Meta-Learning as Prediction Map Approximation

Wessel Bruinsma

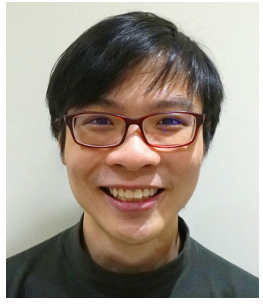
University of Cambridge and Invenia Labs

Research Talk at Sheffield Machine Learning Group, 24 Feb 2022

Collaborators

Wessel Bruinsma

Jonathan Gordon



Andrew Foong

James Requeima

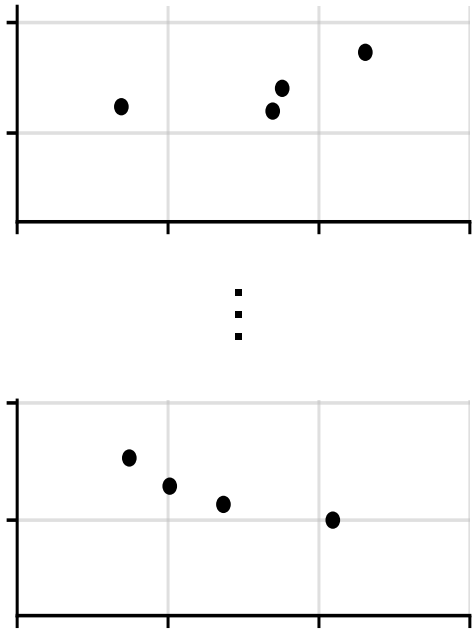
Stratis Markou

Anna Vaughan

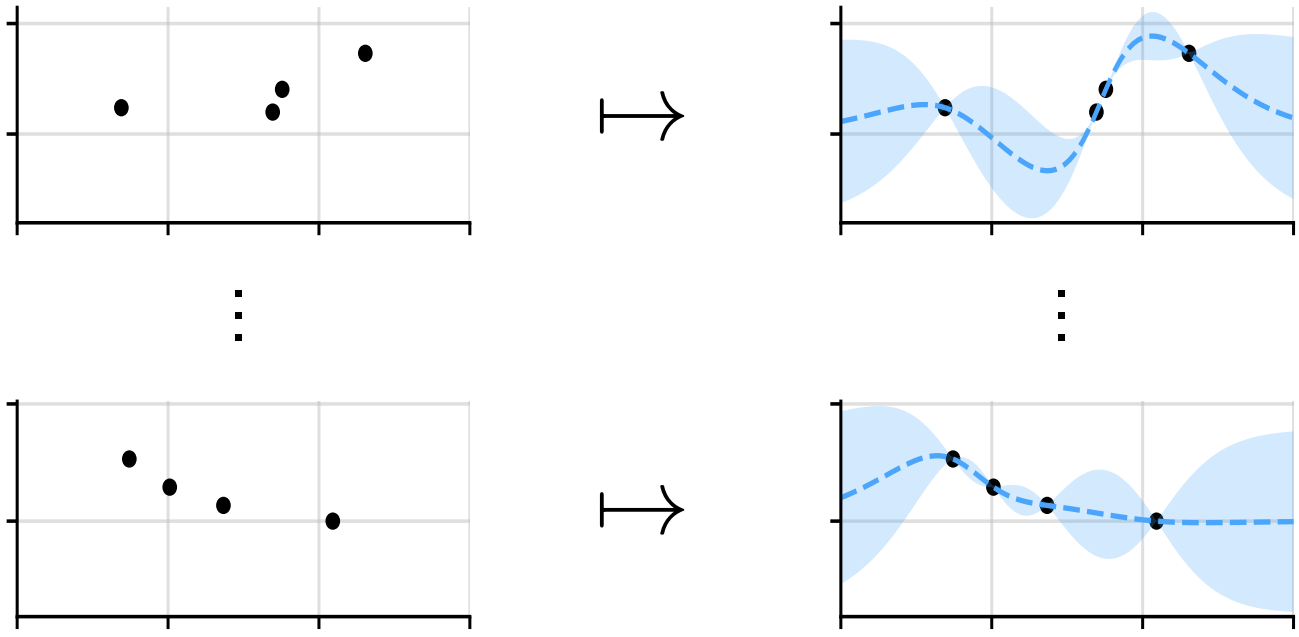
Yann Dubois

Rich Turner

Meta-Learning and Neural Processes

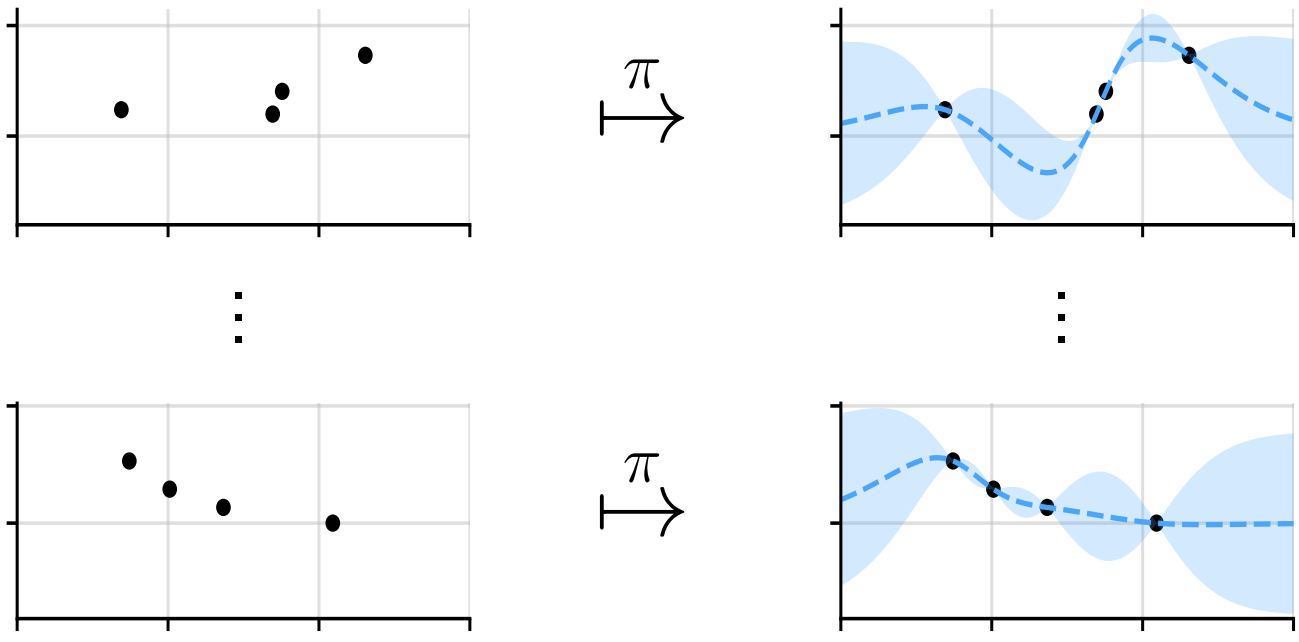


Meta-Learning and Neural Processes



Meta-Learning and Neural Processes

π : data sets $\mathcal{D}$ $\longrightarrow$ predictions $\mathcal{P}$



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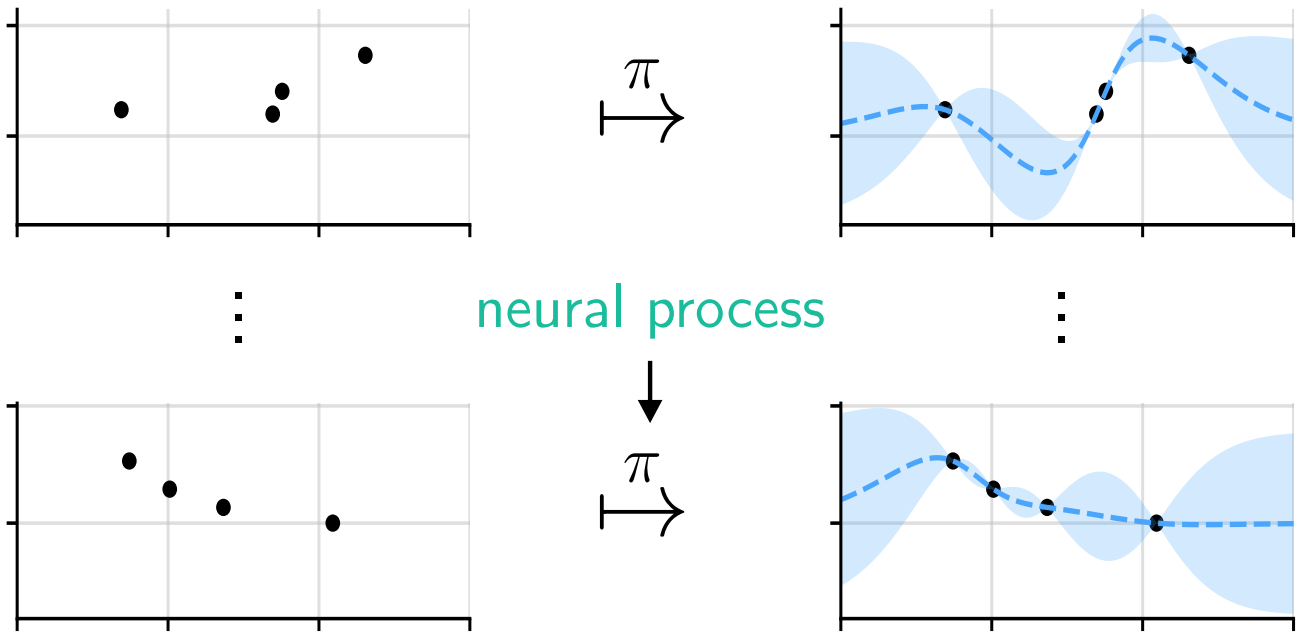

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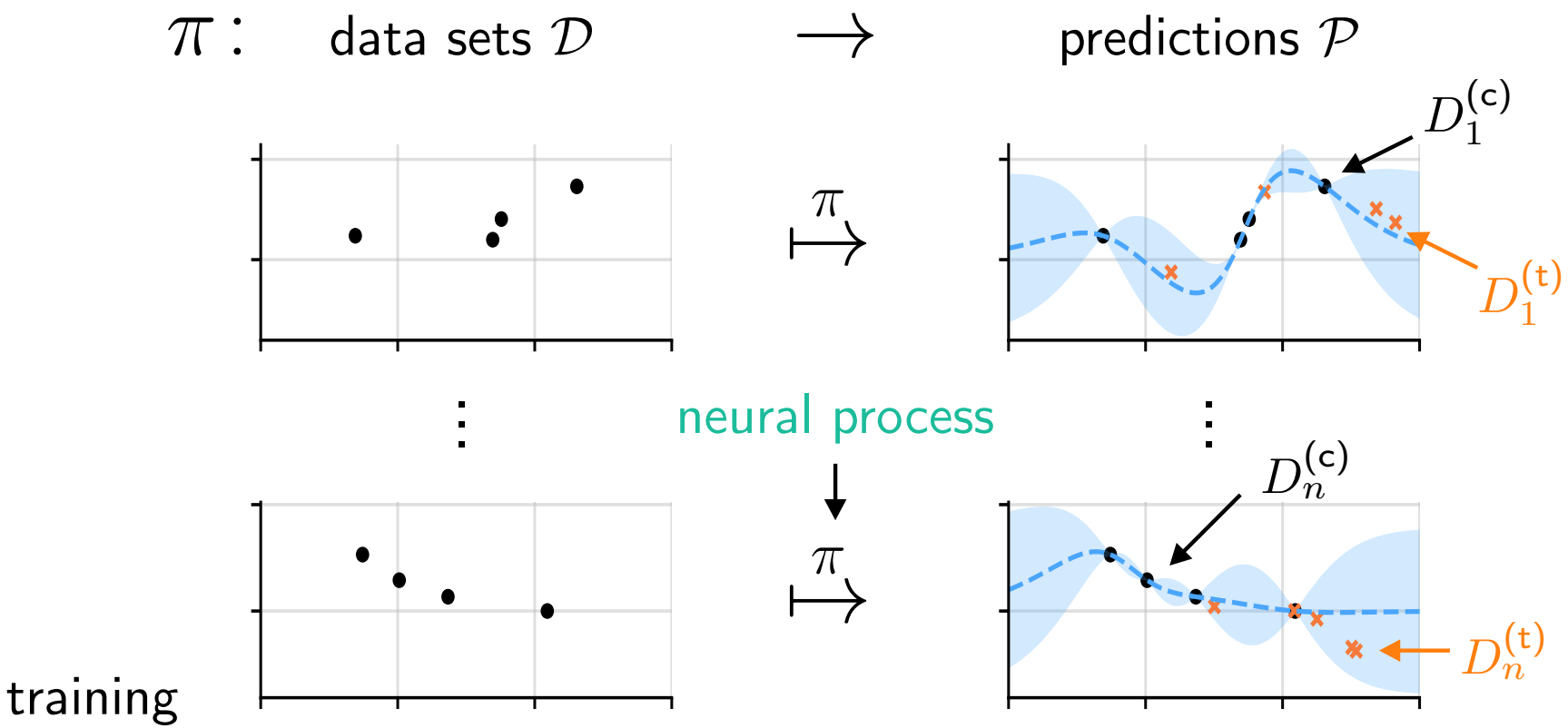

