Meta-Learning as Prediction Map Approximation

Wessel Bruinsma

University of Cambridge and Invenia Labs

Job Research Talk at Microsoft Research, 6 Jan 2022

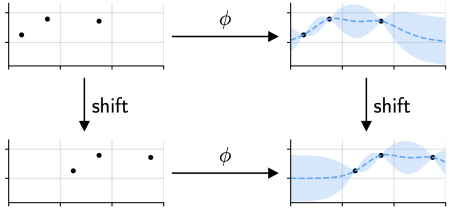
Hello! 👋

- PhD student at Cambridge MLG, supervised by Rich Turner.
- Researcher at Invenia Labs.

- MPhil in MLMI (Cam).
- BSc in EE (Delft).

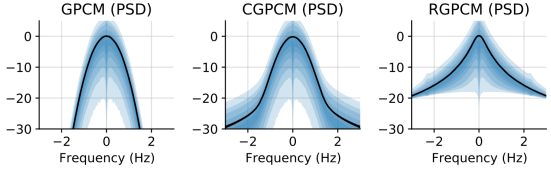
Neural processes:

- equivariance,
- correlated predictions



Gaussian processes:

- multiple outputs,
- nonpar. kernel priors



Theory:

- MFVI BNNs $\Rightarrow$ prior,
- PAC Bayes

$$\|\mathbb{E}_Q[\mathbf{f}(\mathbf{x})] - \mathbb{E}_P[\mathbf{f}(\mathbf{x})]\|_2 \leq c_1 c_2^{L-1} \frac{1 + \frac{1}{\sqrt{D_i}}\|\mathbf{x}\|_2}{\sqrt{M}} \mathrm{KL}(Q,P)(\mathrm{KL}(Q,P)^{\frac{L-1}{2}} \vee 1),$$

$$\|\mathbb{E}_Q[\mathbf{f}^2(\mathbf{x})] - \mathbb{E}_P[\mathbf{f}^2(\mathbf{x})]\|_\infty \leq c_3 c_4^{L-1} \frac{1 + \frac{1}{D_i}\|\mathbf{x}\|_2^2}{\sqrt{M}} \mathrm{KL}(Q,P)(\mathrm{KL}(Q,P)^{L-1} \vee 1)$$

Hello! 👋 (2)

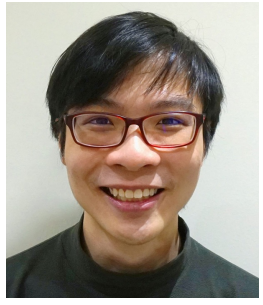
- Stheno (`github.com/wesselb/stheno`)
- Plum (`github.com/wesselb/plum`)
- Matrix (`github.com/wesselb/matrix`)

```
>>> from matrix import Diagonal, LowRank, Woodbury, Kronecker, LowerTriangular, ...

>>> d = Diagonal(np.array([1, 2, 3]))

>>> B.inv(d + 1)
<Woodbury matrix: batch=(), shape=(3, 3), dtype=float64
 diag=<diagonal matrix: batch=(), shape=(3, 3), dtype=float64
       diag=[1.    0.5   0.333]>
 lr=<low-rank matrix: batch=(), shape=(3, 3), dtype=float64, rank=1
                 ...
                 [0.333]]>>>

>>> B.inv(B.inv(d + 1)) - 1
<diagonal matrix: batch=(), shape=(3, 3), dtype=float64
 diag=[1. 2. 3.]>
```

