In-Context In-Context Learning with Transformer Neural Processes

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1. Neural Processes

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- Seek to approximate the posterior predictive map of a ground-truth $\mathcal{Y}$-valued stochastic process on input space $\mathcal{X}$

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(so we might consider a transformer-based model…)

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- Model using an encoder $e : \mathcal{X} \times \mathcal{S} \to \mathcal{Z}$ and a decoder $d : \mathcal{X} \times \mathcal{Z} \to \Theta$

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(Use a Monte-Carlo estimate of this expectation using the tasks you actually have access to.)

2. Transformer Neural Processes

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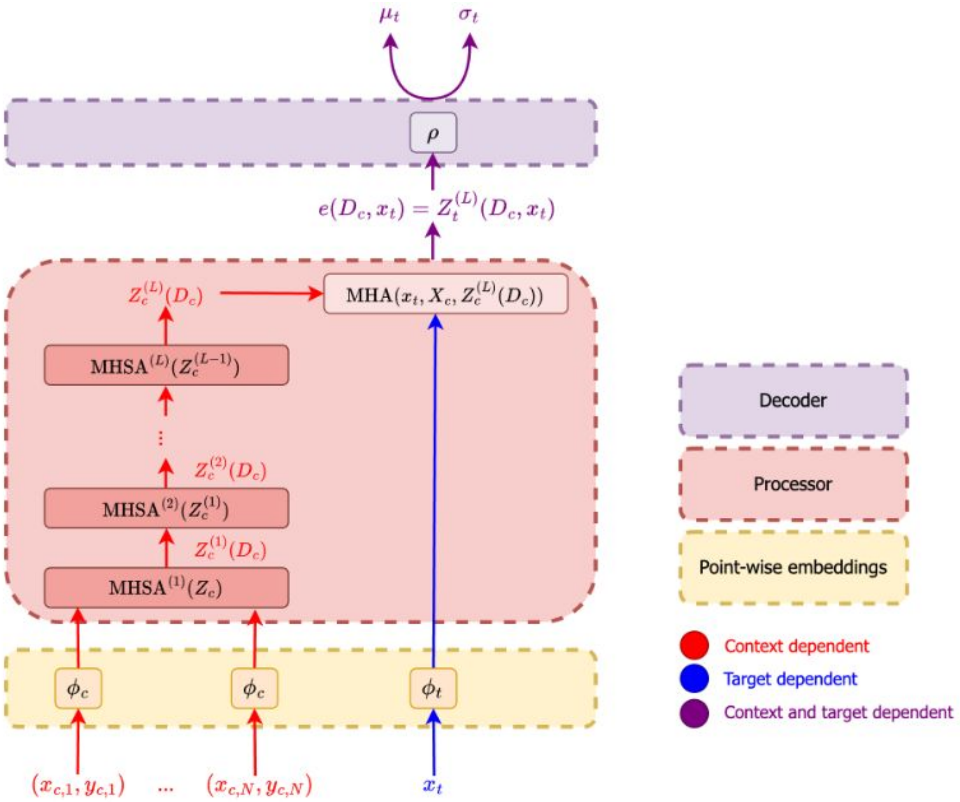

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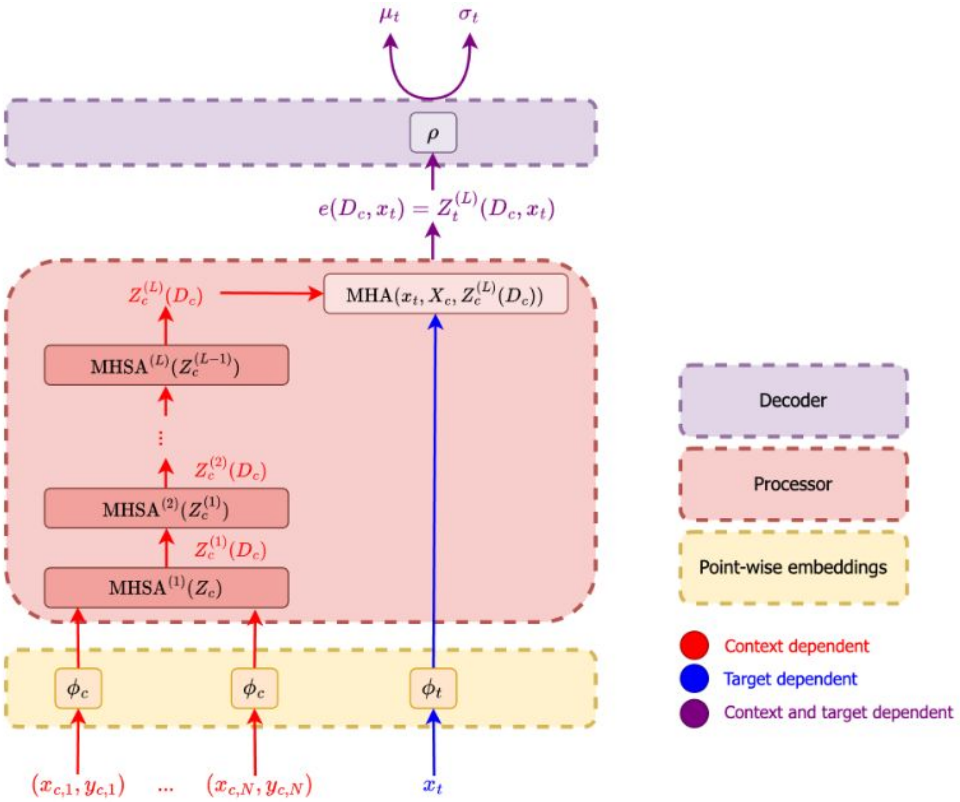