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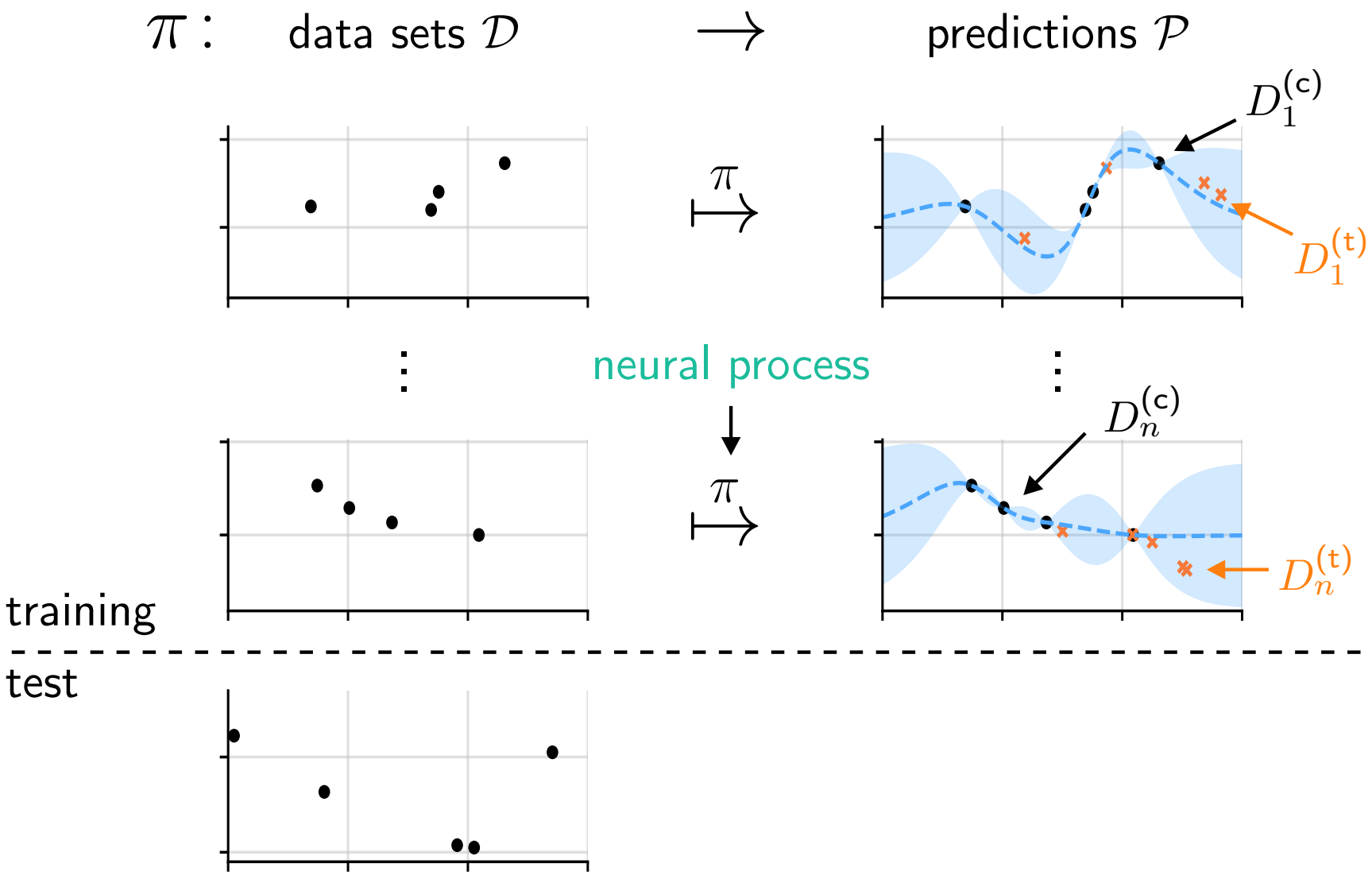

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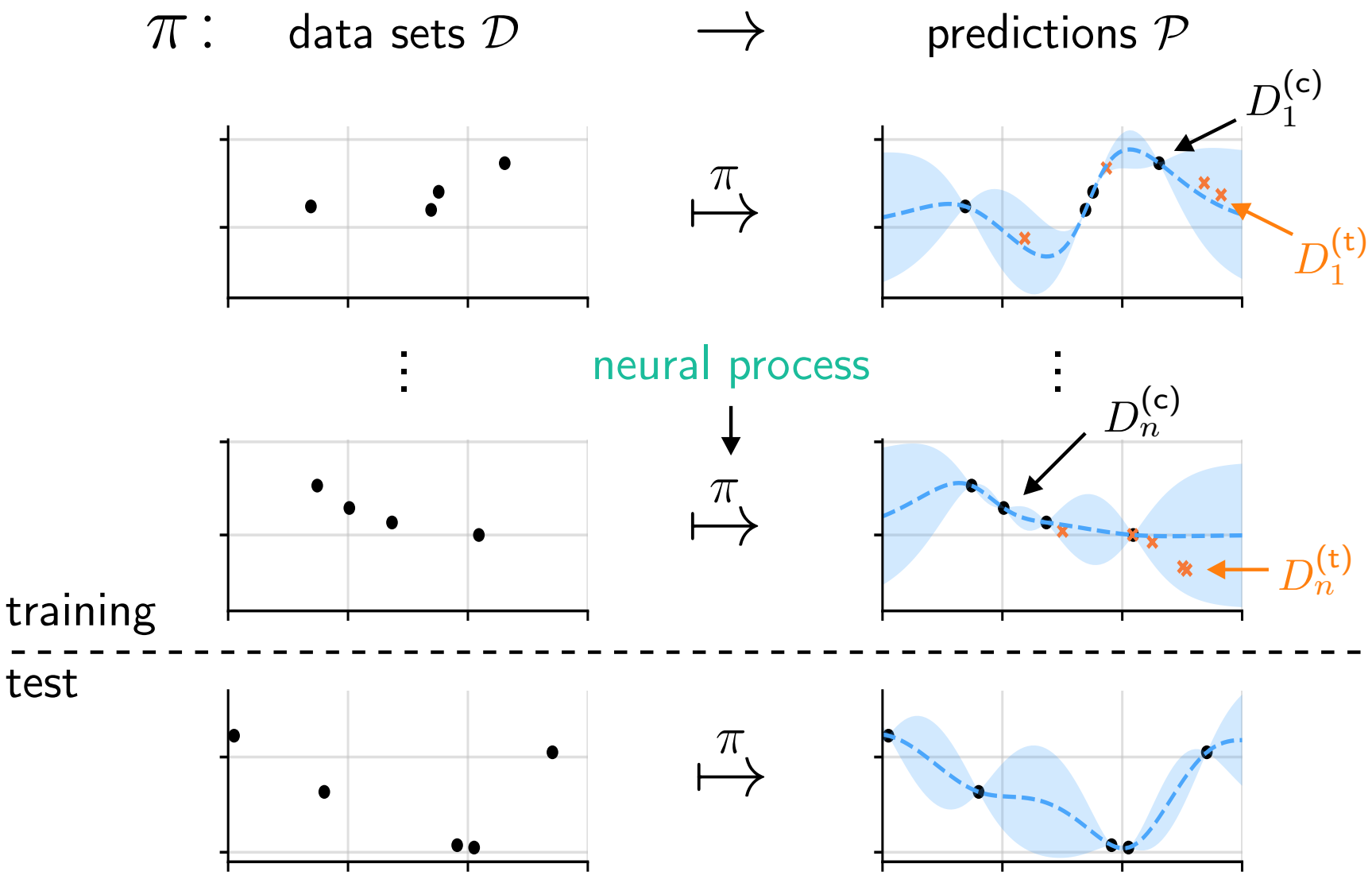
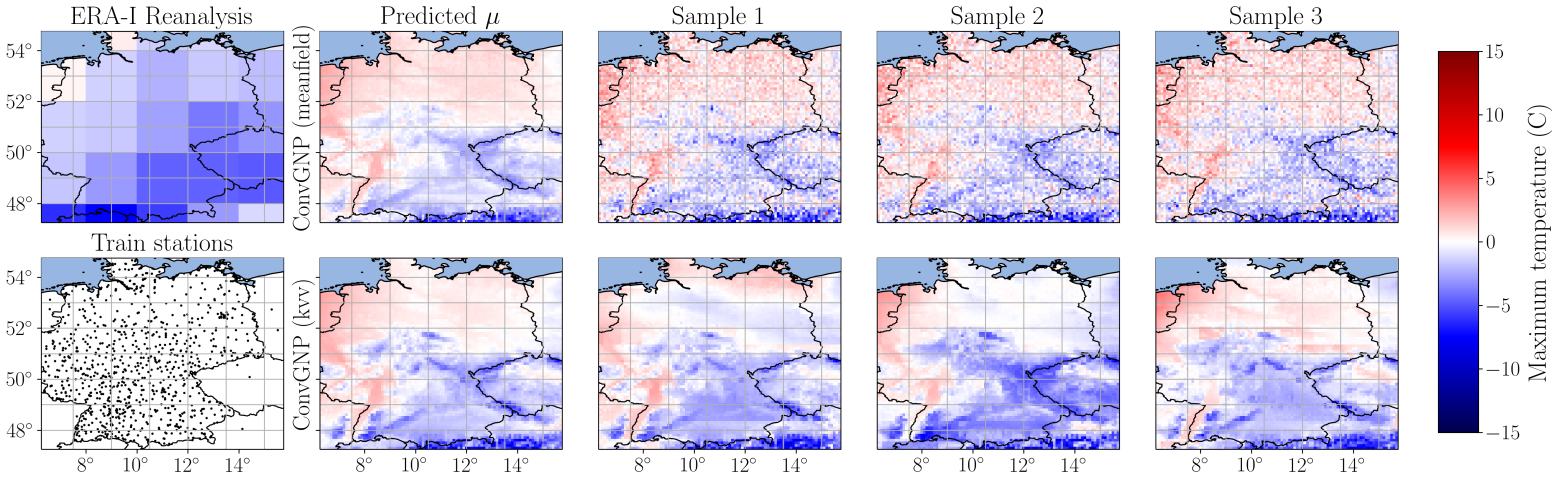


Applications of Neural Processes

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



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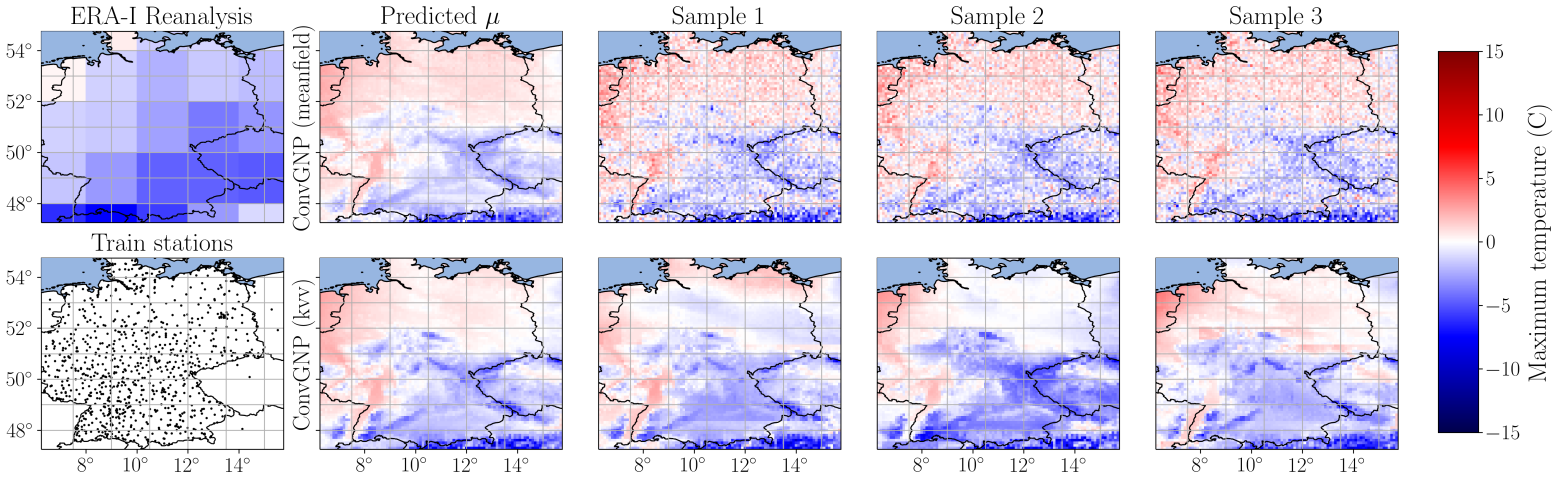
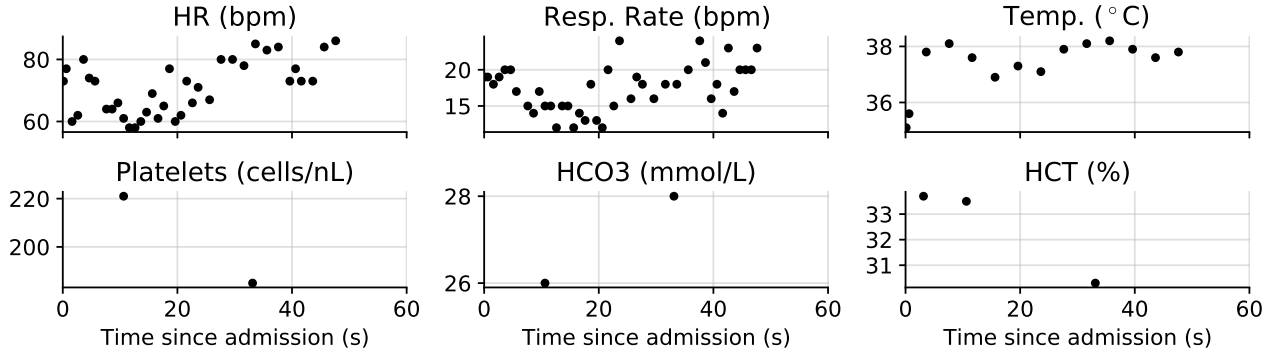


- ICU monitoring (Silva et al., 2012; Shysheya, 2020):



Today: Prediction Map Approximation

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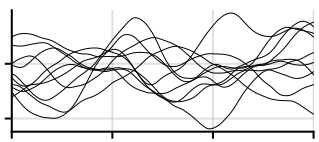
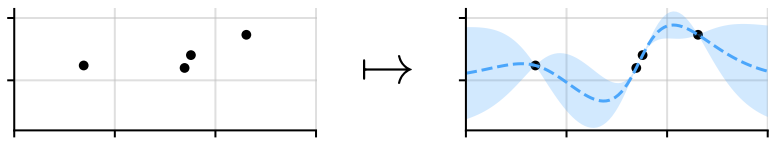
$$f \sim p(f)$$

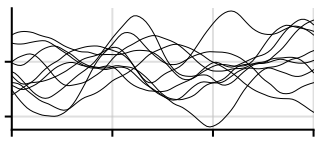


Today: Prediction Map Approximation

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



$f \sim p(f)$ → pred. map π_f



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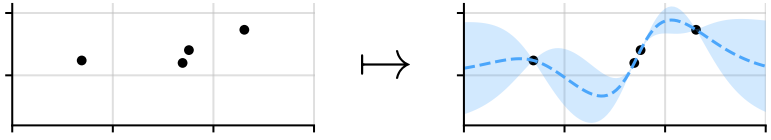

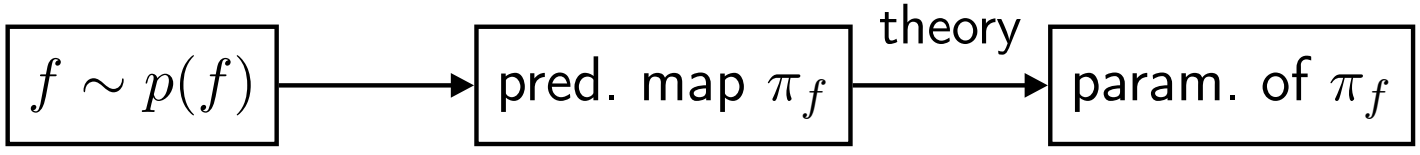

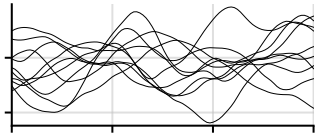

$$m(D) = \rho\big(\sum_{(x,y)\in D} \phi(x,y)\big)$$

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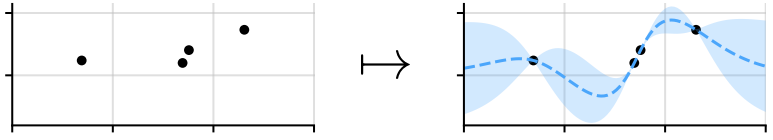

