universal approximation properties
- ✓ Properties of $f \Rightarrow$ symmetries of $\pi_f \Rightarrow$ param. efficient archs!

Prediction Map Approximation

Setup

e.g., a sawtooth wave

- Let f be some ground-truth stochastic process.
- Posterior prediction map: $\pi_f \colon \mathcal{D} \to \mathcal{P}$, $\pi_f(D) = p(f \mid D)$.
- Goal: find Gaussian approximation $\tilde{\pi} \colon \mathcal{D} \to \mathcal{P}_{\mathsf{G}}$.
- Approach:

$$\tilde{\pi}(D) \in \operatorname*{arg\,min}_{\mu \in \mathcal{P}_{\mathsf{G}}} \mathrm{KL}(\pi_f(D), \mu).$$

✗ Approximate f and perform inference in approximation.

✓ Directly approximate posteriors of f.

- $\mathrm{KL}(\mathcal{GP}(0, 1 \cdot e^{-|\cdot|}), \mathcal{GP}(0, \sigma^2 e^{-|\cdot|})) = \infty$ unless $\sigma^2 = 1$!
- If $\mathrm{KL}(\pi_f(D), \mu_0) < \infty$ for some $\mu_0 \in \mathcal{P}_{\mathsf{G}}$, then

$$\tilde{\pi}(D) = \pi_{\mathsf{MM}}(D) := \mathcal{GP}(m_{f \mid D}, k_{f \mid D}).$$

Neural Processes

- Practical objective:

if $f \sim \pi(D)$, then $(f(x_1), ..., f(x_n)) \sim P_{\mathbf{x}}\pi(D)$

à la variational family $\tilde{\pi} \in \arg\min_{\pi \in \mathcal{Q}} \mathcal{L}(\pi)$,

$$\mathcal{L}(\pi) = \mathbb{E}_{p(D)p(\mathbf{x})} \mathrm{KL}(P_{\mathbf{x}}\pi_f(D), P_{\mathbf{x}}\pi(D))$$

$$\approx -\frac{1}{N}\sum_{n=1}^{N} \log q(D_n^{(\mathsf{t})} \mid D_n^{(\mathsf{c})}) := \mathcal{L}_n(\pi)$$

density of $\pi(D_n^{(\mathsf{c})})$

- Call π continuous if $D_i \to D$ implies $\pi(D_i) \rightharpoonup \pi(D)$.
- Setting $\mathcal{Q}$ to

$$\mathcal{M}_{\mathsf{G}} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\mathsf{G}} : \pi \text{ continuous}\},$$

minimiser exists, is unique, and coincides with original problem!

Parametrising Prediction Maps

GPs without correlations, *i.e.* $k(x, x') = 0$ if $x \neq x'$

- For now, consider $\mathcal{Q}_{\text{G,MF}} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\text{G,MF}}\}$.
- Separately parametrise mean map and variance map:

$$m \colon \mathcal{D} \to C(\mathbb{R}, \mathbb{R}), \qquad \sigma^2 \colon \mathcal{D} \to C(\mathbb{R}, (0, \infty)).$$

Thm (Zaheer et al., 2017; Wagstaff et al., 2019). A continuous function $f \colon \mathcal{D}_{\leq M} \to Z$ has the form of a deep set:

$$f(D) = \rho\big(\textstyle\sum_{(x,y)\in D} \phi(x, y)\big)$$

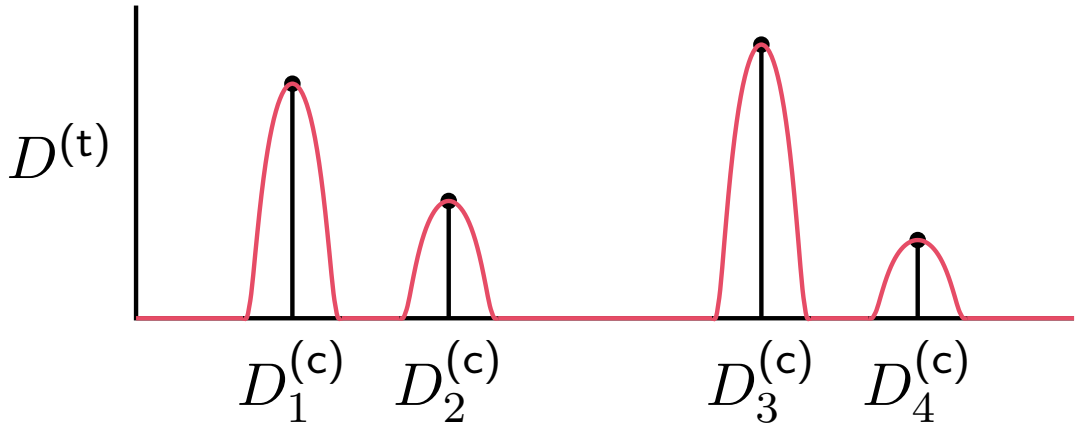
where $\phi \colon \mathbb{R}^2 \to \mathbb{R}^M$ and $\rho \colon \mathbb{R}^M \to Z$ are continuous.