Collaborators

Wessel Bruinsma

Jonathan Gordon



Andrew Foong

James Requeima

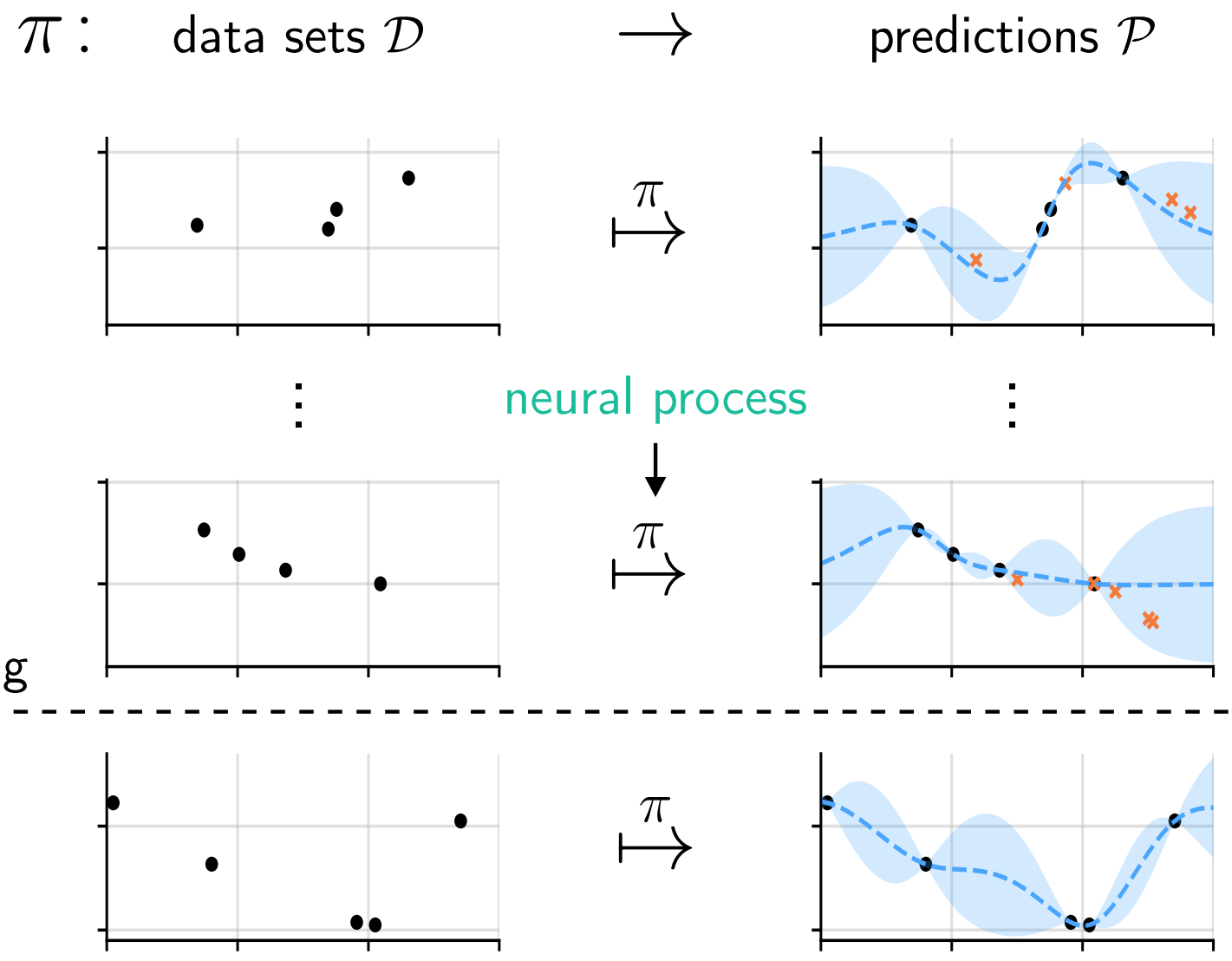
Stratis Markou

Yann Dubois

Anna Vaughan

Rich Turner

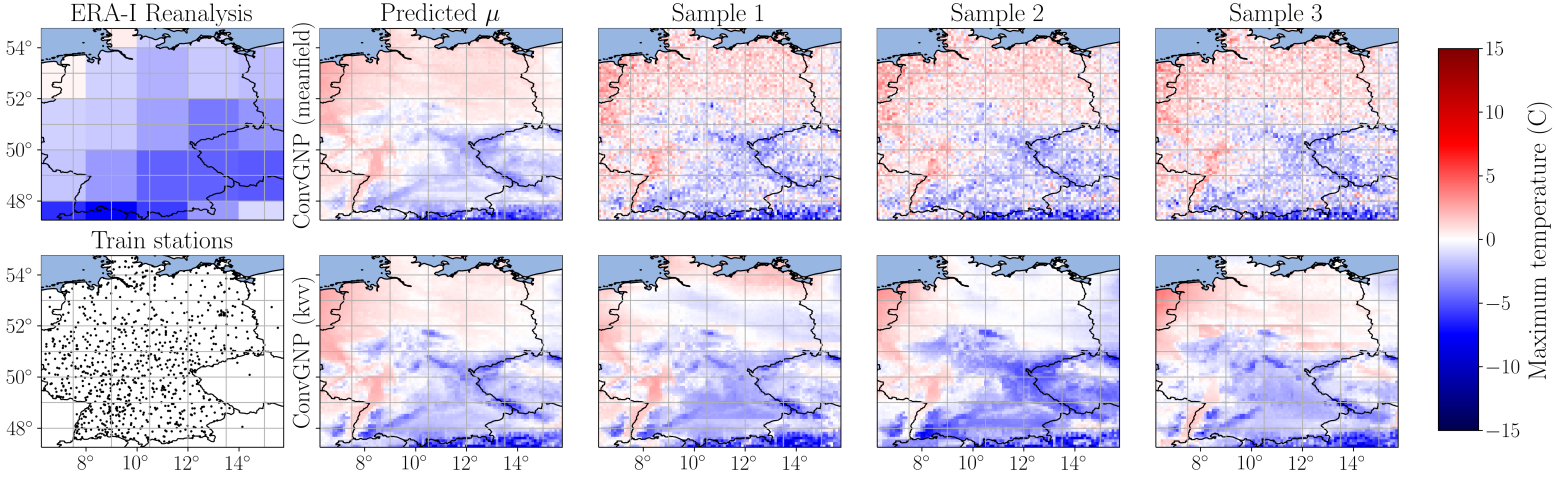
Meta-Learning and Neural Processes



Examples of Neural Processes

- Image completion (Gordon, Bruinsma, et al., 2020):

- Climate model downscaling (Markou et al., 2021):



Examples of Neural Processes (2)

- Potential energy surface prediction:

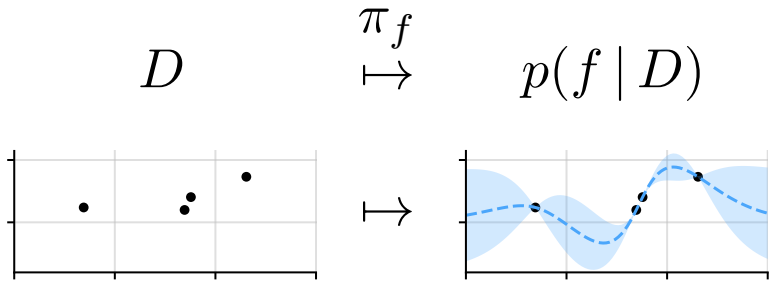