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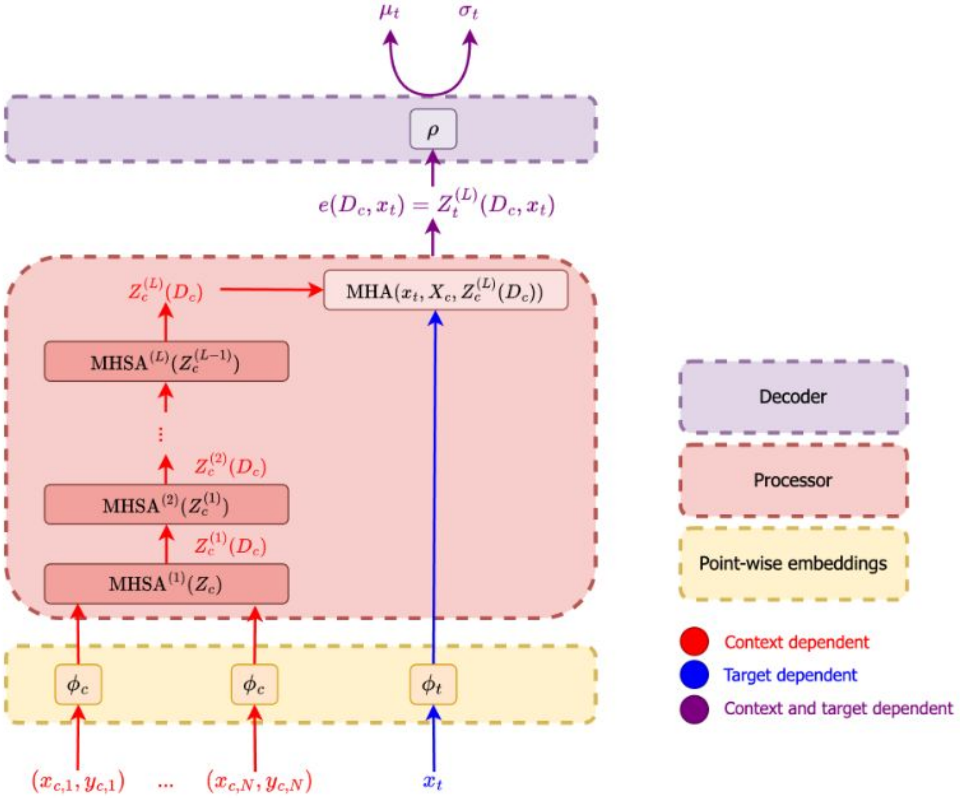

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- Pass output through decoder ρ (a 2-layer, 128-width MLP) to get predictive distribution (mean and variance of a Gaussian).

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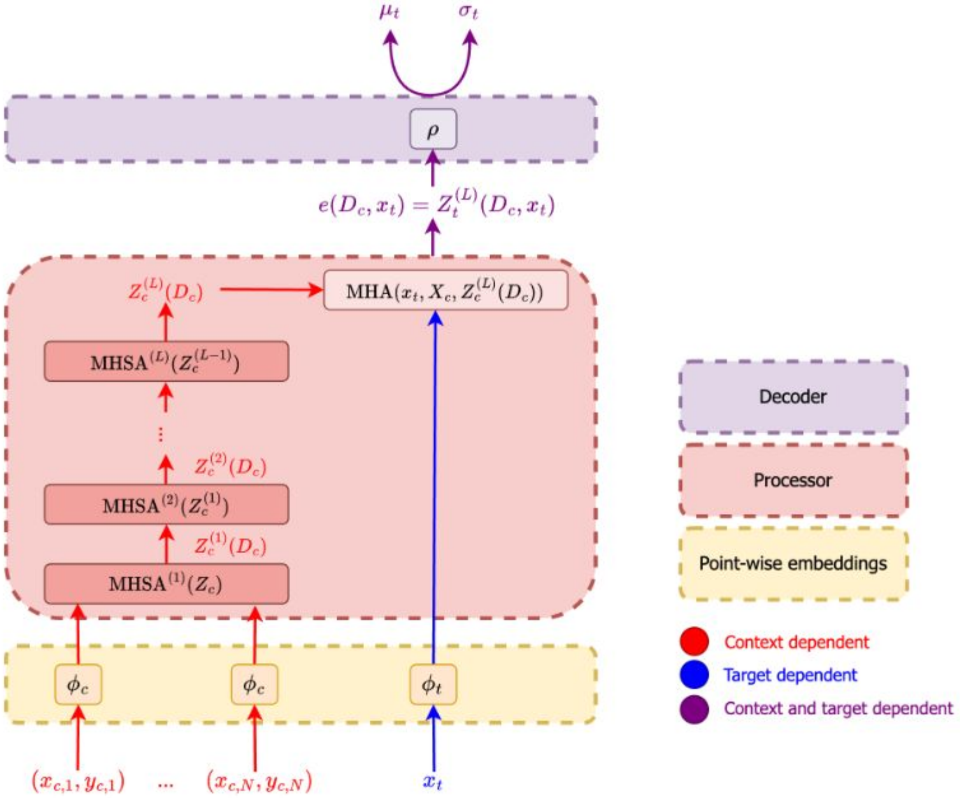

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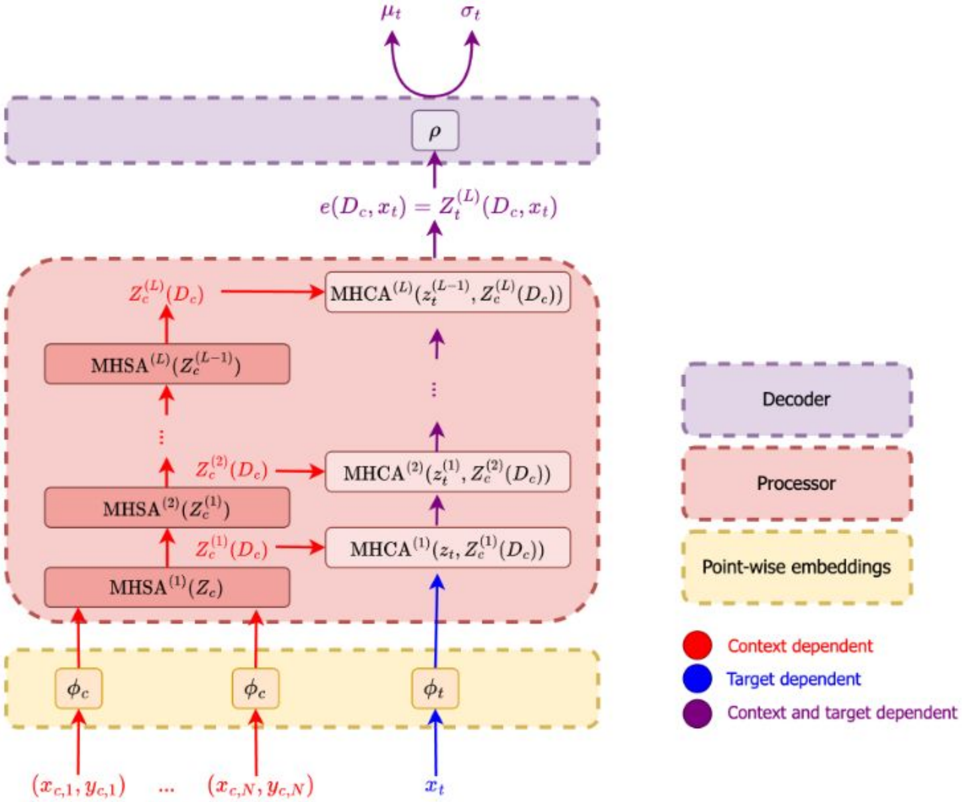