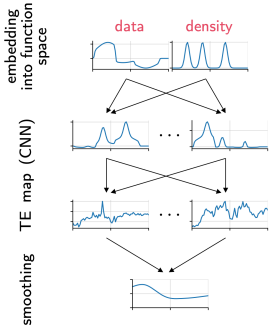

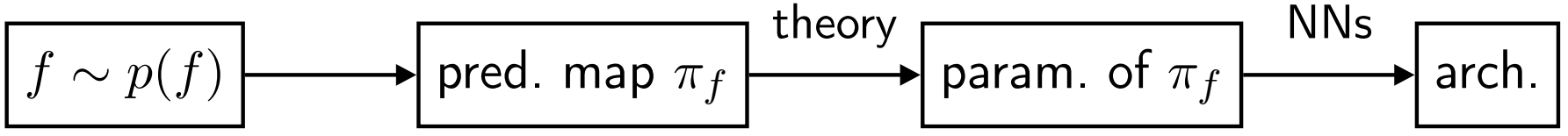

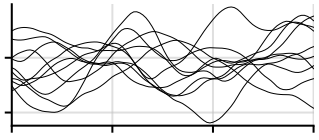

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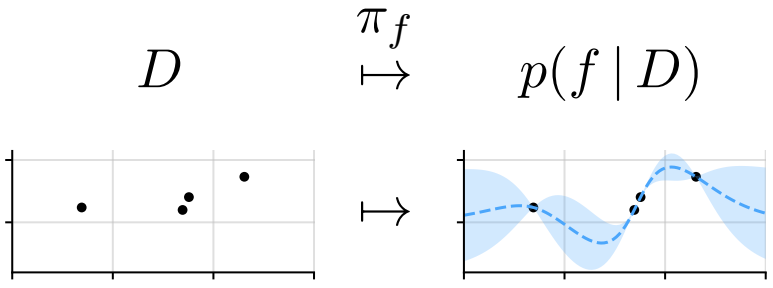

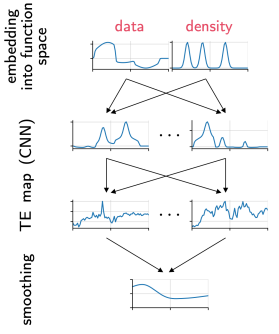

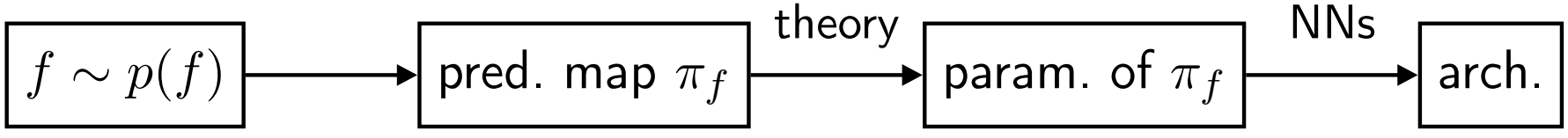

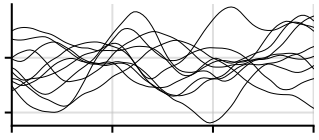

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- ✓ Theoretical framework

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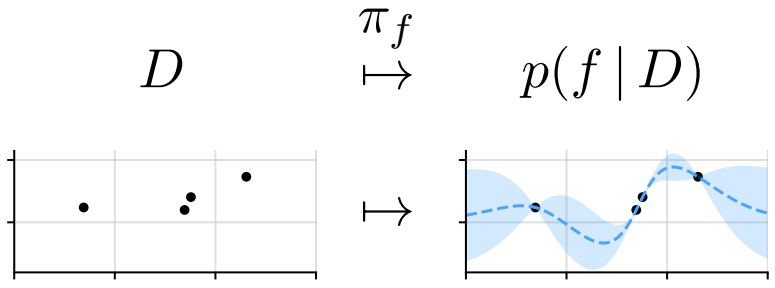

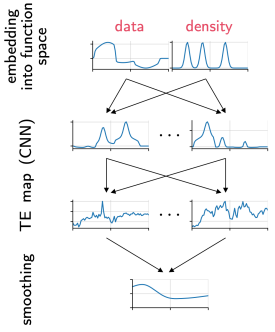

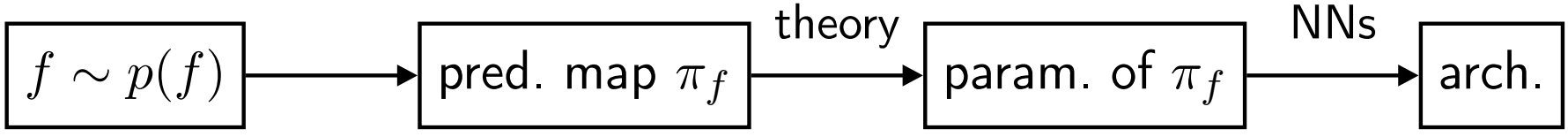

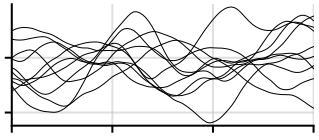

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- ✓ Theoretical framework
- ✓ Architectures with universal approximation properties

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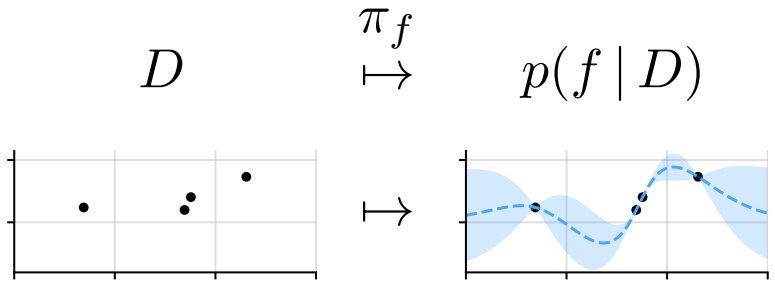

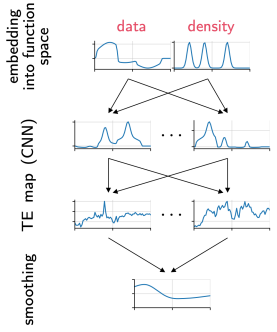

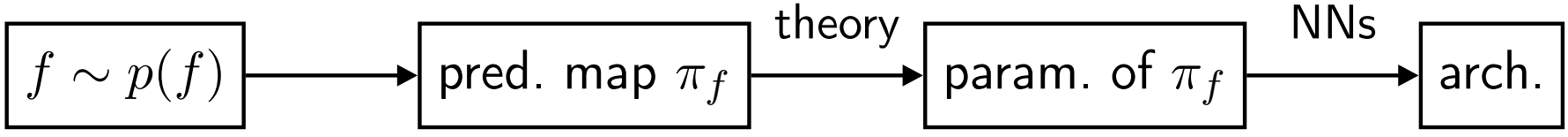

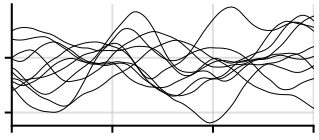

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- ✓ Theoretical framework
- ✓ Architectures with universal approximation properties
- ✓ Properties of $f \Rightarrow$ symmetries of $\pi_f \Rightarrow$ param. efficient archs!

Prediction Map Approximation

Setup

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e.g., a sawtooth wave

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

- Practical objective:

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

Neural Processes

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à la variational family $\longrightarrow$

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

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

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

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

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

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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 $\mathcal{Q}_{\mathsf{G,MF}} = \{\pi : \mathcal{D} \to \mathcal{P}_{\mathsf{G,MF}}\}$.

Parametrising Prediction Maps

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

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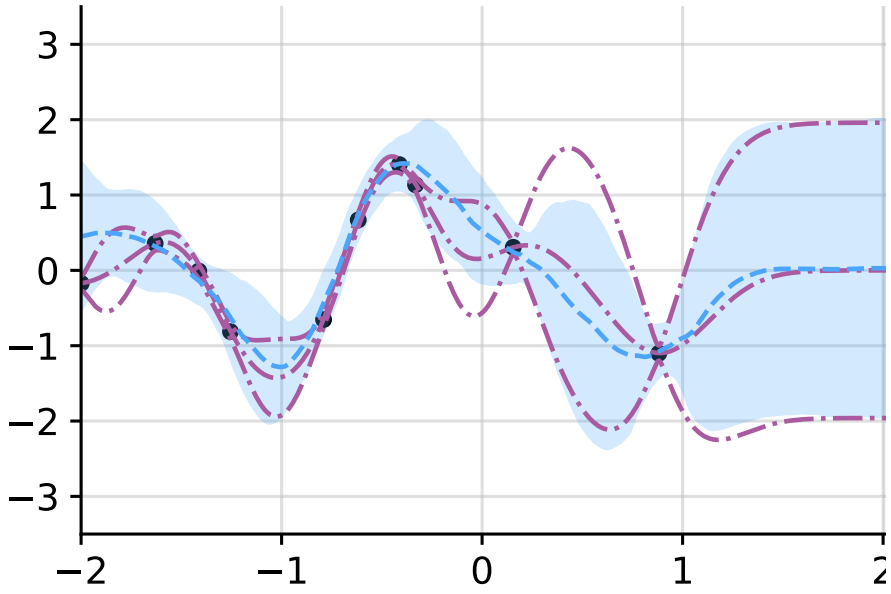
- Conditional neural process (Garnelo et al., 2018):

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

The Conditional Neural Process



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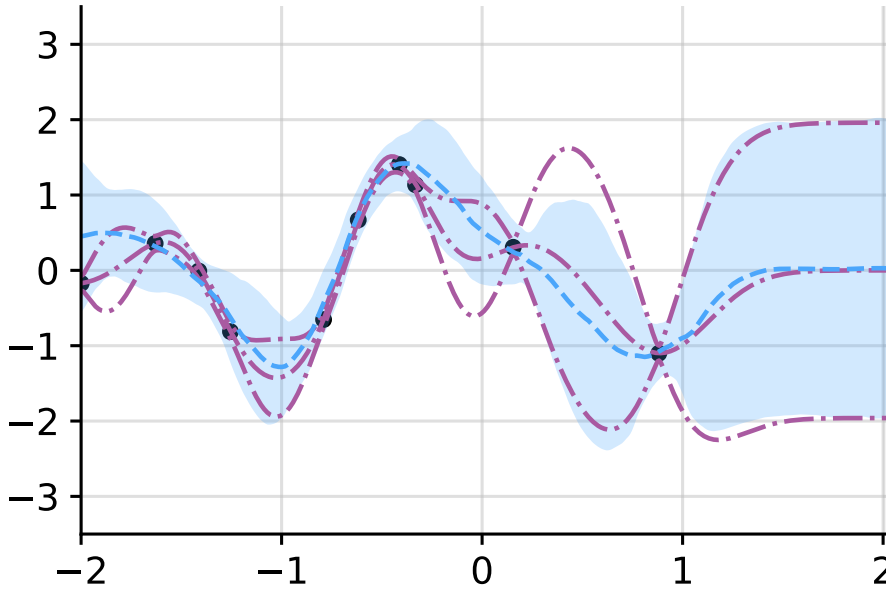

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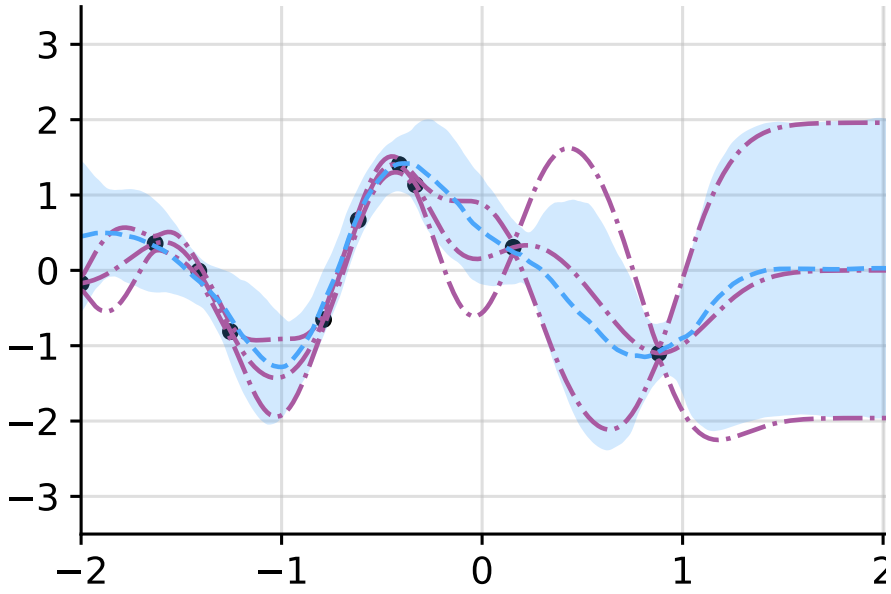

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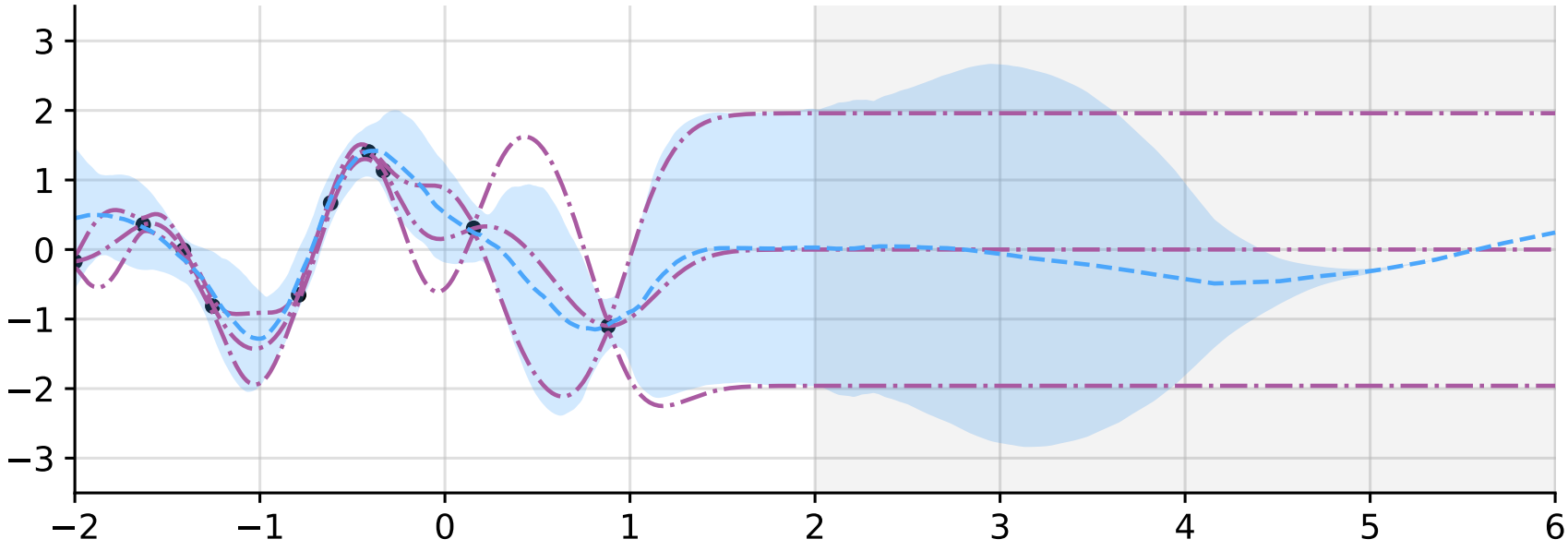