```
C    0.0072 -0.5687  0.0
C   -1.2854  0.2499  0.0
O    1.1304  0.3147  0.0
H    0.0392 -1.1972  0.89
H    0.0392 -1.1972 -0.89
H   -1.3175  0.8784  0.89
H   -1.3175  0.8784 -0.89
H   -2.1422 -0.4239  0.0
H    1.9857 -0.1365  0.0
```

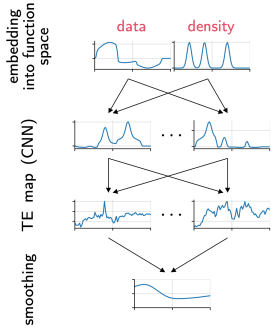
$\longmapsto$

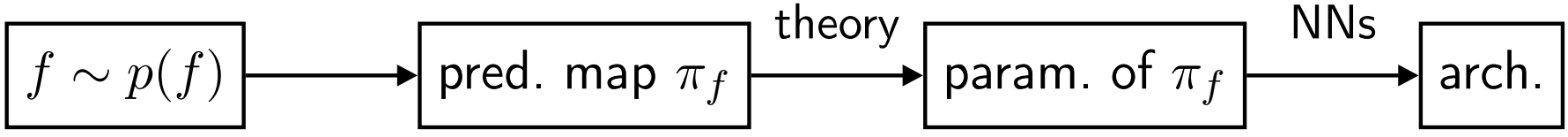
$$U_{\mathrm{BO}}(\mathbf{r}_1, \ldots, \mathbf{r}_{n_{\mathrm{atoms}}})$$
and/or
$$(\mathbf{f}_1, \ldots, \mathbf{f}_{n_{\mathrm{atoms}}})$$