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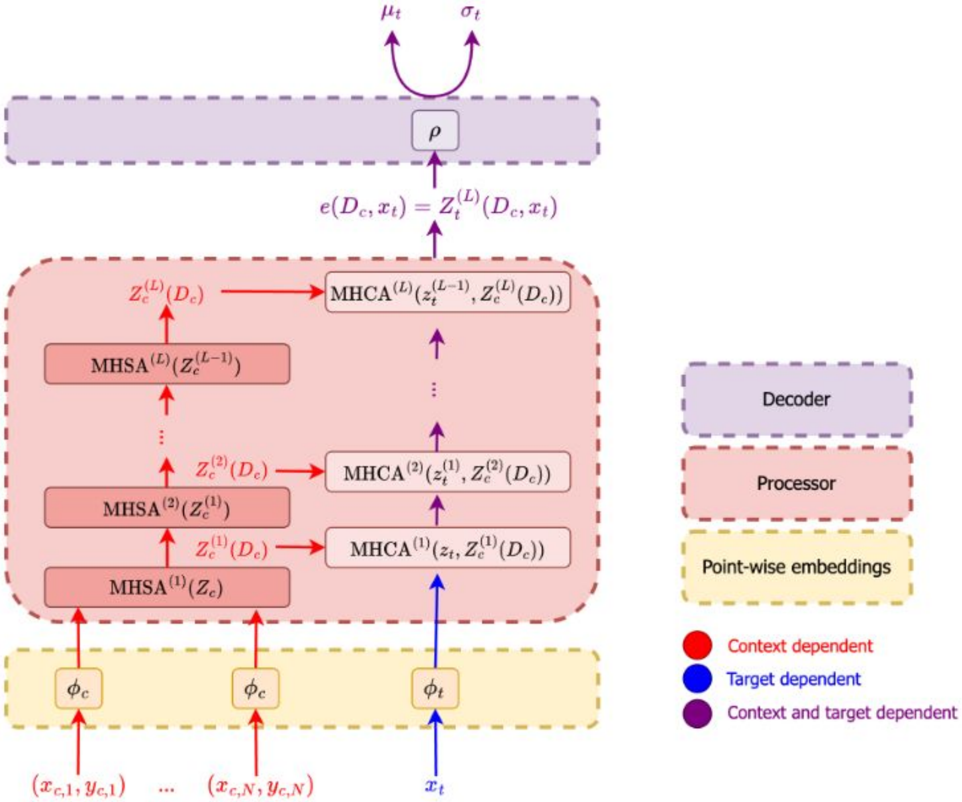

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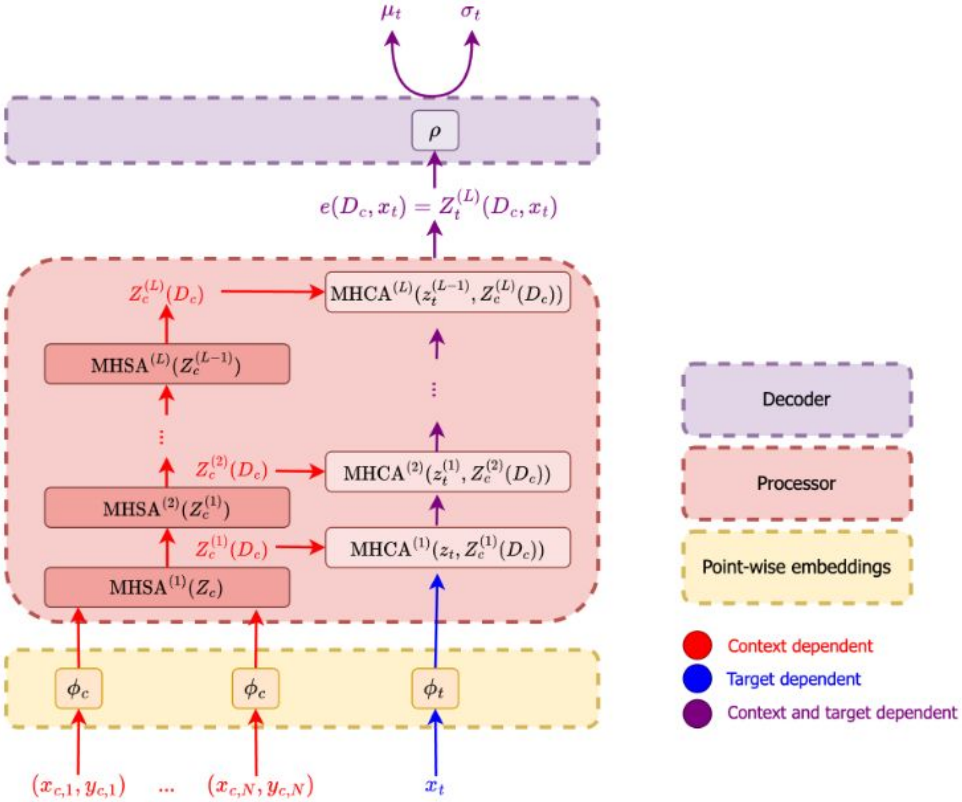
- Problem: $\mathcal{O}\left(N_c^2 + N_c N_t\right)$
- Solution: pseudo tokens



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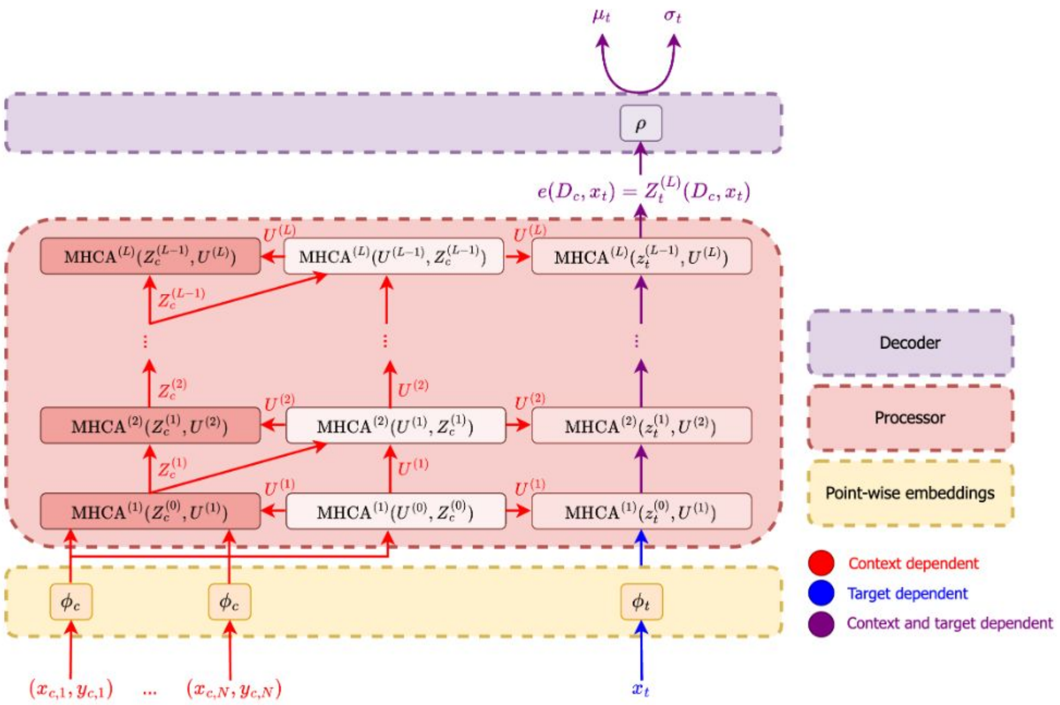
Pseudo Token TNP (PT-TNP)