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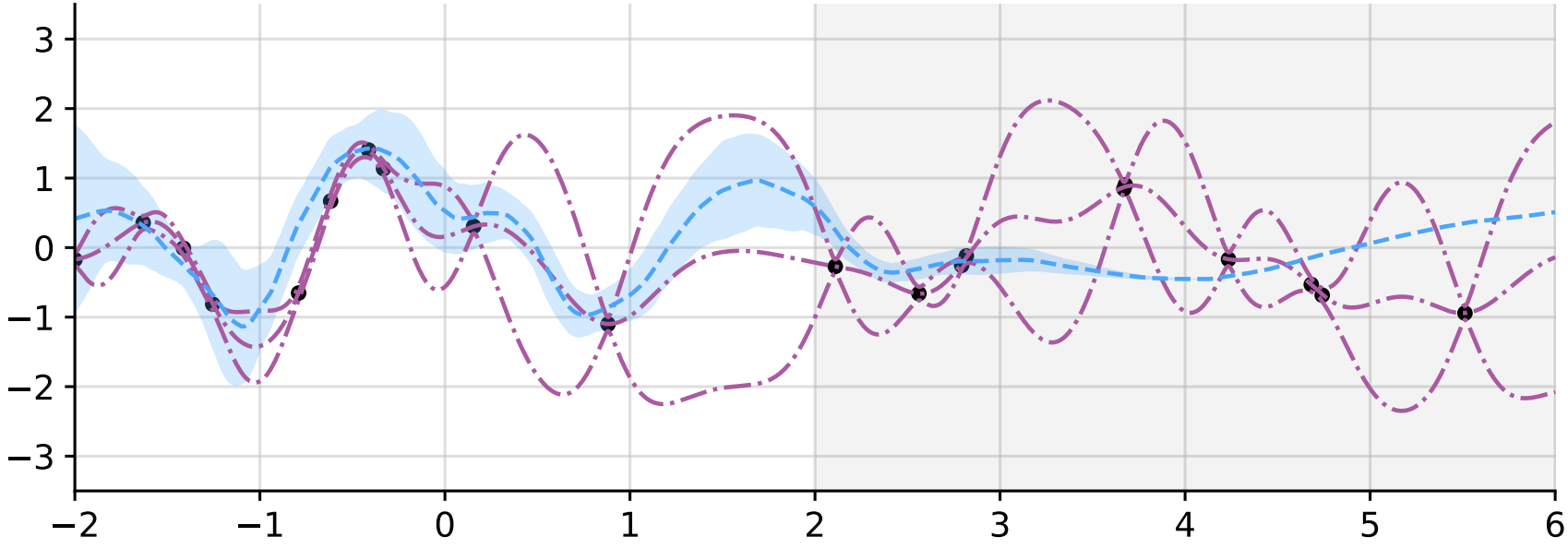

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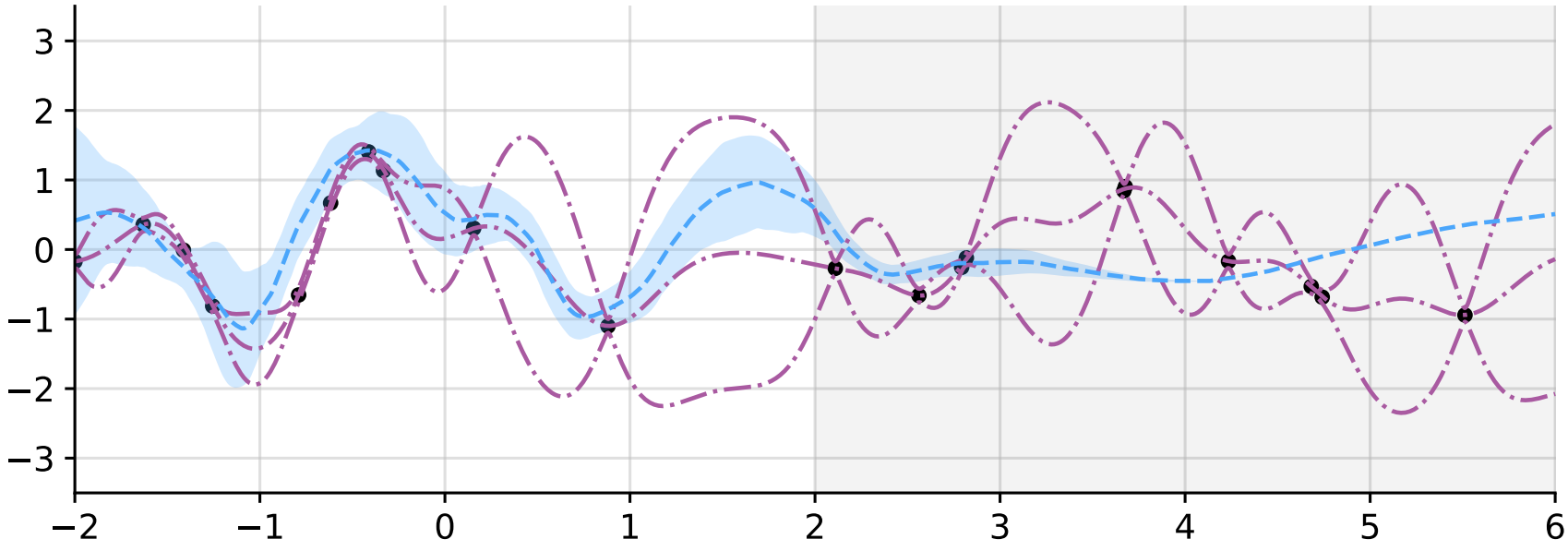

- ✗ Learns very slowly
- ✗ Underfits
- ✗ Generalises poorly

Exploiting Stationarity

Translation-Equivariant Prediction Maps

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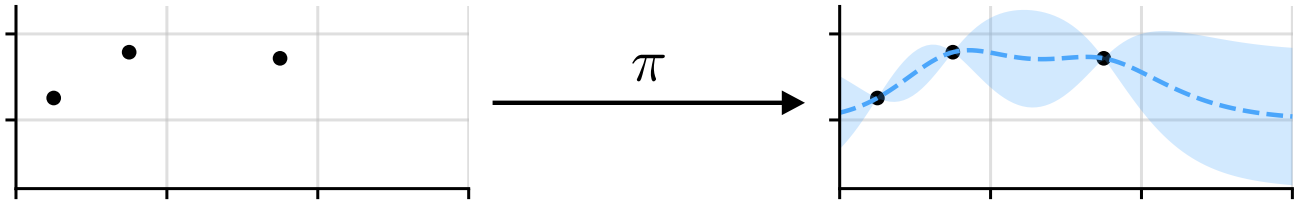

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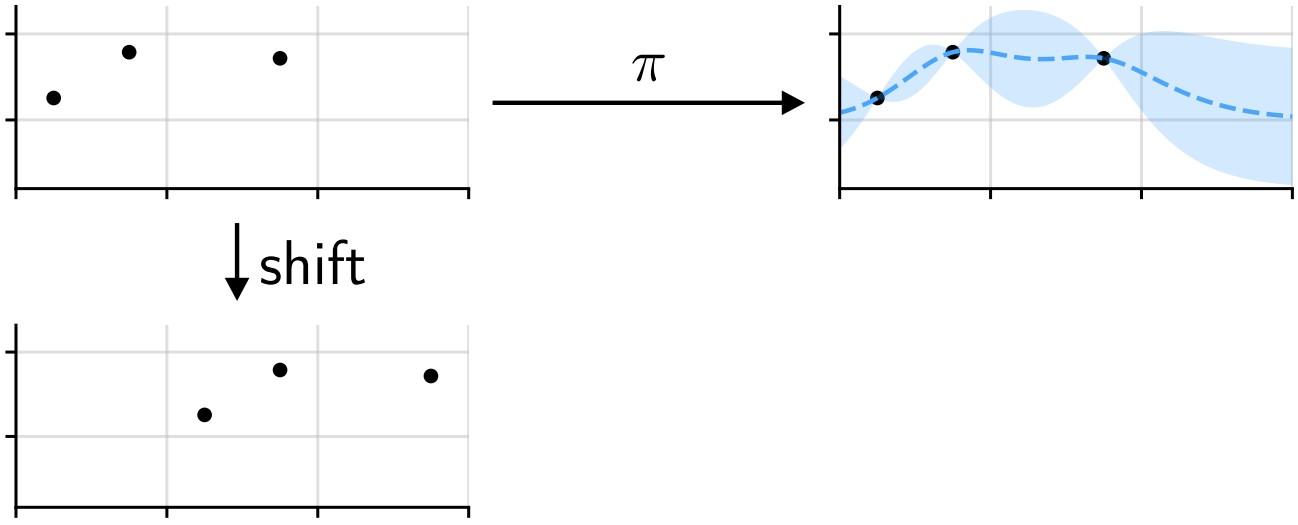

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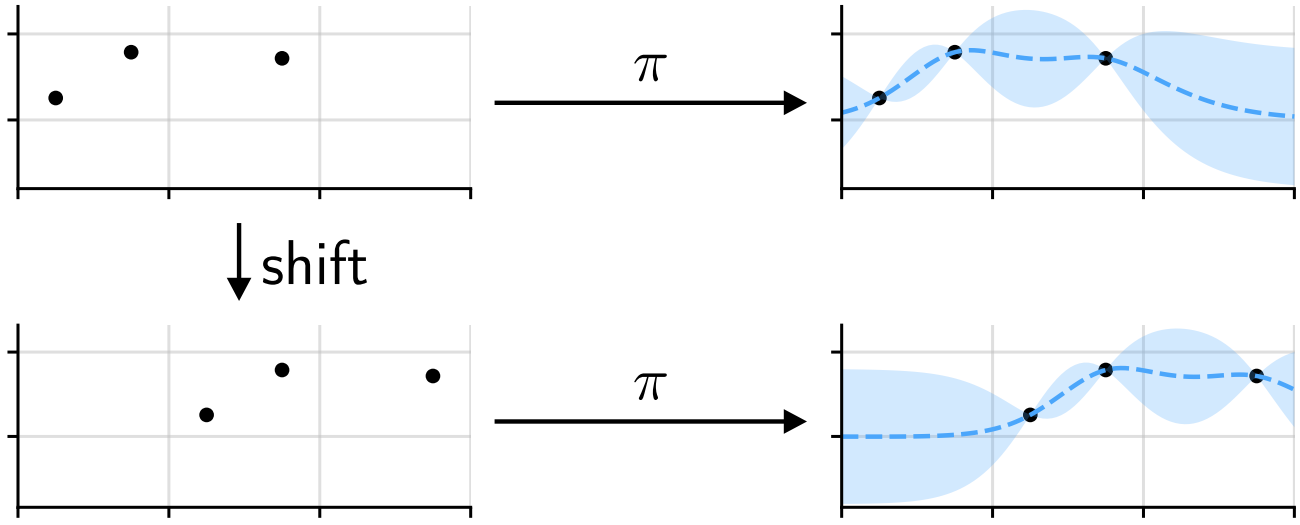

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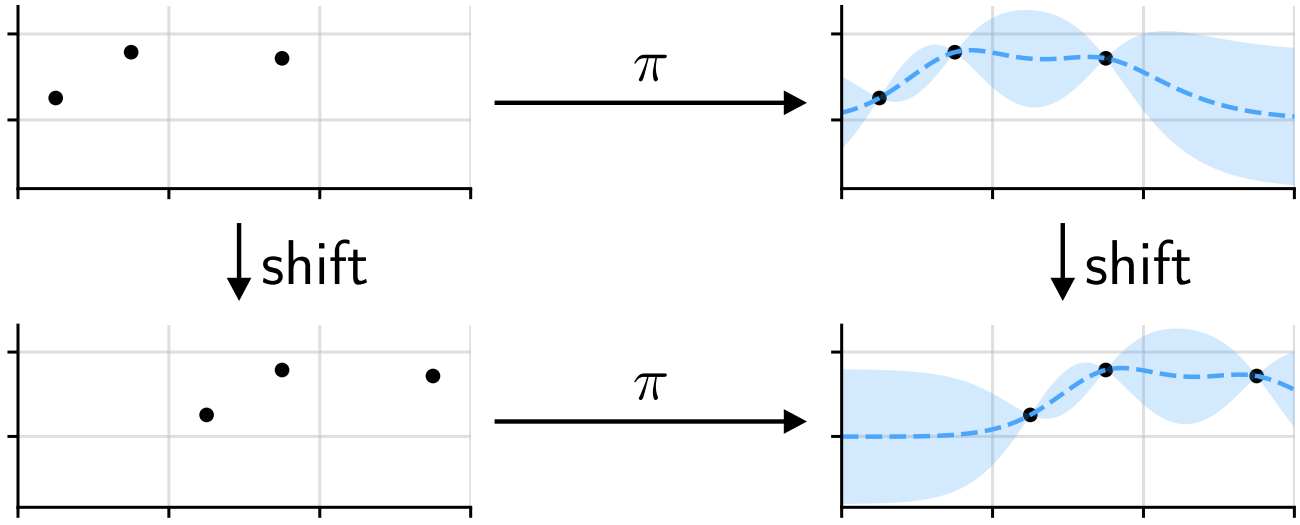

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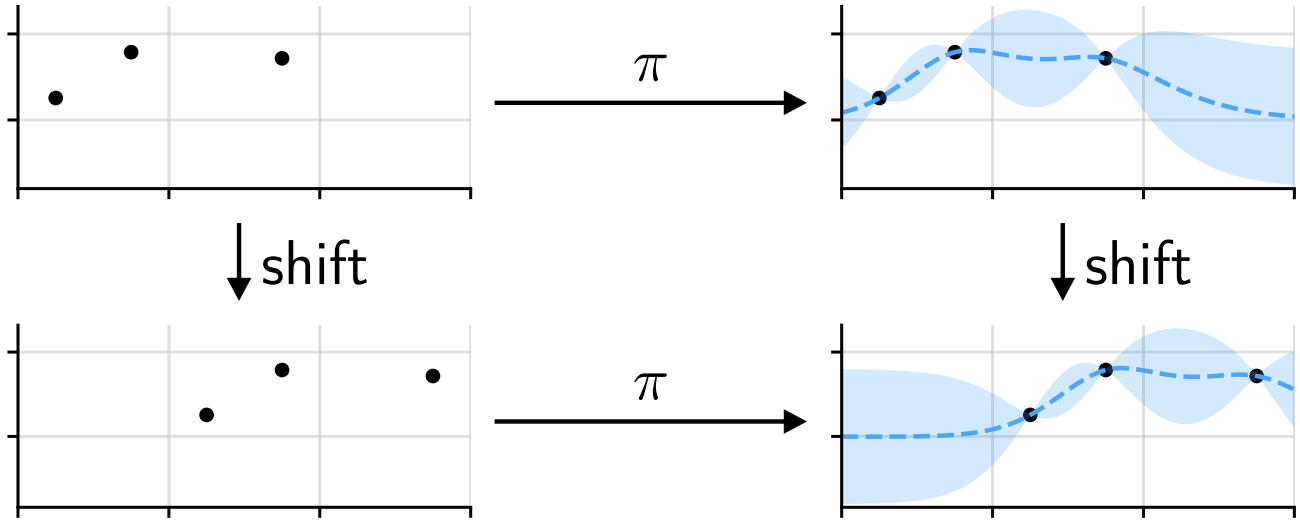

Prop (Foong et al., 2020). f is stationary $\iff$ π_f is TE.