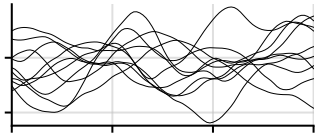
1. Variable number and permutation invariance of atoms
2. Energy conservation of forces
3. Rototranslation invariance (energy) or equivariance (forces)

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: approximate π_f with $\tilde{\pi} \in \mathcal{Q}$ (à la variational family).
- Approach: Minimise loss function:

$$\tilde{\pi} \in \operatorname*{arg\,min}_{\pi \in \mathcal{Q}} \mathcal{L}_{\mathrm{Div}}(\pi), \quad \mathcal{L}_{\mathrm{Div}}(\pi) = \sup_{D \in \mathcal{D}} \mathrm{Div}(\pi_f(D), \pi(D)).$$

↑ some divergence; *e.g.*, $\mathrm{Div} = \mathrm{KL}$

- Regularity of π_f? Existence of $\tilde{\pi}$?
  - $\mathrm{KL}(\mathcal{GP}(0, 1 \cdot e^{-|\cdot|}), \mathcal{GP}(0, \sigma^2 e^{-|\cdot|})) = \infty$ unless $\sigma^2 = 1$!

✗ Approximate f and perform inference in approximation.

✓ Directly approximate posteriors of f.

Parametrising Prediction Maps

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

- For now, consider $\mathcal{Q}_{\text{G,MF}} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\text{G,MF}}\}$.
- How do we parametrise a $\pi \colon \mathcal{D} \to \mathcal{P}_{\text{G,MF}}$?

$\Rightarrow$ 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.

A Practical Objective

- Appealing objective, but theoretical issues:

$$\mathcal{L}_{\mathsf{KL}}(\pi) = \sup_{D \in \mathcal{D}} \mathrm{KL}(\pi_f(D), \pi(D)).$$

- Practical objective (Garnelo, Rosenbaum, et al., 2018; Gordon, Bronskill, et al., 2019):