- Add in $M \ll N_c$ ‘pseudo tokens’, $\mathrm{U} \in \mathbb{R}^{M \times D_z}$, to distill/summarise the latent context tokens, Z_c .



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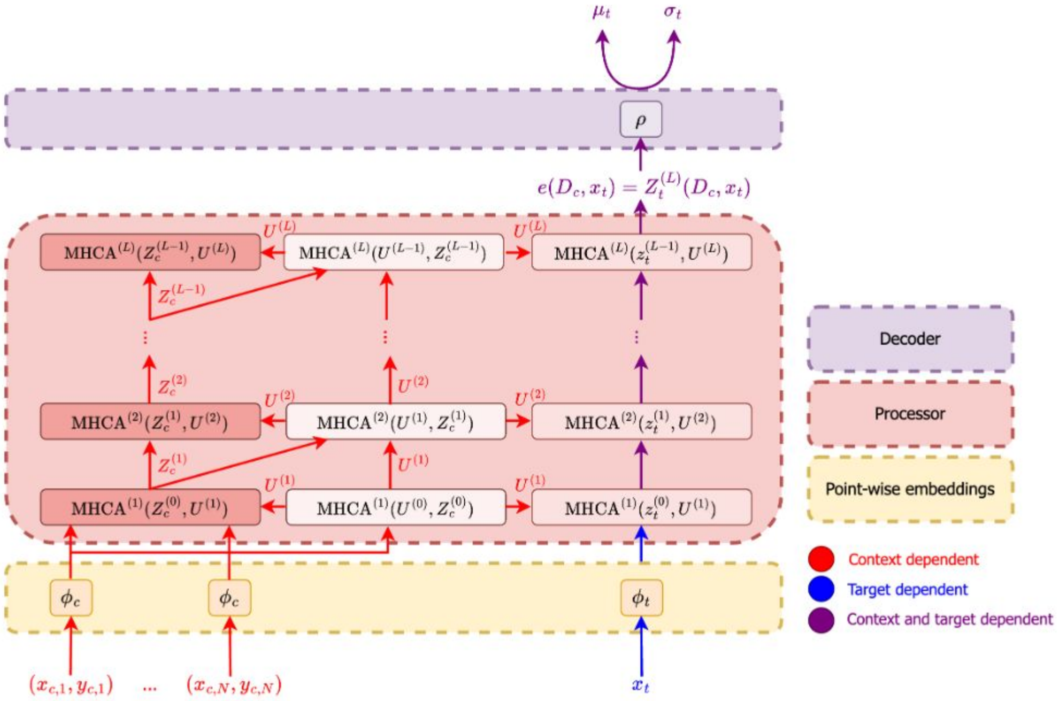
$$\mathcal{O}\left(MN_c + MN_t + M^2\right)$$



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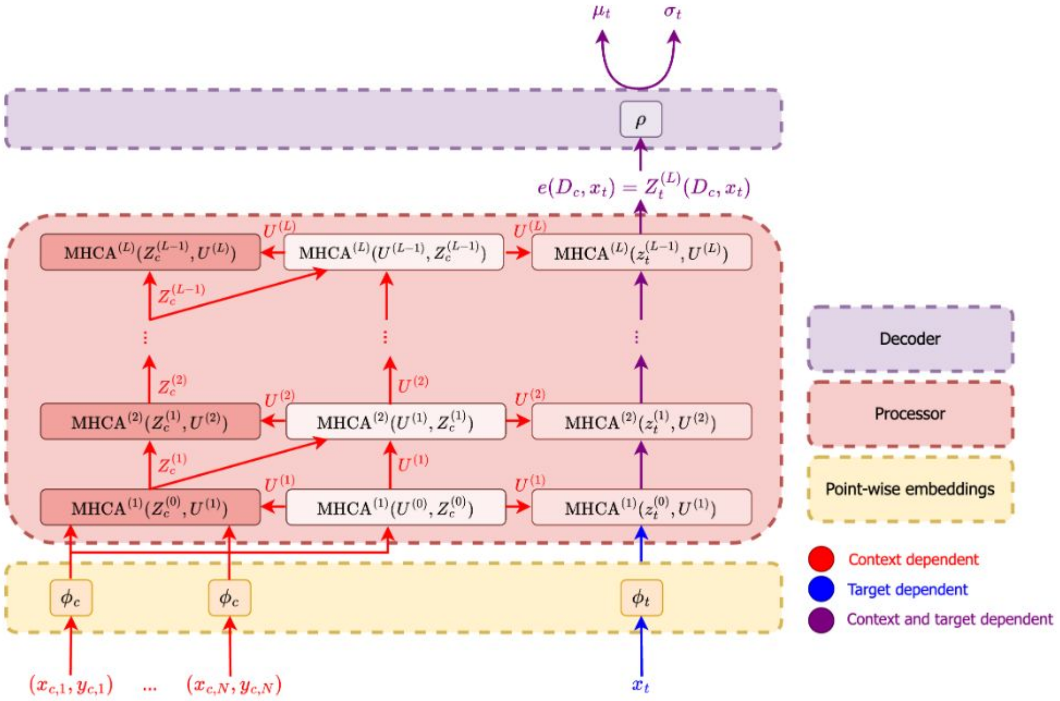
- Now we're linear in dataset size



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3. In-Context In-Context Learning

What if we have related (‘in-context’) data?

