Meta-Learning as Prediction Map Approximation

Wessel Bruinsma

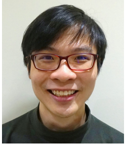
University of Cambridge and Invenia Labs

Research Talk at CBL, 23 Feb 2022

Collaborators

Wessel Bruinsma

Jonathan Gordon



Andrew Foong

James Requeima

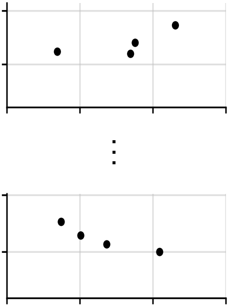
Stratis Markou

Anna Vaughan

Yann Dubois

Rich Turner

Meta-Learning and Neural Processes



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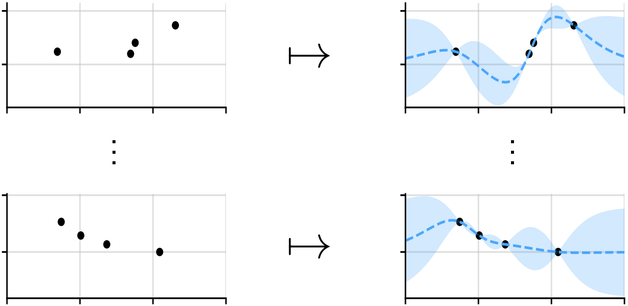

Meta-Learning and Neural Processes

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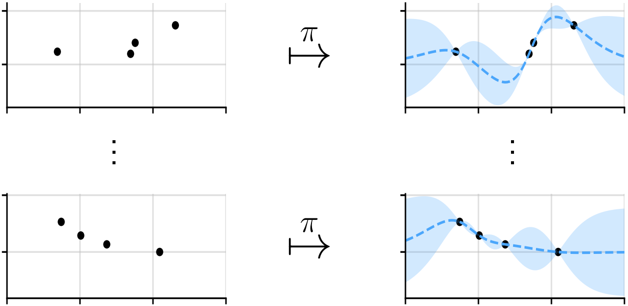

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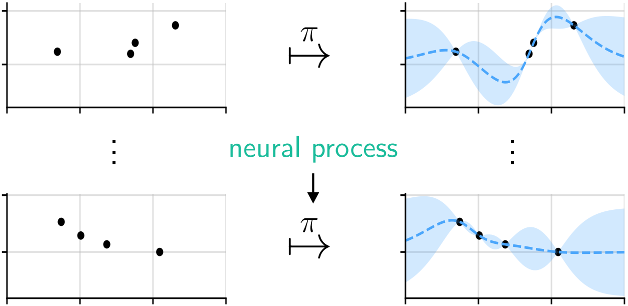

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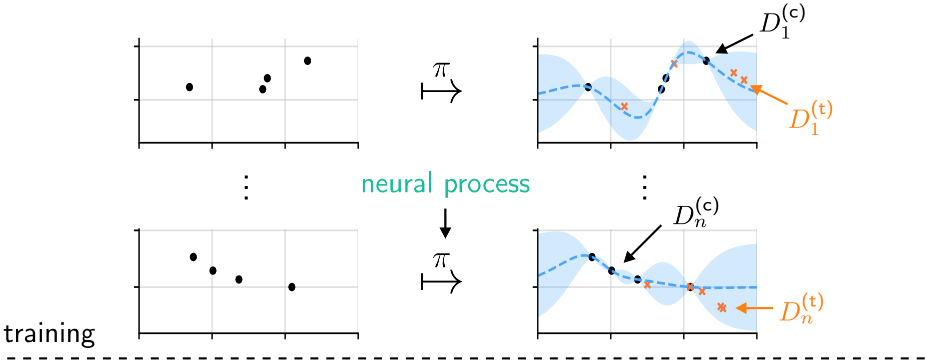

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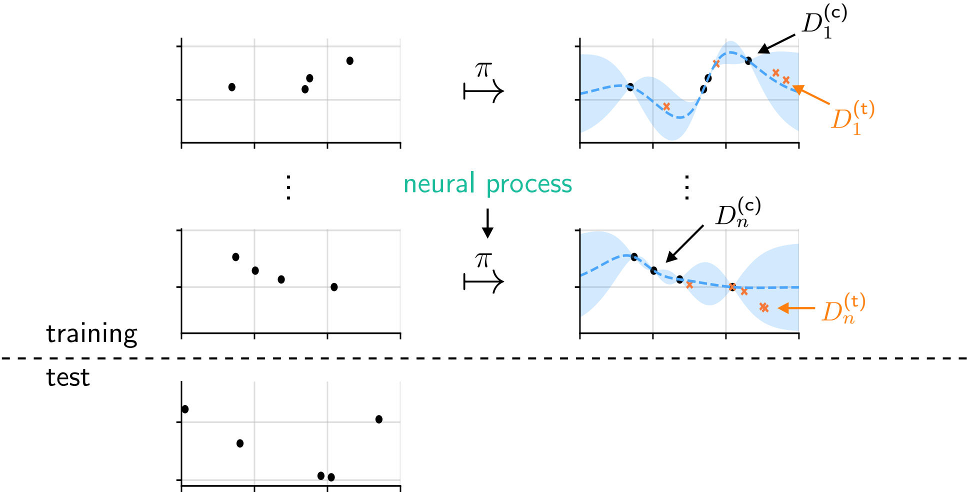