Parametrising TE Prediction Maps

Deep Set

(Zaheer et al., 2017)

$f : \mathcal{D}_{\leq M} \to Z$ is cont.

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$\iff$

$$E : \mathcal{D}_{\leq M} \to \mathbb{R}^M,$$
$$E(D) = \sum_{(x,y)\in D} \phi(x, y)$$

$$\rho : \mathbb{R}^M \to Z,$$
$$f(D) = \rho(E(D))$$

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Parametrising TE Prediction Maps

Deep Set (Zaheer et al., 2017)	Convolutional Deep Set (Gordon et al., 2020)
$f\colon \mathcal{D}_{\leq M} \to Z$ is cont.	$f\colon \mathcal{D}_{\leq M} \to Z$ is cont. and TE
$\iff$	T_τ?!
encoder $E\colon \mathcal{D}_{\leq M} \to \mathbb{R}^M$, $E(D) = \sum_{(x,y)\in D} \phi(x,y)$	
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	$\iff$	$\iff$
	T_τ?!	
encoder	$E\colon \mathcal{D}_{\leq M} \to \mathbb{R}^M$, $E(D) = \sum_{(x,y)\in D} \phi(x,y)$	$E\colon \mathcal{D}_{\leq M} \to \mathbb{H}$, $E(D) = \sum_{(x,y)\in D} k(\bullet - x)\phi(y)$
decoder	$\rho\colon \mathbb{R}^M \to Z$, $f(D) = \rho(E(D))$	$\rho\colon \mathbb{H} \to Z$, $f(D) = \rho(E(D))$

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	$f\colon \mathcal{D}_{\leq M} \to Z$ is cont.	$f\colon \mathcal{D}_{\leq M} \to Z$ is cont. and TE
	$\Longleftrightarrow$ T_τ?!	$\Longleftrightarrow$ functional embedding (RKHS)
encoder	$E\colon \mathcal{D}_{\leq M} \to \mathbb{R}^M$, $E(D) = \sum_{(x,y)\in D} \phi(x,y)$	$E\colon \mathcal{D}_{\leq M} \to \mathbb{H}$, $E(D) = \sum_{(x,y)\in D} k(\bullet - x)\phi(y)$
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	$\iff$ ↓ T_τ?!	$\iff$ ↓ functional embedding (RKHS)
encoder	$E\colon \mathcal{D}_{\leq M} \to \mathbb{R}^M$, $E(D) = \sum_{(x,y)\in D} \phi(x,y)$	$E\colon \mathcal{D}_{\leq M} \to \mathbb{H}$, $E(D) = \sum_{(x,y)\in D} k(\bullet - x)\phi(y)$
decoder	$\rho\colon \mathbb{R}^M \to Z$, $f(D) = \rho(E(D))$	TE map between function spaces ≈ CNN → $\rho\colon \mathbb{H} \to Z$, $f(D) = \rho(E(D))$

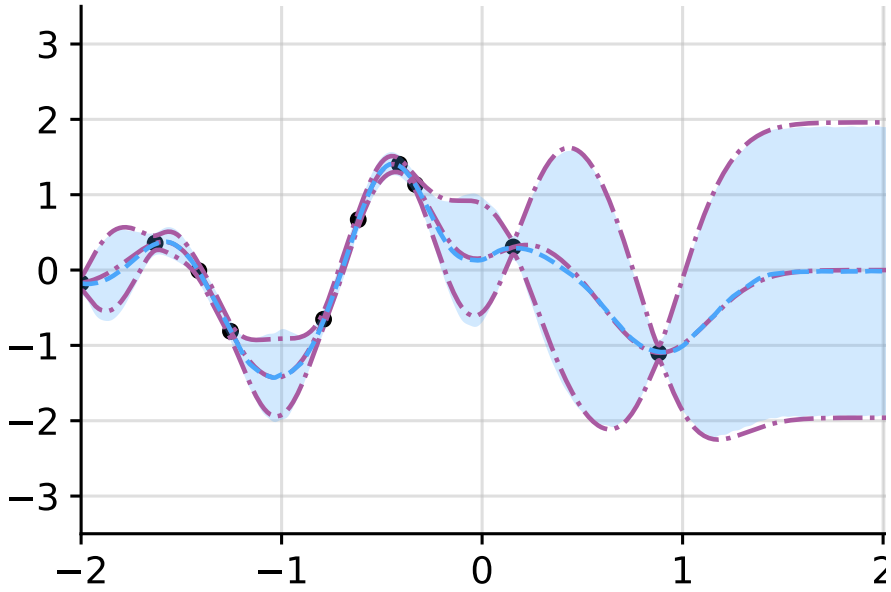
Parametrising TE Prediction Maps

	Deep Set (Zaheer et al., 2017)	Convolutional Deep Set (Gordon et al., 2020)
	$f : \mathcal{D}_{\leq M} \to Z$ is cont.	$f : \mathcal{D}_{\leq M} \to Z$ is cont. and TE
	$\iff$ T_τ?!	$\iff$ 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 et al., 2020):

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

The Convolutional CNP



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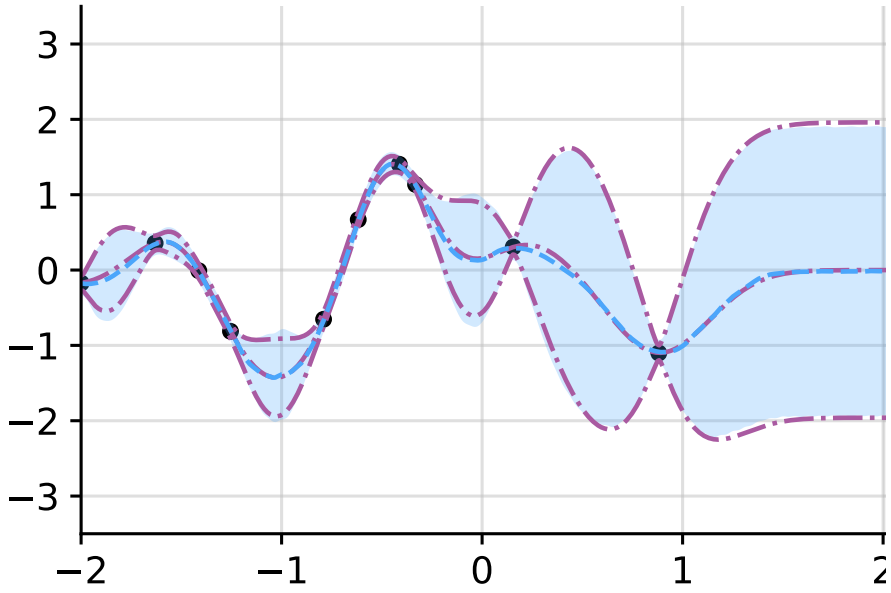

✓ Learns pretty quickly

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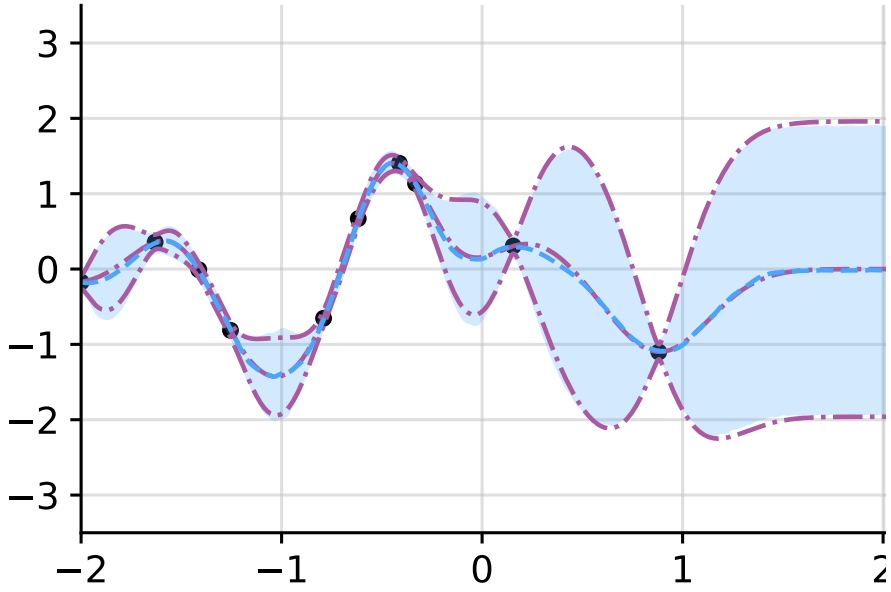

- ✓ Learns pretty quickly
- ✓ Recovers target (diagonalised ground-truth GP)

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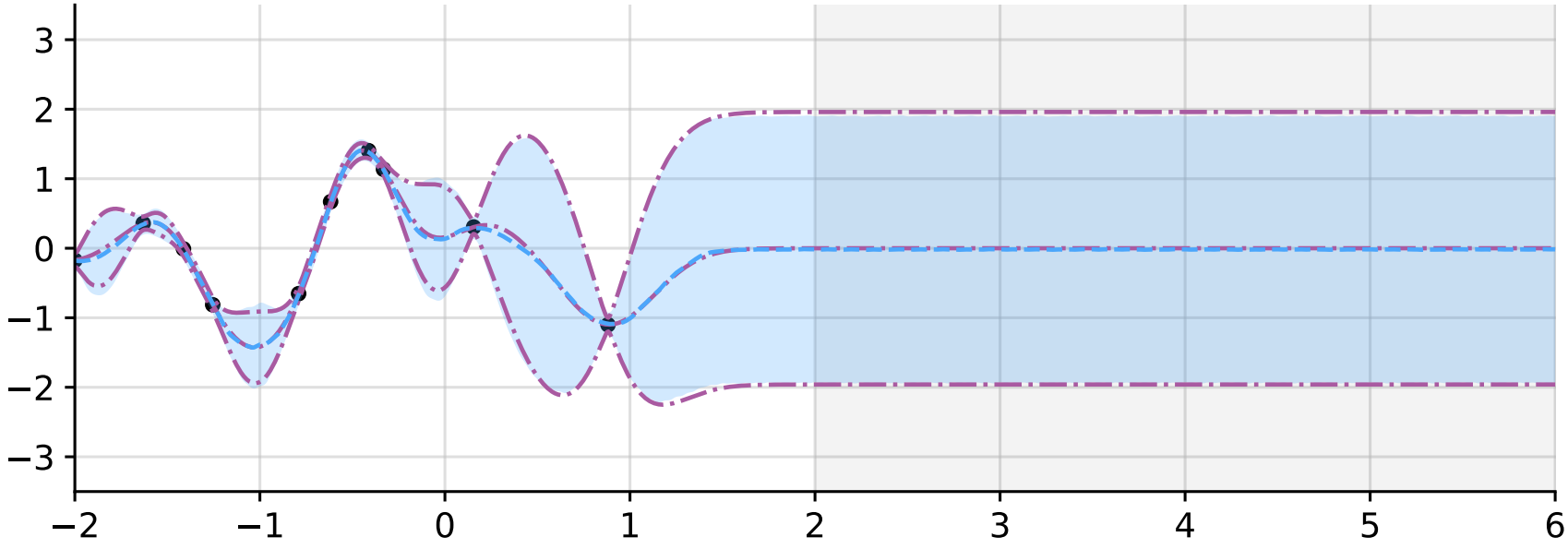

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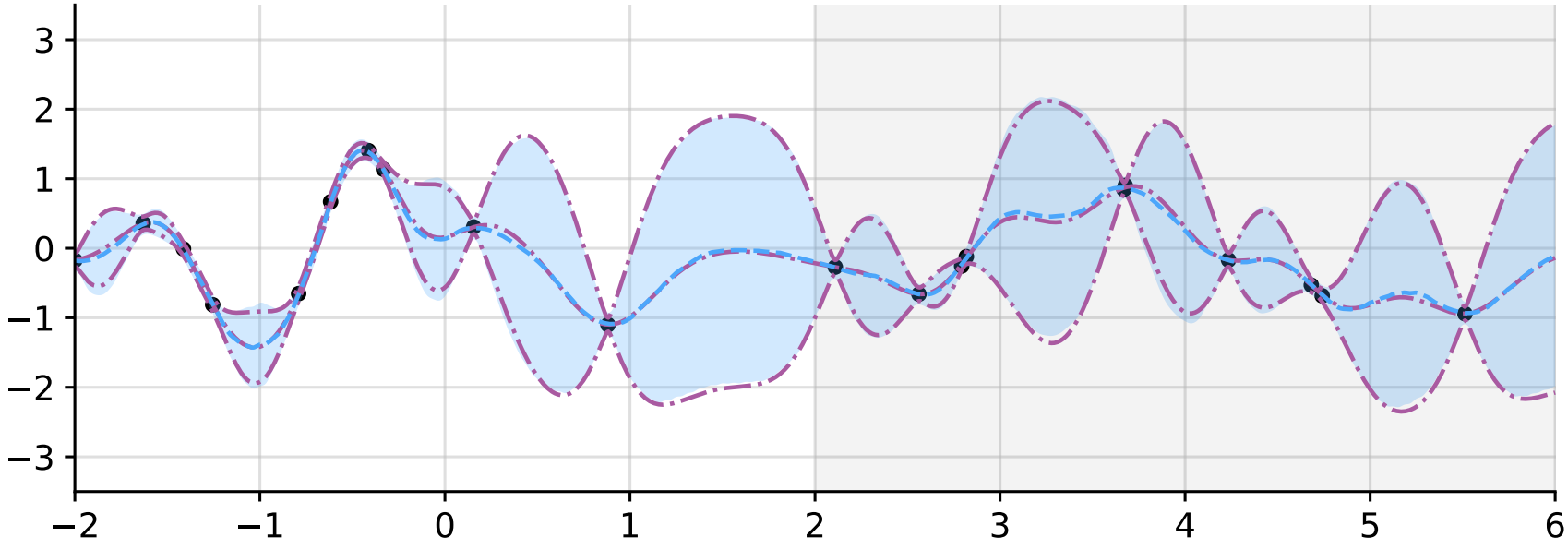