- We may have multiple related datasets from the target stochastic process
- E.g. a meta-dataset of PDE-simulated Navier-Stokes equations*
    - Could be partitioned into multiple sets based on the Reynold’s number (dimensionless parameter describing fluid flow)
    - Infeasible: train one NP per Reynold’s number (from 10^-6 to 10^12)
    - Idea: learn a single NP that can condition on each partition of the meta-dataset
- “*In-context in-context learning*”
    - “*amortizing the learning of stochastic-process specific NPs*”

(*) Note: training a single NP on the whole non-partitioned meta-dataset would give the predictive distribution of the marginal stochastic process

Theorem: More data is good

Theorem 1 (In-context in-context learning) *Let* $\xi_i \sim p(\xi)$, $\mathcal{D}_i, \{\mathcal{D}_j\} \sim P(\xi_i)$. *Let* $p(\mathbf{y}|\mathbf{x}, \mathcal{D}_i, \xi_i)$ *be the marginal posterior distribution of* $P(\xi_i)$ *given* $\mathcal{D}_i$, $p(\mathbf{y}|\mathbf{x}, \mathcal{D}_i, \{\mathcal{D}_j\})$ *be the marginal posterior distribution of the stochastic process* P *given* $\mathcal{D}_i$ *and* $\{\mathcal{D}_j\}$, *and* $p(\mathbf{y}|\mathbf{x}, \mathcal{D}_i)$ *be the marginal posterior distribution of the stochastic process* P *given* $\mathcal{D}_i$. *Then,*

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If we have extra datasets $\{\mathcal{D}_j\}$from the stochastic process $P(\xi_i)$ (on top of $\mathcal{D}_i$), then it can't hurt to condition on those too.

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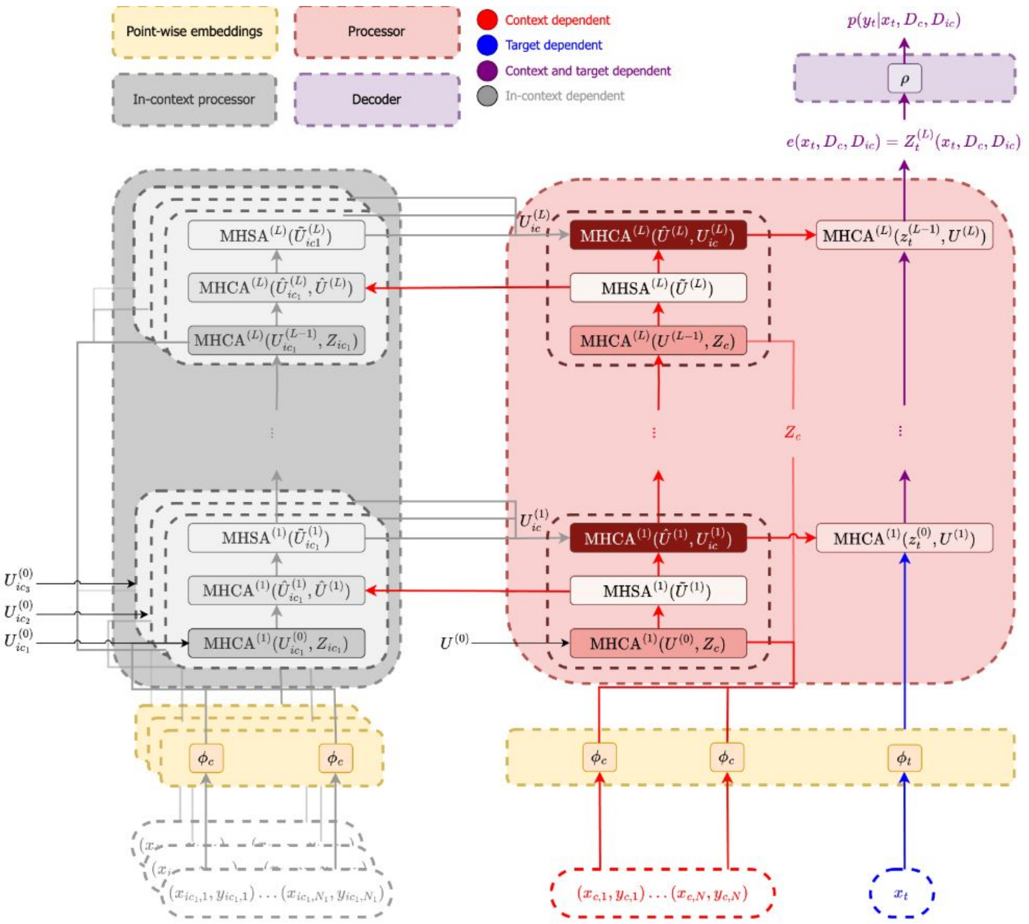
We refer to the additional datasets as the *in-context datasets* $\{\mathcal{D}_{ic,j}\}_{j=1}^{N_{ic}}$

In-Context In-Context Learning with TNPs (ICICL-TNP)

Create extra pseudo-tokens for each of the in-context datasets, U_{ic_i}.



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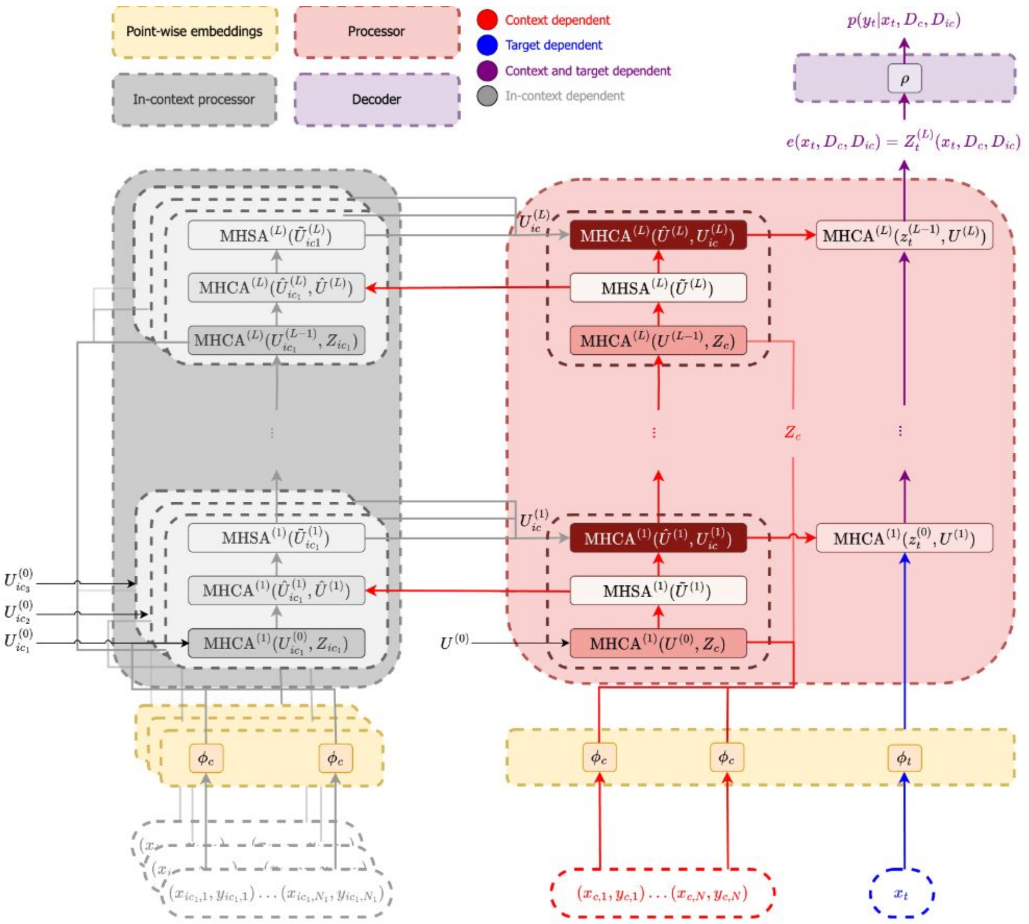