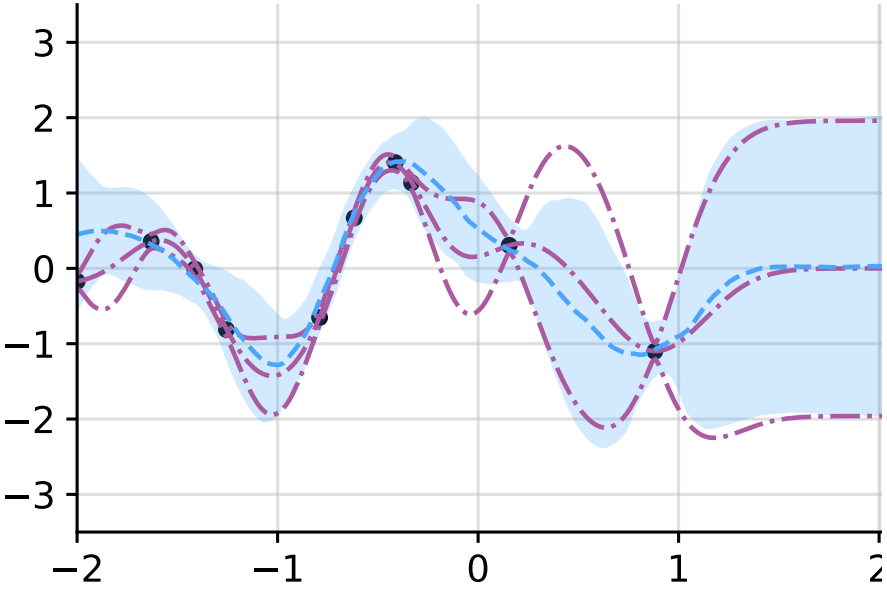
density of $\pi(D^{(\mathsf{c})})$

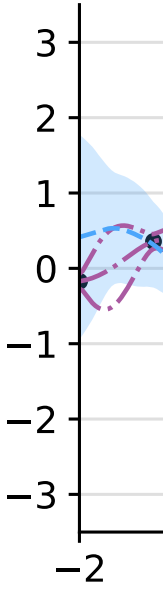
$$\begin{aligned}\mathcal{L}_{\mathsf{ML}}(\pi) &= \mathbb{E}_{p(D)}[\log q(D^{(\mathsf{t})} \mid D^{(\mathsf{c})})] \\ &\approx \tfrac{1}{M} \textstyle\sum_{m=1}^{M} \log q(D_m^{(\mathsf{t})} \mid D_m^{(\mathsf{c})}).\end{aligned}$$

- Under conditions, minimisers coincide (Bruinsma et al., 2021)!
- Conditional neural process (Garnelo, Rosenbaum, et al., 2018):

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

The Conditional Neural Process





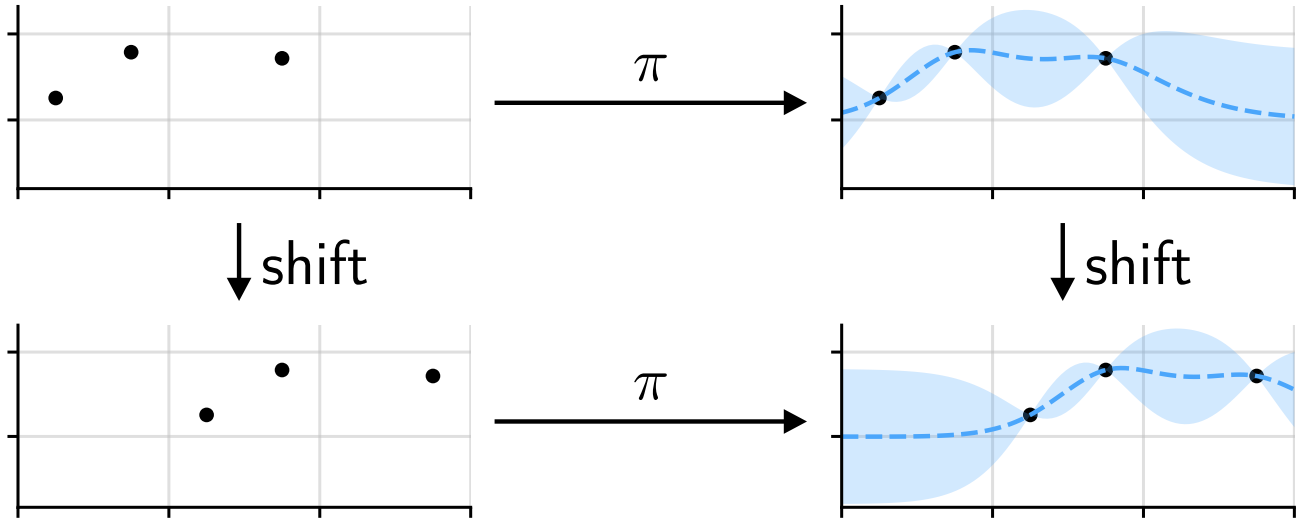
- ✗ Learns very slowly
- ✗ Underfits
- ✗ Generalises poorly

Exploiting Stationarity

Translation-Equivariant Prediction Maps

- Let T_τ represent a translation by τ.
- A prediction map $\pi : \mathcal{D} \to \mathcal{P}$ is translation equivariant (TE) if

$$\pi(\mathsf{T}_\tau D) = \mathsf{T}_\tau \pi(D).$$



Prop (Foong et al., 2020). f is stationary $\iff$ π_f is TE.