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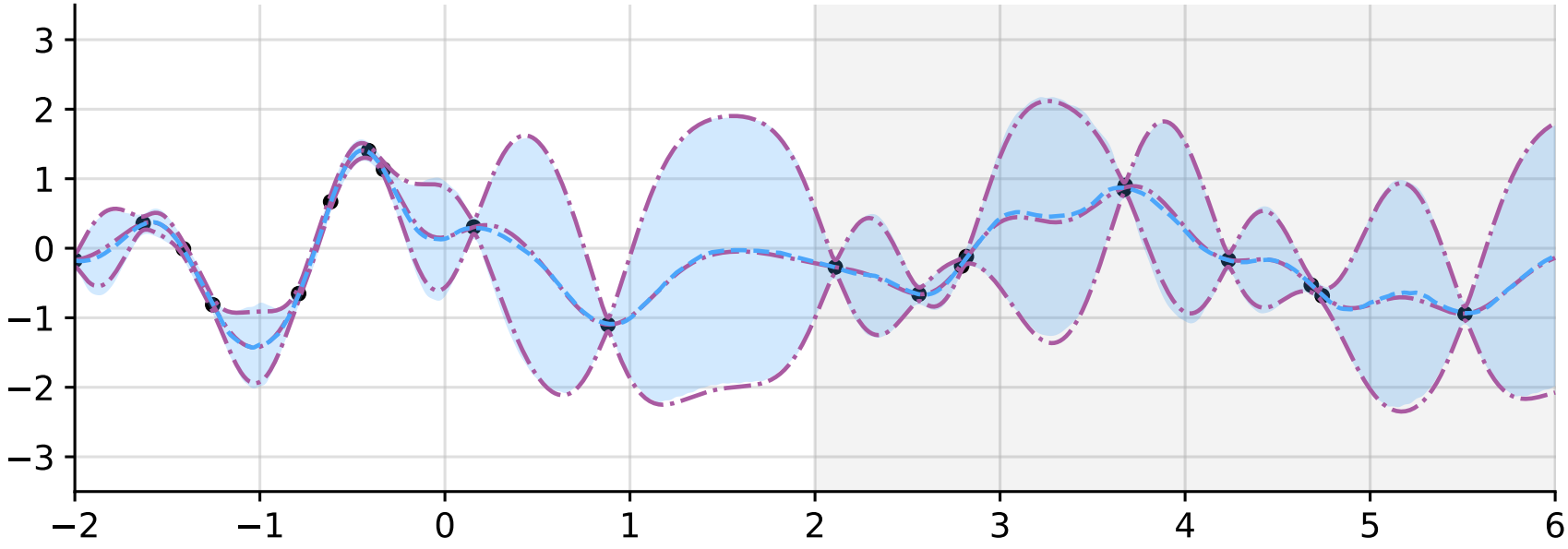
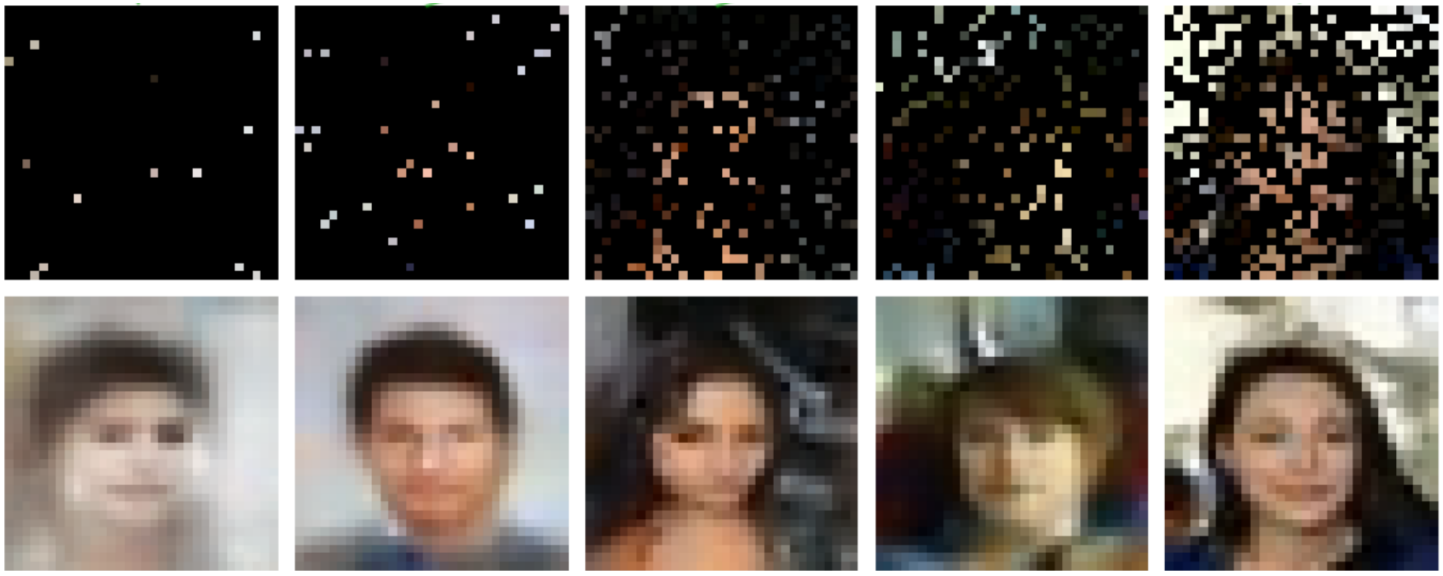


- ✓ Learns pretty quickly
- ✓ Recovers target (diagonalised ground-truth GP)
- ✓ Generalises well

The Convolutional CNP (2)



Gordon et al. (2020)

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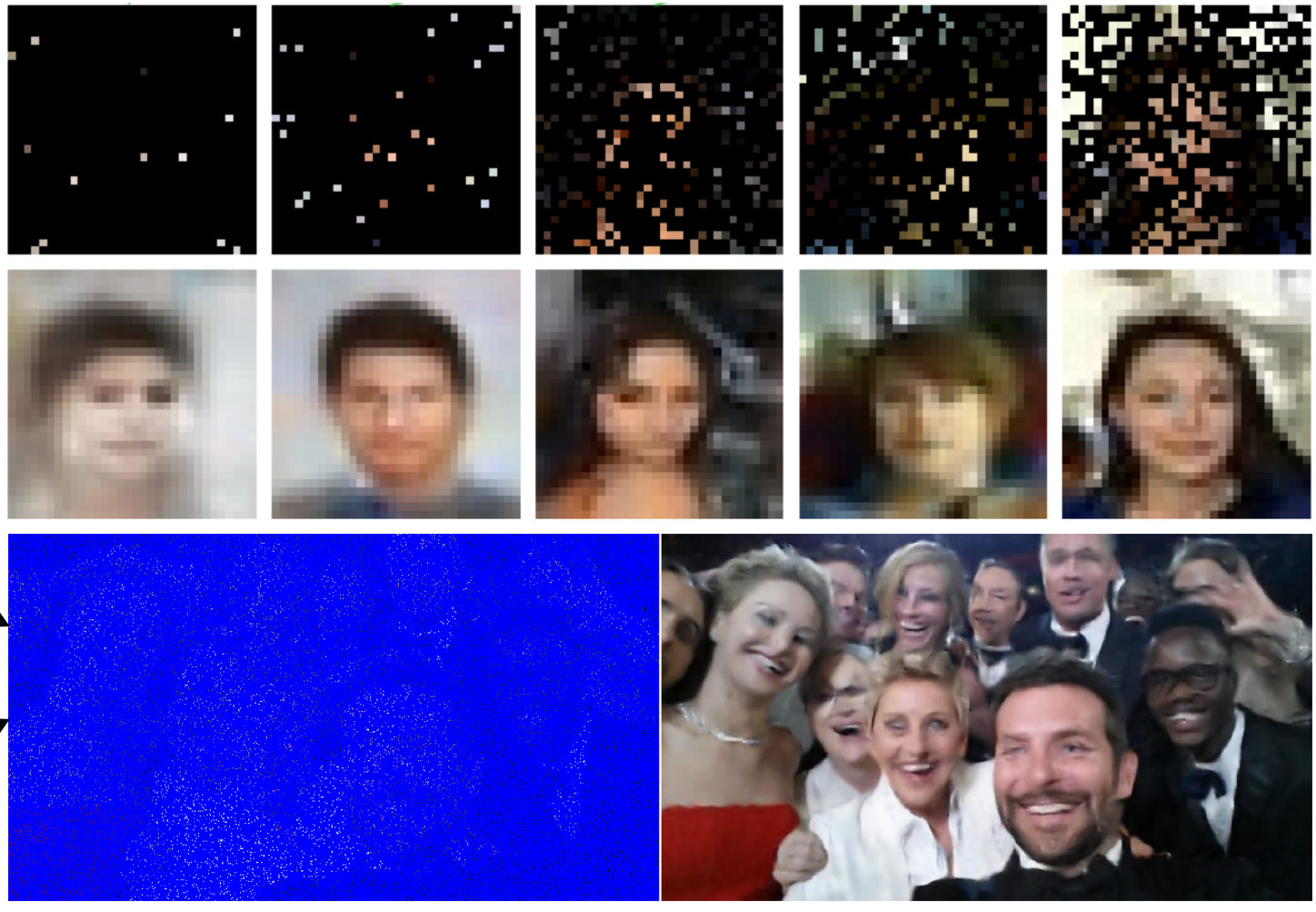
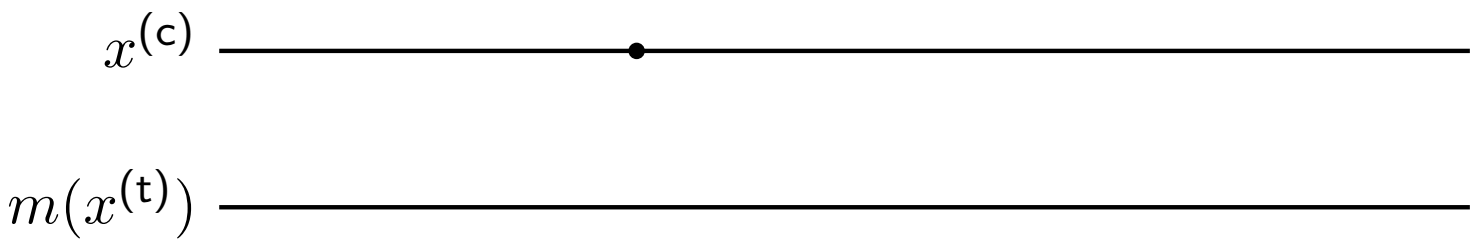


Gordon et al. (2020)

Why Does TE Help Generalise?

- CNNs have receptive field $R > 0$:



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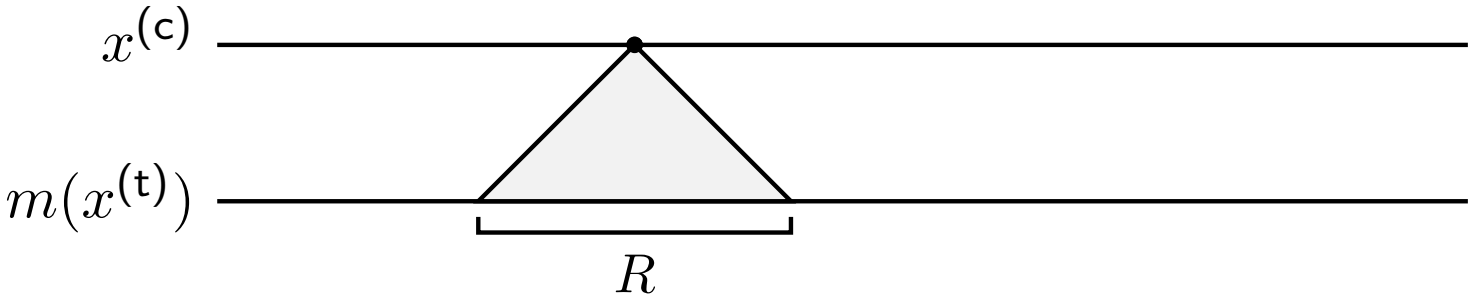

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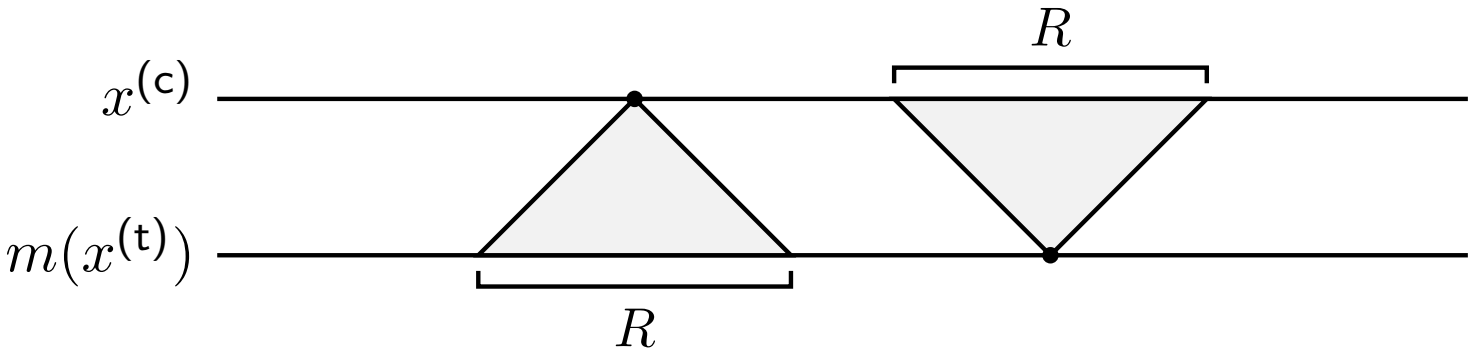

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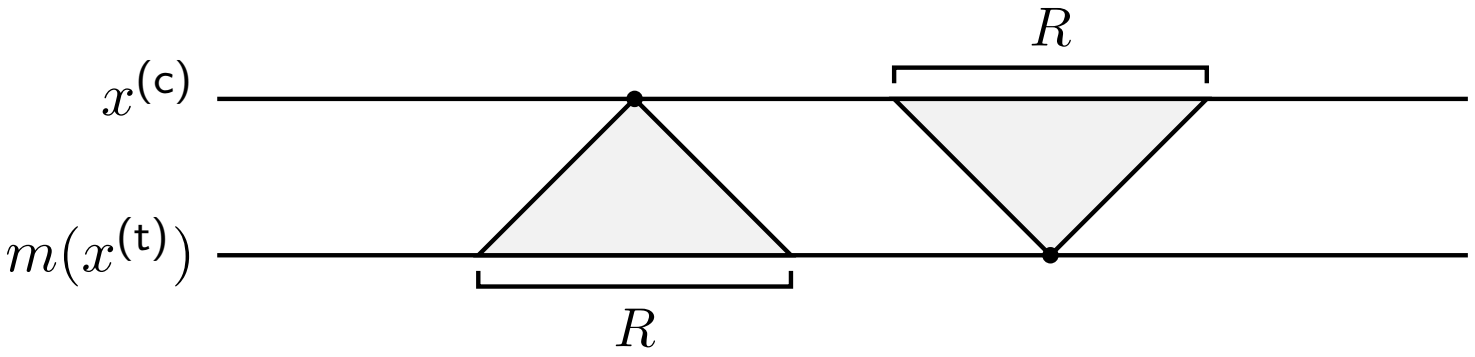