- Conditional neural process (Garnelo et al., 2018):

$$\boxed{\mathcal{L} + \mathcal{Q}_{\text{G,MF}} + \text{deep sets for } \pi = \text{CNP}}$$

Consistency of Prediction Map Approximation

The Problem



$$\mathcal{L}_n(\pi) = -\frac{1}{N}\sum_{n=1}^{N} \log q(D_n^{(\mathsf{t})} \mid D_n^{(\mathsf{c})}) \text{ “}\approx \frac{1}{N}\sum_{n=1}^{N}(D_n^{(\mathsf{t})} - f(D_n^{(\mathsf{c})}))^2\text{ ”}$$

$\Rightarrow$ Cannot optimise $\mathcal{L}_n(\pi)$ over $\pi \in \mathcal{M}_{\mathsf{G}}$: overfitting!

- Practice: tune NN capacity using black magic.
- Will show that we can reasonably restrict to compact $\mathcal{Q} \subset \mathcal{M}_{\mathsf{G}}$.

Assumptions on Ground-Truth Process

Let $\mathcal{D} \subseteq \bigcup_{n=0}^{\infty} (\mathcal{X} \times \mathbb{R})^n$ be a collection of data sets of interest.

Assumptions:

- $\mathcal{X}$ is compact.
- There exist $p \geq 2$, $q > 1$, $c > 0$, and $r > 0$ such that

$$\mathbb{E}[|f(x) - f(y)|^p] \leq c|x - y|^q \quad \text{whenever} \quad |x - y| < r.$$

- $\mathcal{D}$ is bounded: $|||\mathcal{D}||| := \sup\{|\mathbf{x}| \vee \|\mathbf{y}\|_\infty : (\mathbf{x}, \mathbf{y}) \in \mathcal{D}\} < \infty$.
- $M := \sup_{x \in \mathcal{X}} [|f(x)|^{2+\gamma}] < \infty$ for some $\gamma > 0$.
- Observations under Gaussian noise with $\sigma^2 \in [\underline{\sigma}^2, \overline{\sigma}^2]$.

A Compact Variational Family

- Identify every $\pi \in \mathcal{M}_{\mathsf{G}}$ with

$$m\colon \mathcal{X} \times \mathcal{D} \to \mathbb{R}, \quad k\colon \mathcal{X} \times \mathcal{X} \times \mathcal{D} \to \mathbb{R}, \quad \sigma^2 \in [\underline{\sigma}^2, \overline{\sigma}^2].$$

- Then exist $L^*\colon [0,\infty)^2 \to [0,\infty)$ and $M^* > 0$ such that

$$\pi_{\mathsf{MM}} \in \left\{ \pi \in \mathcal{M}_{\mathsf{G}} \;\middle|\; \begin{array}{c} |m(x_1,D_1) - m(x_2,D_2)| \le L^*(|x_1 - x_2|, \|D_1 - D_2\|) \\ |k(x_1,D_1) - k(x_2,D_2)| \le L^*(|x_1 - x_2|, \|D_1 - D_2\|) \\ \|m\|_\infty, \|k\|_\infty \le M^* \end{array} \right\}.$$

- Call this collection $\mathcal{Q}^*$. Define a metric on $\mathcal{Q}^*$:

$$d(\pi_1, \pi_2) = \|m_1 - m_2\|_\infty + \|k_1 - k_2\|_\infty + |\sigma_1^2 - \sigma_2^2|.$$

- Arzelà–Ascoli theorem: $(\mathcal{Q}^*, d)$ is compact.