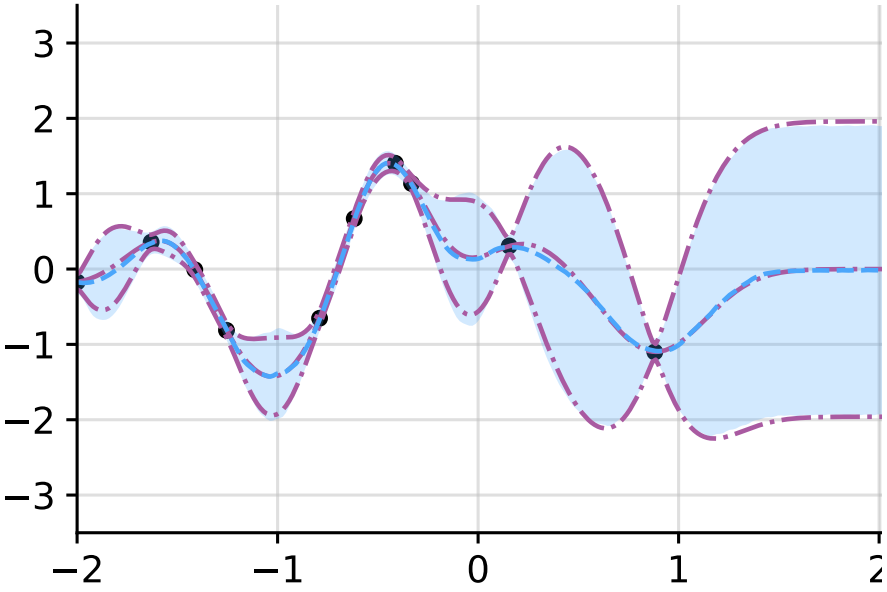
Parametrising TE Prediction Maps

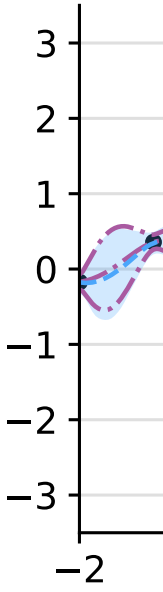
	Deep Set (Zaheer et al., 2017)	Convolutional Deep Set (Gordon, Bruinsma, et al., 2020)
	$f : \mathcal{D}_{\leq M} \to Z$ is cont.	$f : \mathcal{D}_{\leq M} \to Z$ is cont. and TE
	$\iff$	$\iff$
	T_τ?!	functional embedding (RKHS)
encoder	$E : \mathcal{D}_{\leq M} \to \mathbb{R}^M$, $E(D) = \sum_{(x,y)\in D} \phi(x, y)$	$E : \mathcal{D}_{\leq M} \to \mathbb{H}$, $E(D) = \sum_{(x,y)\in D} k(\bullet - x)\phi(y)$
decoder	$\rho : \mathbb{R}^M \to Z$, $f(D) = \rho(E(D))$	TE map between function spaces $\approx$ CNN $\rightarrow$ $\rho : \mathbb{H} \to Z$, $f(D) = \rho(E(D))$

- Gives convolutional CNP (Gordon, Bruinsma, et al., 2020):

$$\boxed{\mathcal{Q}_{\mathsf{G,MF}} + \text{conv. deep sets for } \pi + \mathcal{L}_{\mathsf{ML}} = \text{ConvCNP}}$$

The Convolutional CNP





- ✓ Learns pretty quickly
- ✓ Recovers target (diagonalised ground-truth GP)
- ✓ Generalises well

Further Improvements

Gaussian TE Prediction Maps

- ✗ (Conv)CNP fails to model correlations.
- $\mathcal{Q} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\mathsf{G}}\}$ instead of $\mathcal{Q} = \{\pi \colon \mathcal{D} \to \mathcal{P}_{\mathsf{G,MF}}\}$?
- Bruinsma et al. (2021) establishes repr. thm for kernel map:

$$k \colon \mathcal{D} \to C^{\text{p.s.d.}}(\mathbb{R} \times \mathbb{R}, \mathbb{R})$$