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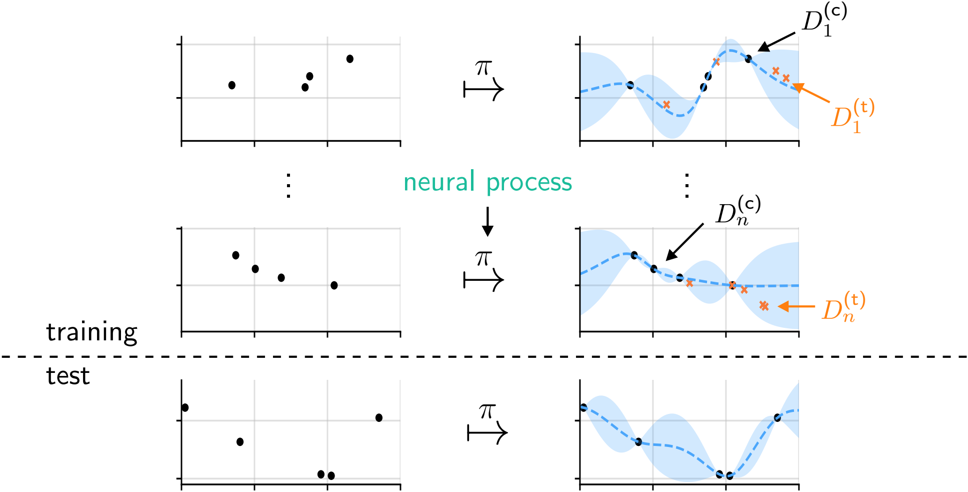
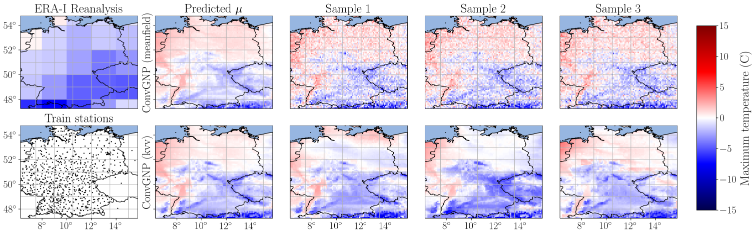


Applications of Neural Processes

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



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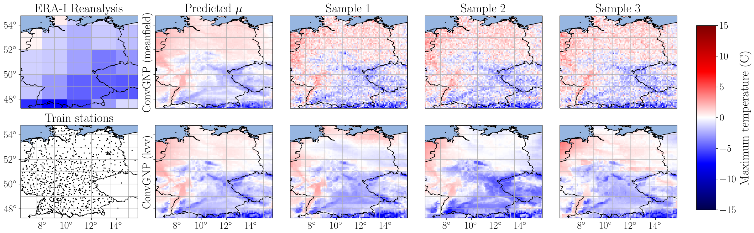
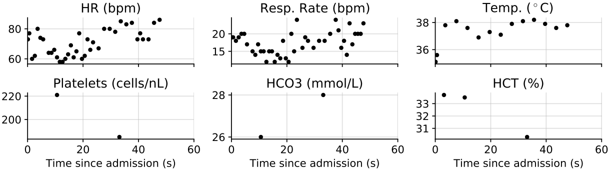


- ICU monitoring (Silva et al., 2012; Shysheya, 2020):



Today: Prediction Map Approximation

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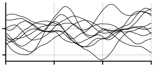
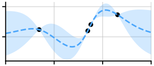


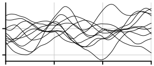
Today: Prediction Map Approximation

$$D \overset{\pi_f}{\mapsto} p(f \mid D)$$

$\mapsto$



$$\boxed{f \sim p(f)} \longrightarrow \boxed{\text{pred. map } \pi_f}$$



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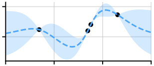
 $\mapsto$ 

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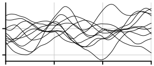

$$m(D) = \rho\Big(\textstyle\sum_{(x,y)\in D} \phi(x,y)\Big)$$

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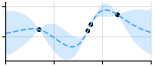