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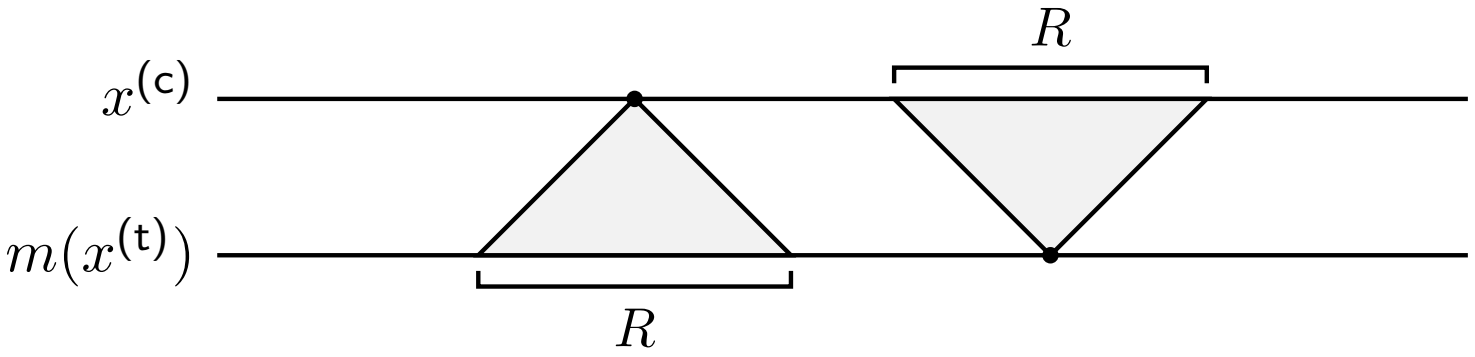
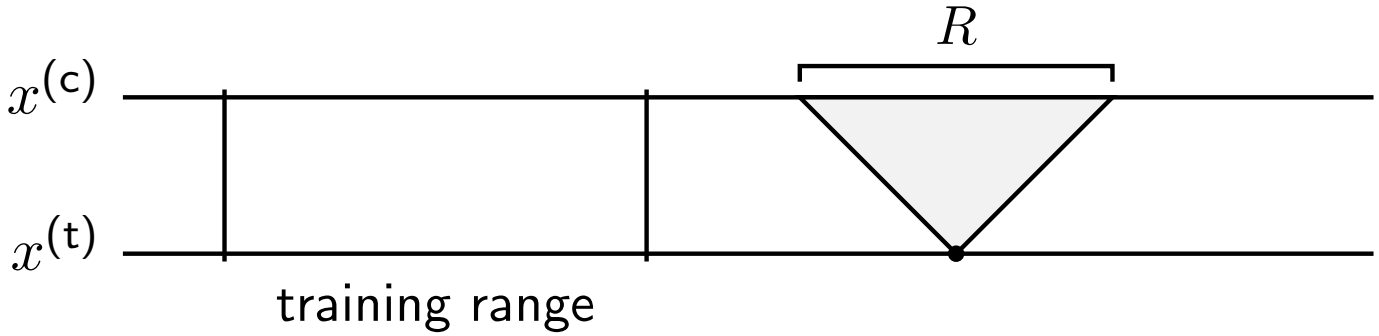


- In combination with TE, helps ConvCNP to generalise:



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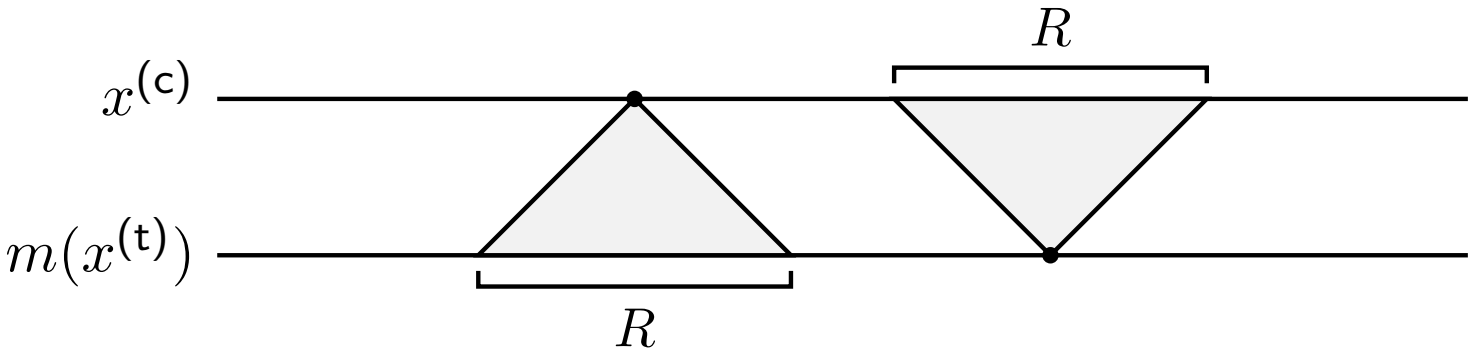

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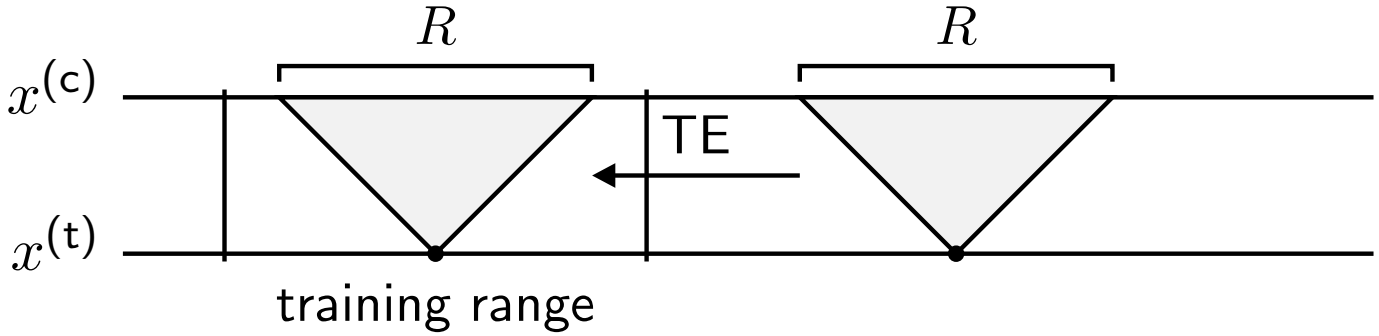

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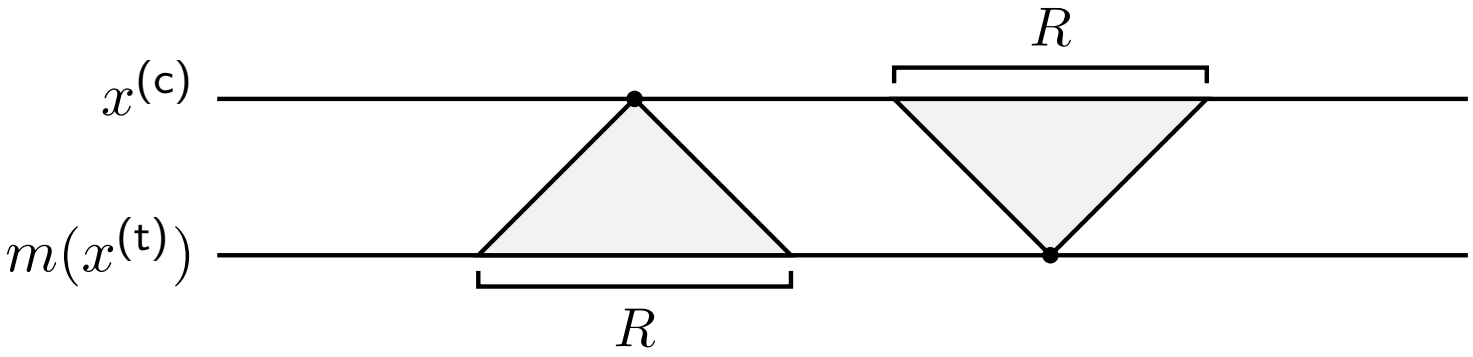

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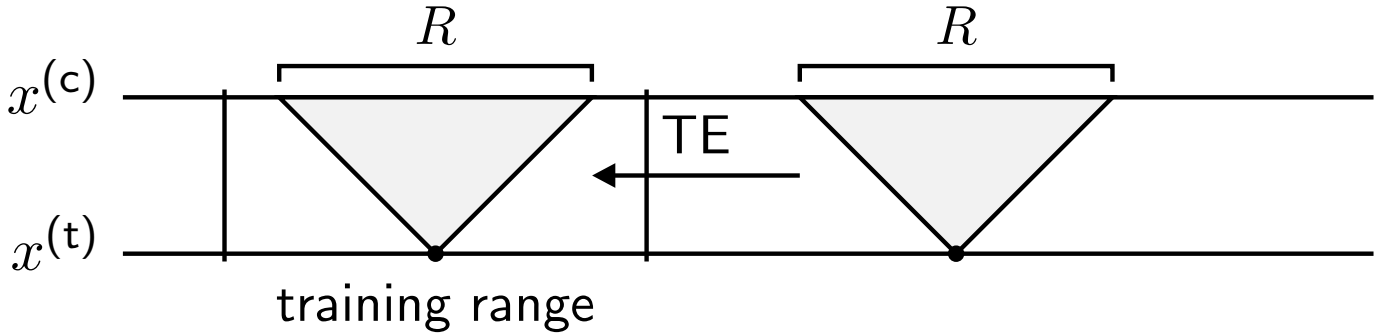
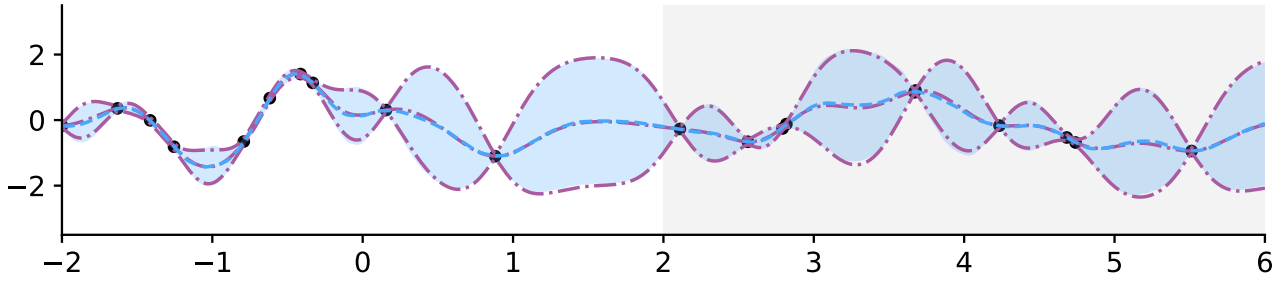


Thm. Suppose that $\mathcal{L}(\pi) \leq \varepsilon$ for data sampled from $[0, R + \ell]$. Then $\mathcal{L}(\pi) \leq \lceil M/\ell \rceil \varepsilon$ for data from any interval of width M.

Further Improvements

Gaussian TE Prediction Maps



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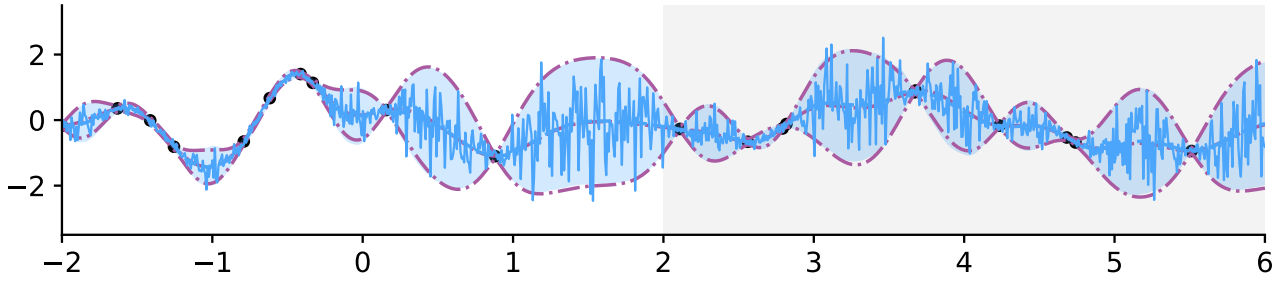

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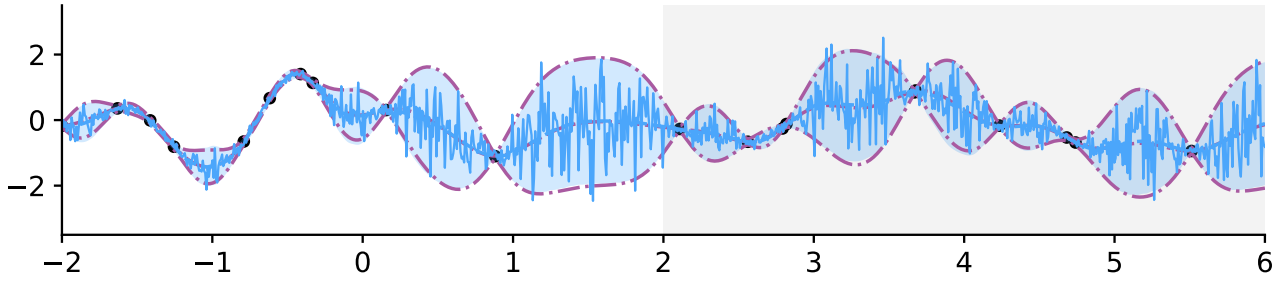

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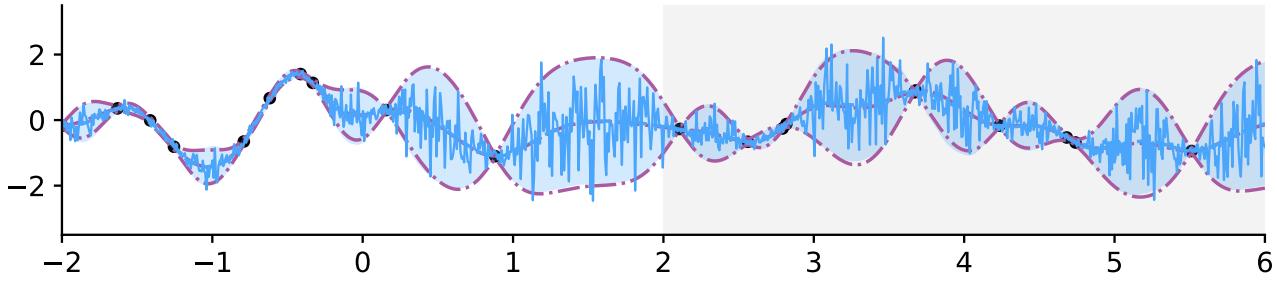