  - Kernel map is diagonally TE: CNNs?
  - ✓ Exploits TE using CNNs, learns quickly, and generalises well
  - ✗ D-dimensional inputs require $2D$-dimensional convolutions
- Markou et al. (2021) provide practical params for $D > 1$.
  - ✓ Approximation with TE basis functions works well

Non-Gaussian TE Prediction Maps

- Neural process (Garnelo, Schwarz, et al., 2018) uses latent variable $\mathbf{z}$ to model correlations: $\mathcal{Q}$ consists of maps π such that

$$f \sim \pi(D) \quad \Longleftrightarrow \quad \mathbf{z} \sim q(\mathbf{z} \mid D), \quad f \mid \mathbf{z} \sim p(f \mid \mathbf{z}).$$

  - ✓ Non-Gaussian and models correlations
  - ✗ $\mathcal{L}_{\mathsf{ML}}$ now intractable
  - ✗ Two ways to approximate $f \mid D^{(\mathsf{c})}, D^{(\mathsf{t})}$:

$$q(\mathbf{z} \mid D^{(\mathsf{c})}, D^{(\mathsf{t})}) \quad \text{and} \quad \tfrac{1}{Z} q(\mathbf{z} \mid D^{(\mathsf{c})}) p(D^{(\mathsf{t})} \mid \mathbf{z})$$

- NP objective tackles both simultaneously (Foong et al., 2020):

$$\mathcal{L}_{\mathsf{NP}}(\pi) = \underbrace{\mathcal{L}_{\mathsf{ML}}(\pi)}_{\approx \log p(\mathbf{y})} \underbrace{- \mathbb{E}_{p(D)}[\mathrm{KL}(q(\mathbf{z} \mid D^{(\mathsf{c})}, D^{(\mathsf{t})}), \tfrac{1}{Z} q(\mathbf{z} \mid D^{(\mathsf{c})}) p(D^{(\mathsf{t})} \mid \mathbf{z}))]}_{\approx \mathrm{KL}(q(\mathbf{z}), p(\mathbf{z} \mid \mathbf{y})),\ \text{encourages Bayes' consistency}}$$

Non-Gaussian TE Prediction Maps (2)

- Latent variable + ConvCNP = ConvNP (Foong et al., 2020)
- ✗ All constructions of NPs use mean-field approximation!
- Promising future direction:

  Combine latent variables with Gaussian TE prediction maps.

  - ✓ Improved uncertainty estimates
  - ✓ Enables approximation of models like Bernoulli random fields

Future Directions

- Combination of latent variable with correlated prediction maps
- Generalisation to other symmetry groups
  - Kawano et al. (2021) and Holderrieth et al. (2021) extend ConvCNP construction to more general symmetries
- Approximate symmetries:

Conjecture. Under conditions, a cont. function $f : \mathcal{D}_{\leq M} \to Z$ is approximately an augmented G-conv. deep set:

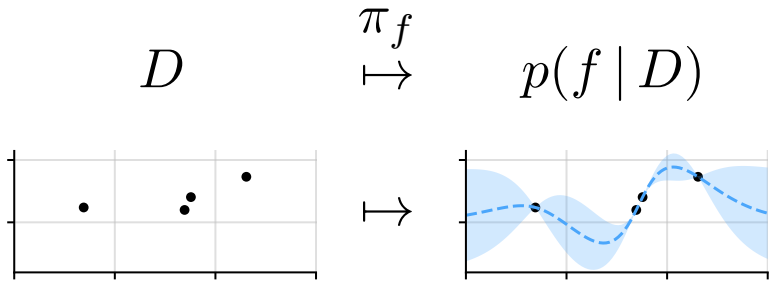
$$f(D) \approx \rho\big(\textstyle\sum_{(x,y)\in D} k(\bullet, x)\phi(y), h_1, \ldots, h_Q\big)$$