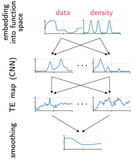

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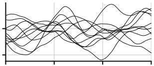

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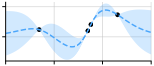

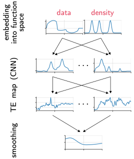

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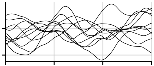

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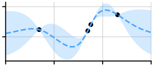
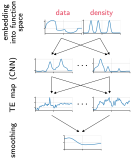
 $\mapsto$ 



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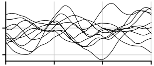

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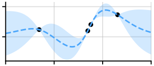

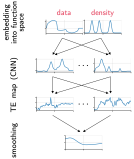

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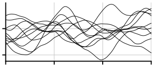

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- ✓ Theoretical framework
- ✓ Architectures with universal approximation properties
- ✓ Properties of $f \Rightarrow$ symmetries of $\pi_f \Rightarrow$ param. efficient archs!

Prediction Map Approximation

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

- Practical objective:

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

- Practical objective:

à la variational family $\longrightarrow$

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$$\begin{aligned}\mathcal{L}(\pi) &= \mathbb{E}_{p(D)p(\mathbf{x})} \operatorname{KL}(P_{\mathbf{x}}\pi_f(D), P_{\mathbf{x}}\pi(D)) \\ &\approx -\frac{1}{N}\sum_{n=1}^{N} \log q(D_n^{(\mathsf{t})} \mid D_n^{(\mathsf{c})}) := \mathcal{L}_n(\pi)\end{aligned}$$

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

Neural Processes

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- 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

- For now, consider $\mathcal{Q}_{\mathsf{G,MF}} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\mathsf{G,MF}}\}$.

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GPs without correlations,
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- Separately parametrise mean map and variance map:

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

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

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

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- 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

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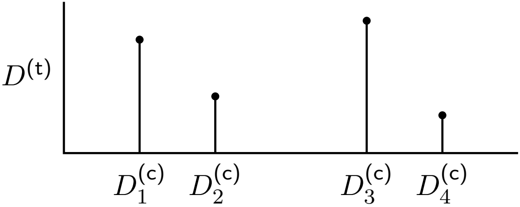

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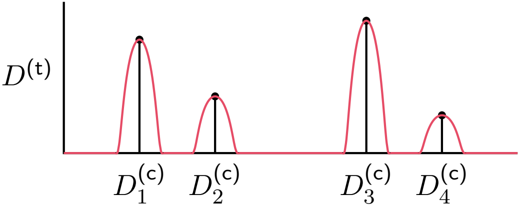

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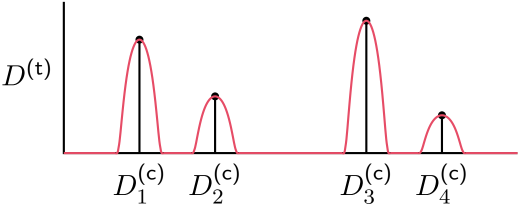

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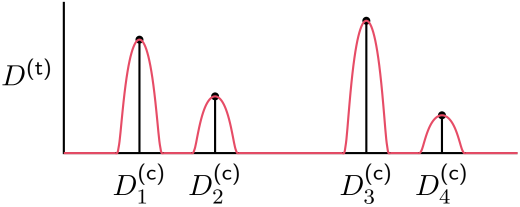

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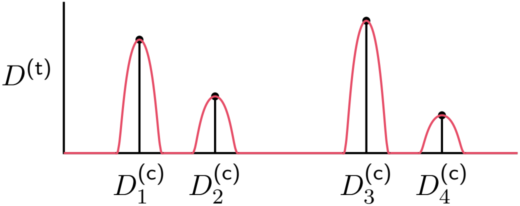

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- Practice: tune NN capacity using black magic.
- Will show that we can reasonably restrict to compact $\mathcal{Q} \subset \mathcal{M}_{\mathsf{G}}$.

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- Observations under Gaussian noise with $\sigma^2 \in [\underline{\sigma}^2, \overline{\sigma}^2]$.

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

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

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

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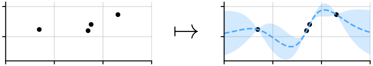
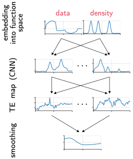
- How much data: finite-sample bounds / rates of convergence?

Wrapping Up

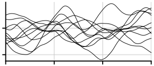
Prediction Map Approximation

$$D \overset{\pi_f}{\mapsto} p(f \mid D)$$





$$\boxed{f \sim p(f)} \longrightarrow \boxed{\text{pred. map } \pi_f} \xrightarrow{\text{theory}} \boxed{\text{param. of } \pi_f} \xrightarrow{\text{NNs}} \boxed{\text{arch.}}$$



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

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

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`.