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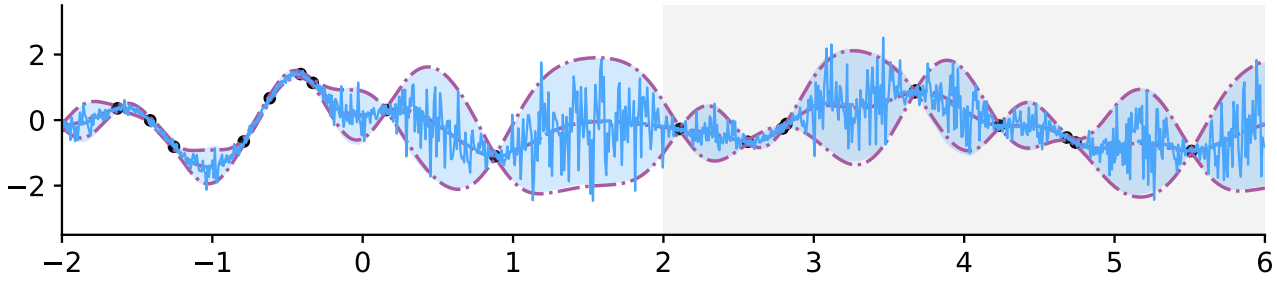

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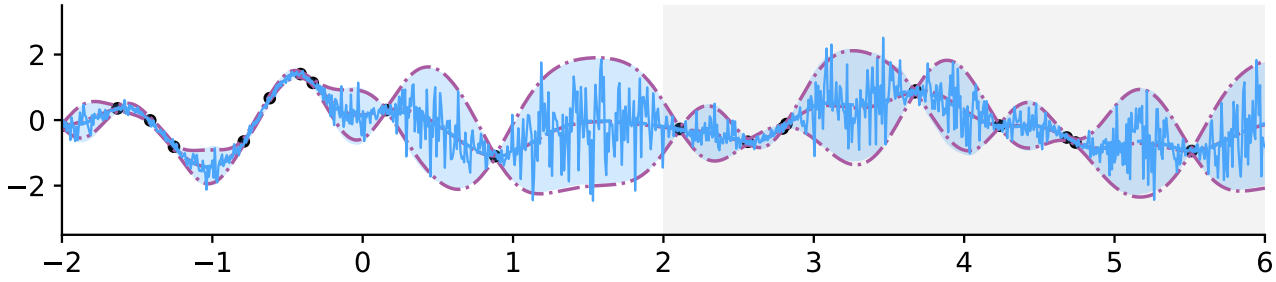

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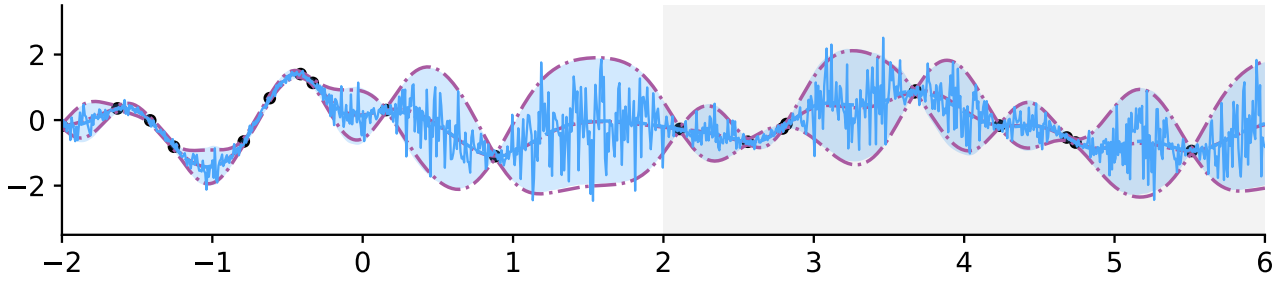

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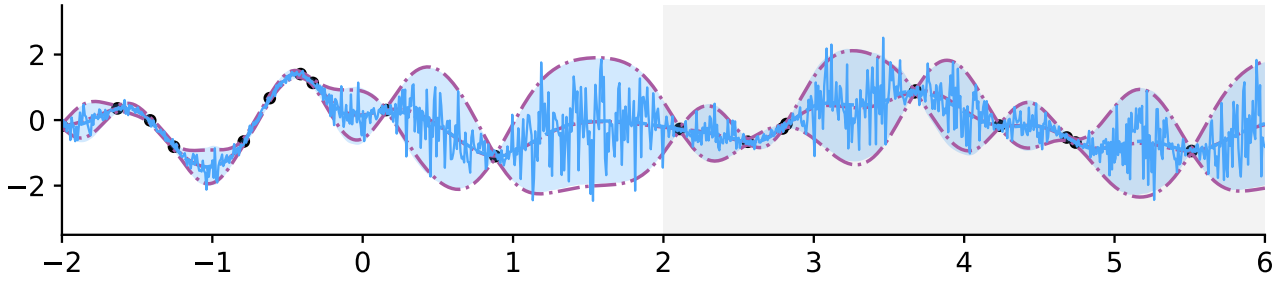

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  - ✗ d-dimensional inputs require $2d$-dimensional convolutions

- Markou et al. (2022) provide practical params for $d > 1$:

$$k(x, x', D) = \langle \mathbf{r}(x, D), \mathbf{r}(x', D) \rangle.$$

TE

Consistency of Prediction Map Approximation

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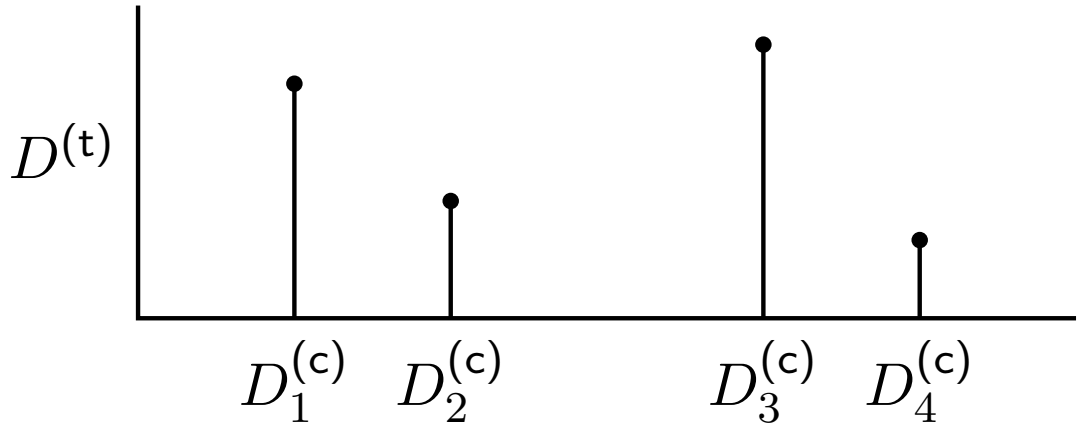

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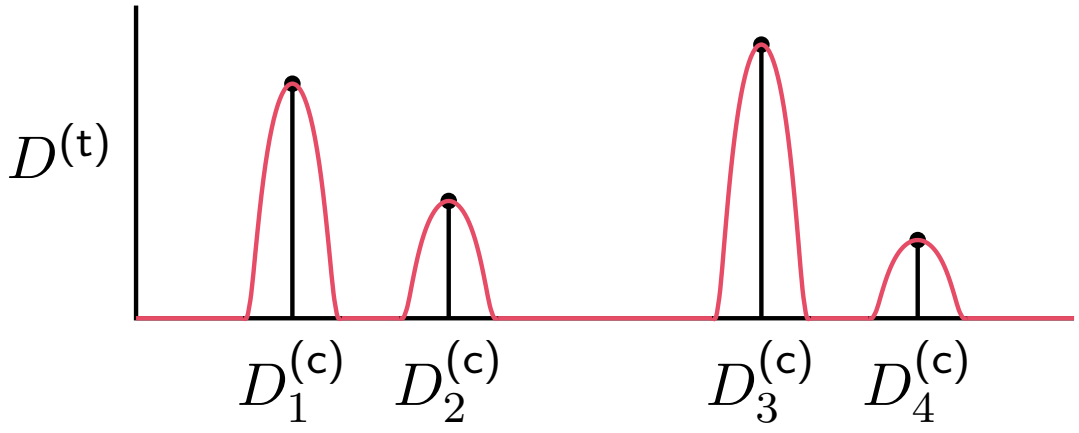

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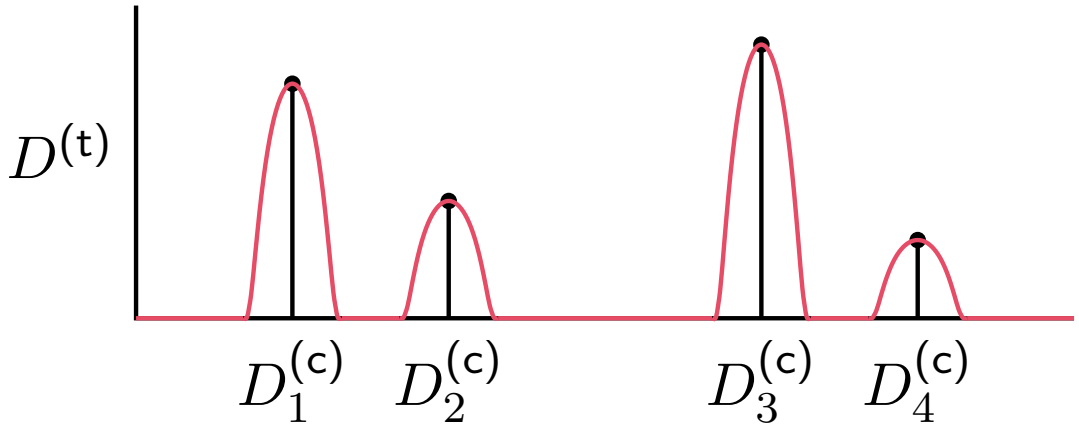

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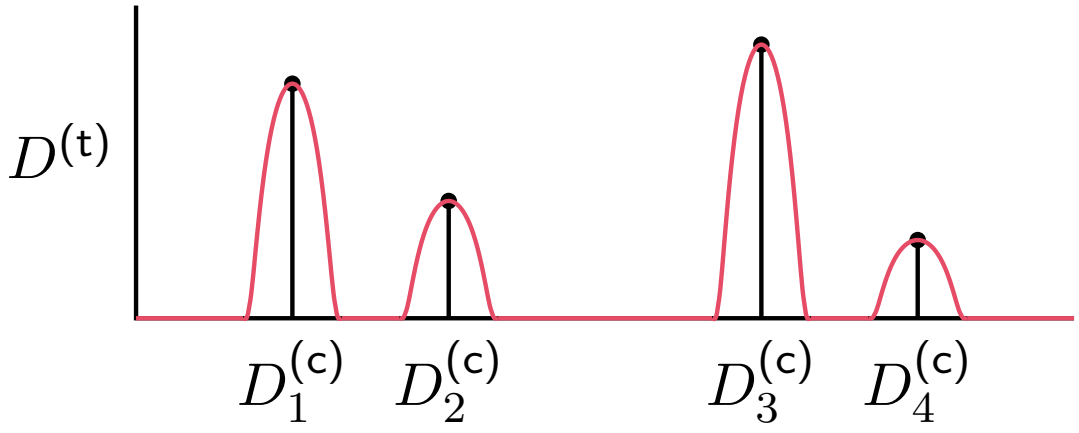

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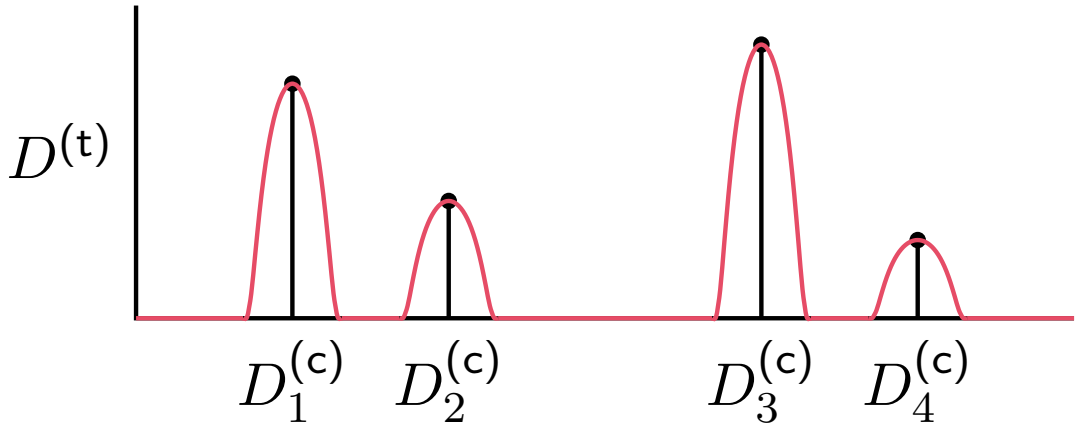

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- Will show that we can reasonably restrict to compact $\mathcal{Q} \subset \mathcal{M}_{\mathsf{G}}$.

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

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

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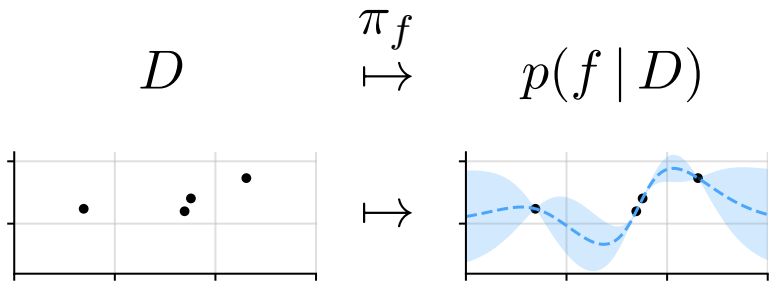
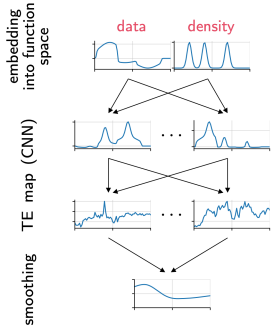
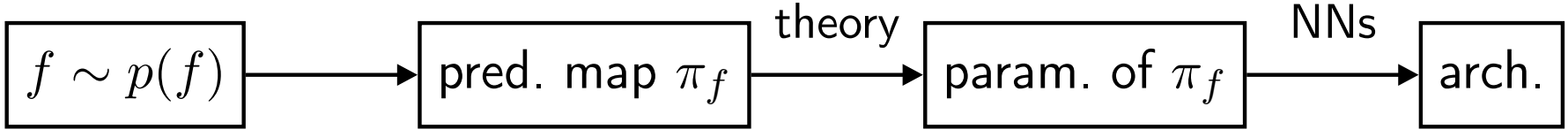
- How much data: finite-sample bounds / rates of convergence?

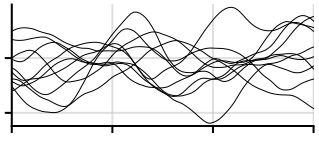
Wrapping Up

Prediction Map Approximation









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

- ✓ 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/predmap`.

Appendix

References

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