Consistency of Prediction Map Approximation

Thm. Let

$$\pi_n \in \operatorname*{arg\,min}_{\pi \in \mathcal{Q}^*} \mathcal{L}_n(\pi), \quad \mathcal{L}_n(\pi) = -\frac{1}{N} \sum_{n=1}^{N} \log q(D_n^{(\mathsf{t})} \mid D_n^{(\mathsf{c})}).$$

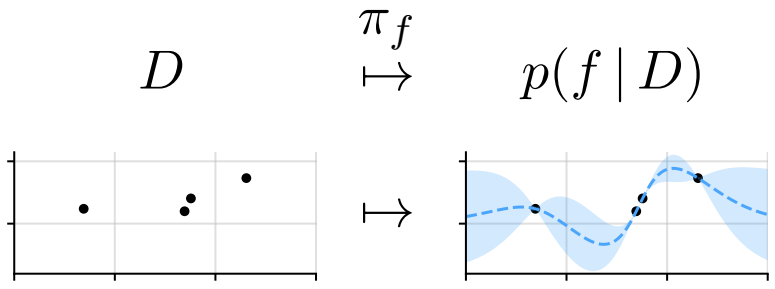
Then, almost surely, $\pi_n(D) \rightharpoonup \pi_{\mathsf{MM}}(D)$ for all $D \in \mathcal{D}$.

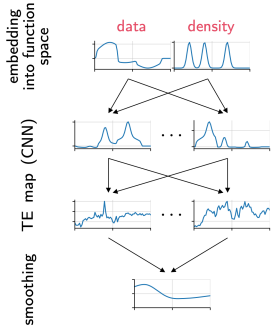
Pending questions:

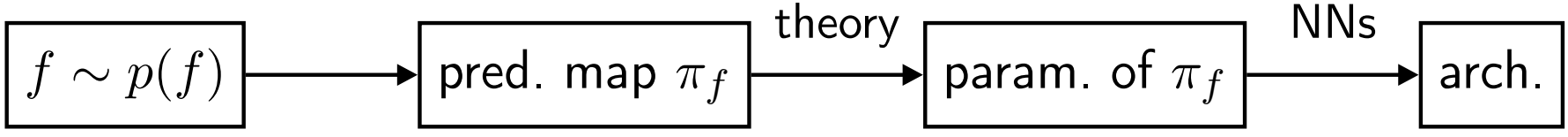
- $\mathcal{Q}_{\mathsf{NN}} = \{(m_\theta, k_\theta, \sigma^2) : \theta \in \mathbb{R}^P\}$?
- How much data: finite-sample bounds / rates of convergence?

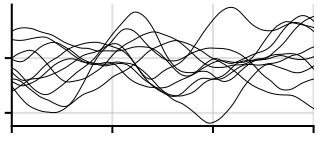
Wrapping Up

Prediction Map Approximation









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These slides: `https://wesselb.github.io/pdf/cbl-predmap`.

Appendix

References

Garnelo, M., D. Rosenbaum, C. J. Maddison, T. Ramalho, D. Saxton, M. Shanahan, Y. Whye Teh, D. J. Rezende, and S. M. A. Eslami (2018). "Conditional Neural Processes". In: *Proceedings of 35th International Conference on Machine Learning*. Vol. 80. Proceedings of Machine Learning Research. PMLR. eprint: https://arxiv.org/abs/1807.01613.

Markou, Stratis, James Requeima, Wessel P. Bruinsma, and Richard E. Turner (2022). "Practical Conditional Neural Processes for Tractable Dependent Predictions". In: *Proceedings of the 10th International Conference on Learning Representations*.

Shysheya, Aliaksandra (2020). "Neural Models for Non-Uniformly Sampled Data". MA thesis. Department of Engineering, University of Cambridge.

References (2)

Silva, Ikaro, George Moody, Daniel J. Scott, Leo A. Celi, and Roger G. Mark (2012). "Predicting In-Hospital Mortality of ICU Patients: The PhysioNet/Computing in Cardiology Challenge 2012". In: *Computing in Cardiology* 39, pp. 245–248.

Wagstaff, E., F. B. Fuchs, M. Engelcke, I. Posner, and M. Osborne (2019). "On the Limitations of Representing Functions on Sets". In: *Proceedings of 36th International Conference on Machine Learning*. Vol. 97. Proceedings of Machine Learning Research. PMLR. eprint: https://arxiv.org/abs/1901.09006.

Zaheer, M., S. Kottur, S. Ravanbakhsh, B. Poczos, R. Salakhutdinov, and A. Smola (2017). "Deep Sets". In: *Advances in Neural Information Processing Systems 30*. Curran Associates, Inc. eprint: https://arxiv.org/abs/1703.06114.