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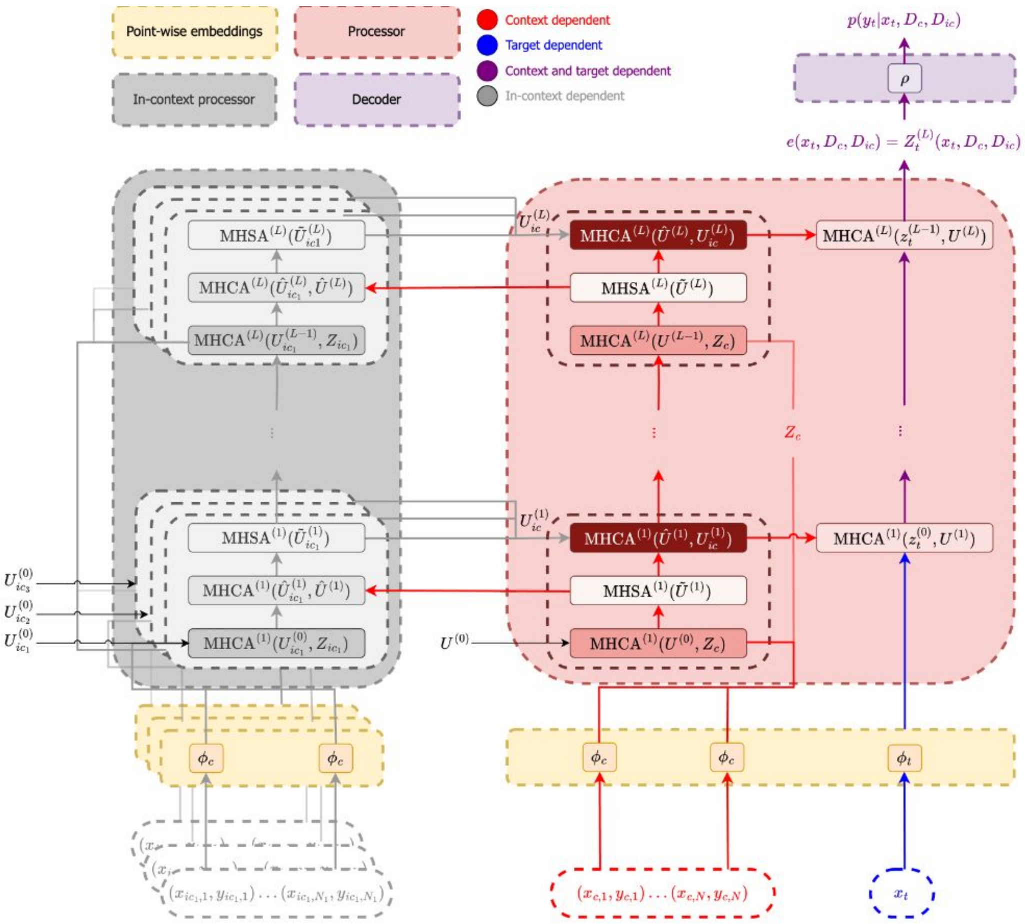

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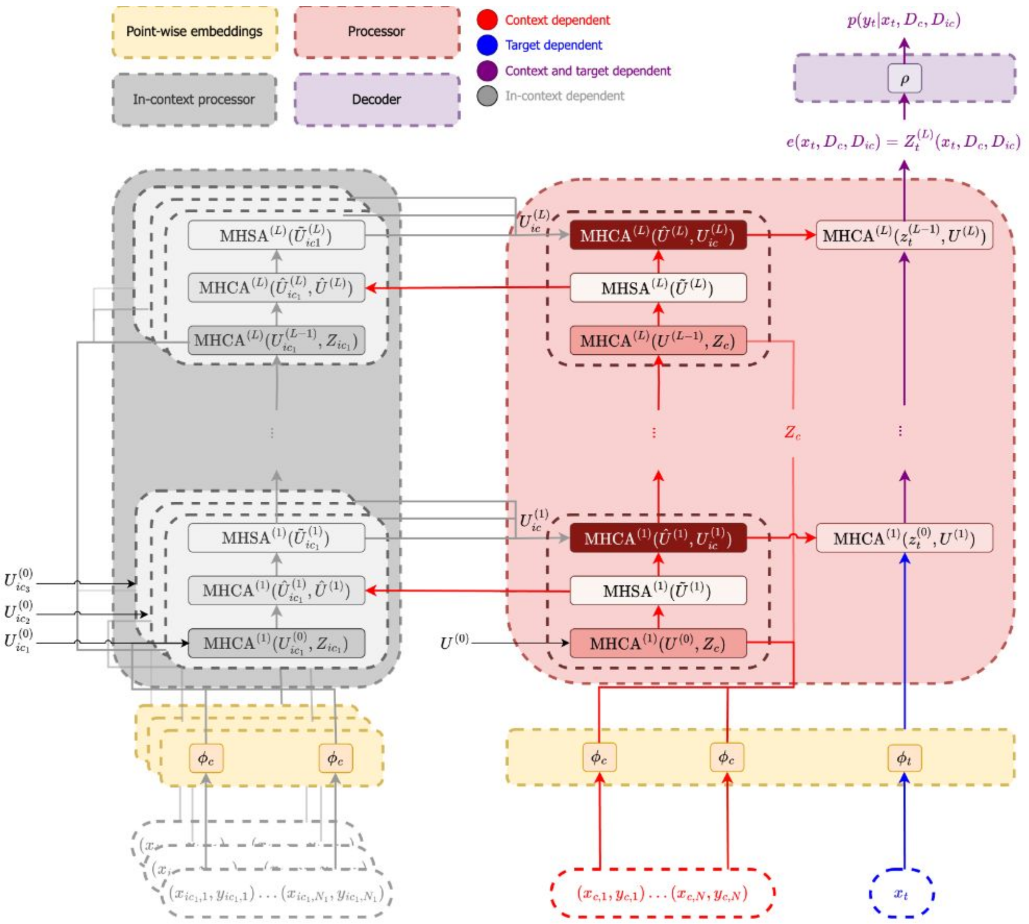