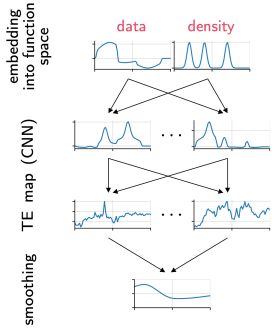
where

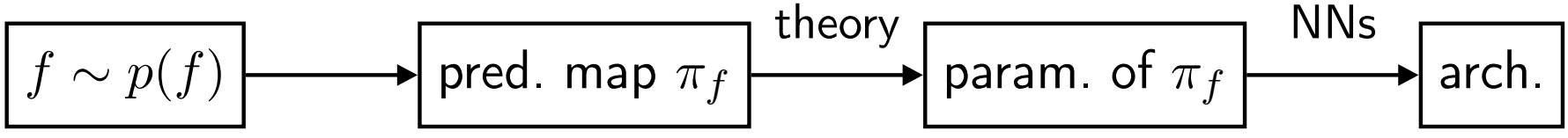
- $\phi\colon \mathbb{R} \to \mathbb{R}^{K+1}$ is continuous,
- $k\colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a G-invariant kernel,
- $h_1, \ldots, h_Q \in \mathbb{H}$ are additional channels, and
- $\rho\colon \mathbb{H} \to Z$ is continuous and G-equivariant.

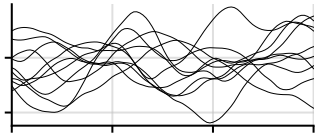
Wrapping Up

Prediction Map Approximation





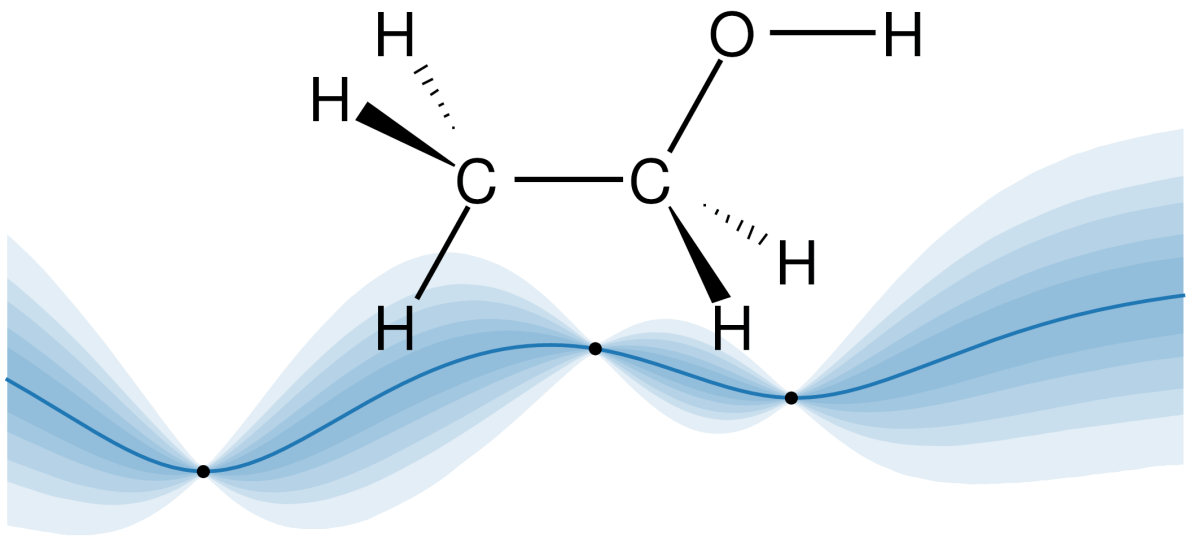




$$m(D) = \rho\big(\textstyle\sum_{(x,y)\in D} \phi(x,y)\big)$$

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

Wessel at Microsoft Research



- Theoretical background and experience in ML
- Practical experience in software engineering (Invenia Labs, OSS)
- Very keen to apply ML to scientific problems!

These slides: `https://wesselb.github.io/pdf/msr`.

Appendix

References

Bruinsma, Wessel P., James Requeima, Andrew Y. K. Foong, Jonathan Gordon, and Richard E. Turner (2021). "The Gaussian Neural Process". In: *Proceedings of the 3rd Symposium on Advances in Approximate Bayesian Inference*. eprint: https://arxiv.org/abs/2101.03606.

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