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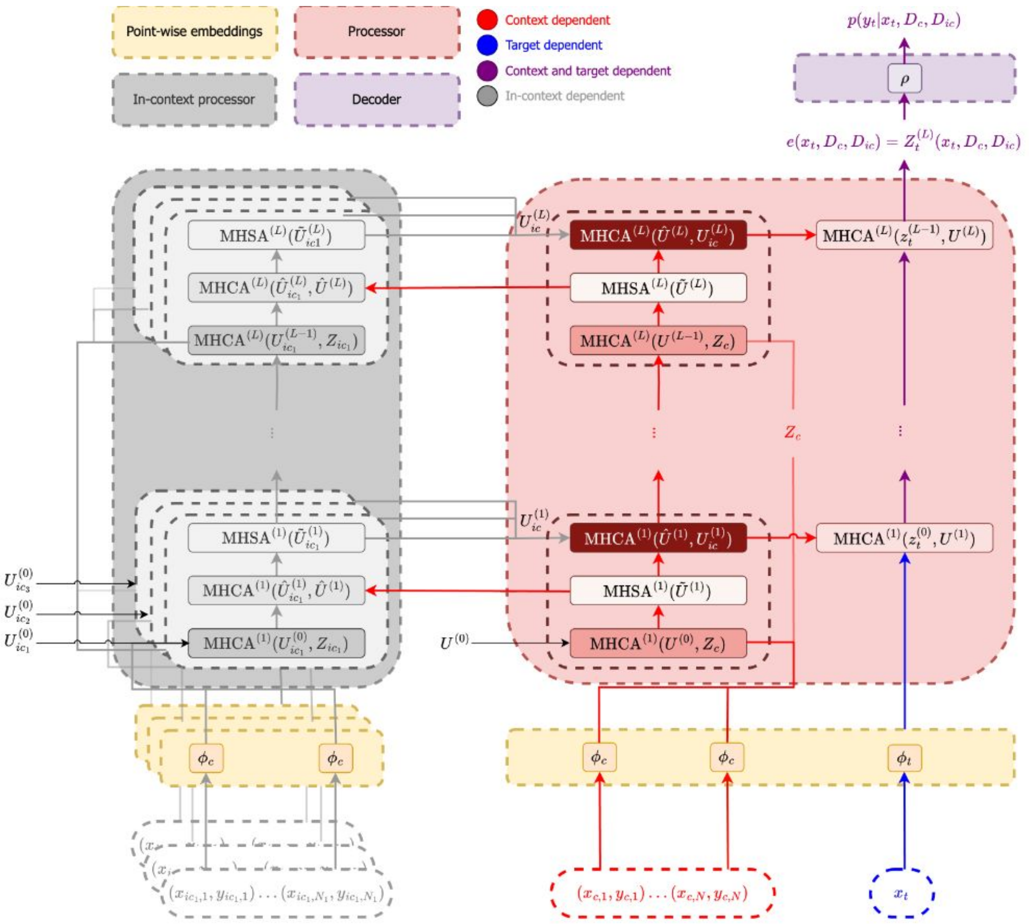

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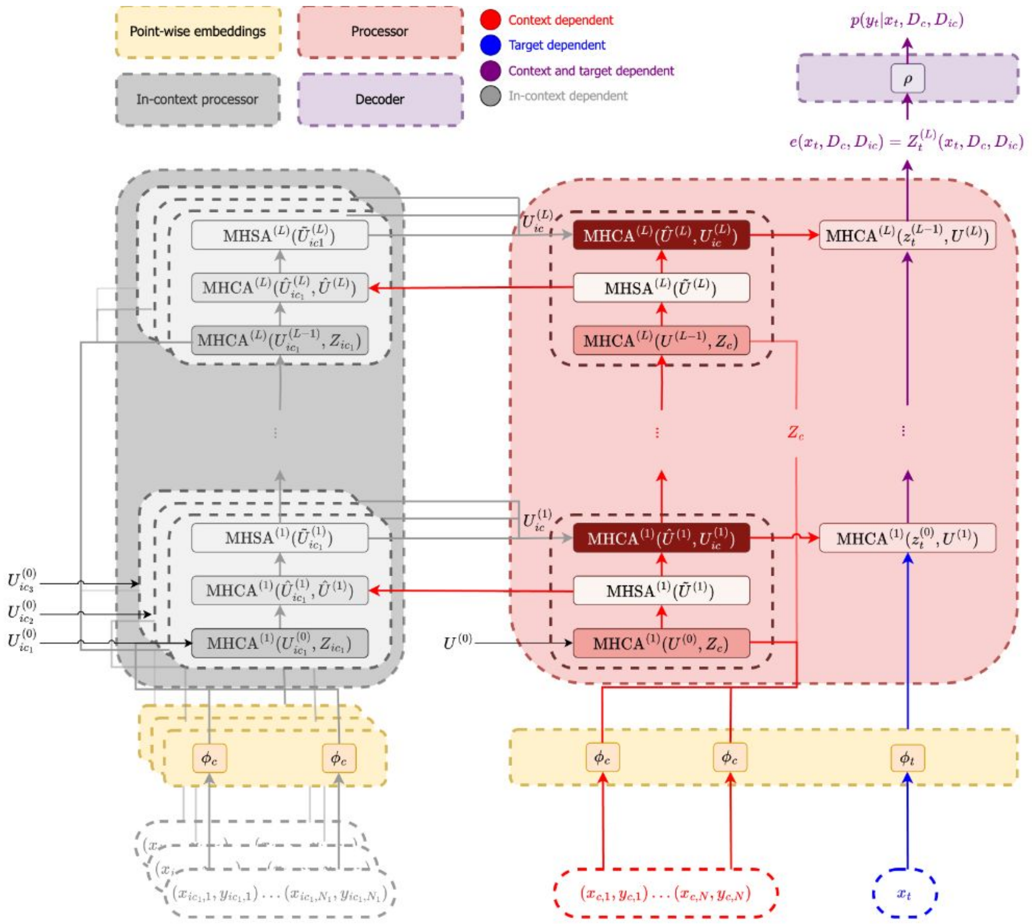
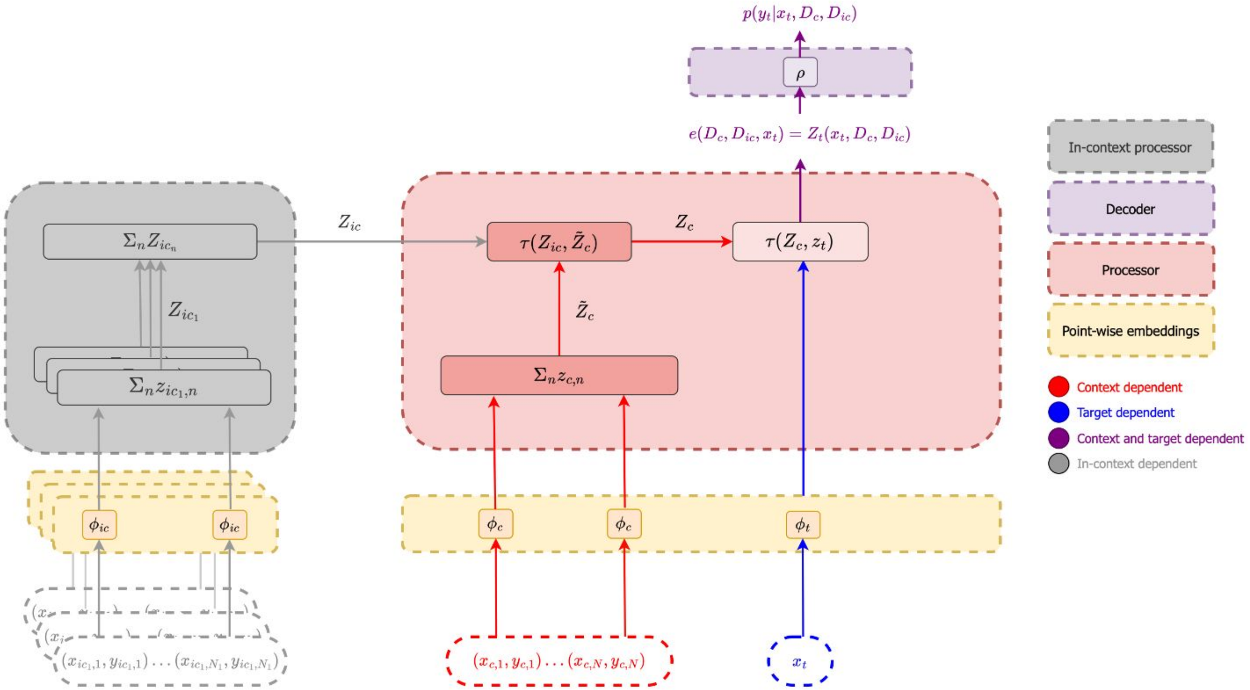


(Simpler model) ICICL Conditional Neural Processes (ICICL-CNPs)



4. Experiments

Experiments

Want to check:

1. Is ICICL still good without any in-context datasets?

2. Does ICICL get better with more in-context datasets (as we’d hope/expect)?

3. How does ICICL fare with OOD contexts?

4. How does ICICL fare with misspecified in-context datasets?

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- Kernel sampled from {RBF, periodic}

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(In-context datasets are drawn using the exact same kernel as the context-dataset.)

Synthetic 1D Regression

Model	Log lik. (↑)
CNP	-0.812 ± 0.005
PT-TNP	-0.598 ± 0.005
ICICL-TNP (0)	-0.607 ± 0.005
ICICL-TNP (1)	-0.499 ± 0.005
ICICL-TNP (2)	-0.474 ± 0.005
ICICL-TNP (3)	-0.469 ± 0.005
ICICL-TNP (4)	-0.467 ± 0.005
ICICL-TNP (5)	$\mathbf{-0.466 \pm 0.005}$

Table 1: Comparison of the predictive performance (in terms of test log likelihood) between the CNP, PT-TNP, and the ICICL-TNP with varying number of in-context datasets (indicated within brackets).

(CNP just uses MLPs instead of transformers.)

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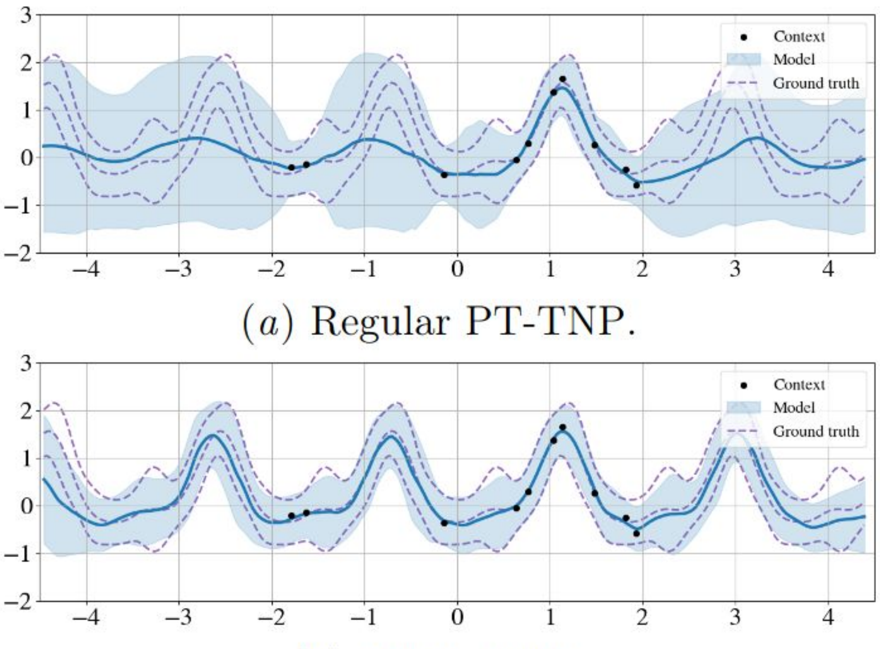
ICICL-TNP (0)	-0.607 ± 0.005
ICICL-TNP (1)	-0.499 ± 0.005
ICICL-TNP (2)	-0.474 ± 0.005
ICICL-TNP (3)	-0.469 ± 0.005
ICICL-TNP (4)	-0.467 ± 0.005
ICICL-TNP (5)	$\mathbf{-0.466 \pm 0.005}$

Table 1: Comparison of the predictive performance (in terms of test log likelihood) between the CNP, PT-TNP, and the ICICL-TNP with varying number of in-context datasets (indicated within brackets).



(a) Regular PT-TNP.

(b) ICICL-TNP.

Figure 2: The difference between the predictive distributions of the regular PT-TNP and the ICICL-TNP when conditioning on three in-context datasets with 128 datapoints (not shown here).

Synthetic 1D Regression - OOD

Test on datasets with bandwidth/period sampled as

$$\log l \sim \mathcal{U}_{[\log 0.1, \log 0.25] \cup [\log 4, \log 10]}$$

Model	Log lik. (↑)
CNP	-0.880 ± 0.006
PT-TNP	-0.798 ± 0.007
ICICL-TNP (0)	-0.783 ± 0.007
ICICL-TNP (1)	-0.721 ± 0.006
ICICL-TNP (2)	-0.702 ± 0.006
ICICL-TNP (3)	$\mathbf{-0.700 \pm 0.006}$

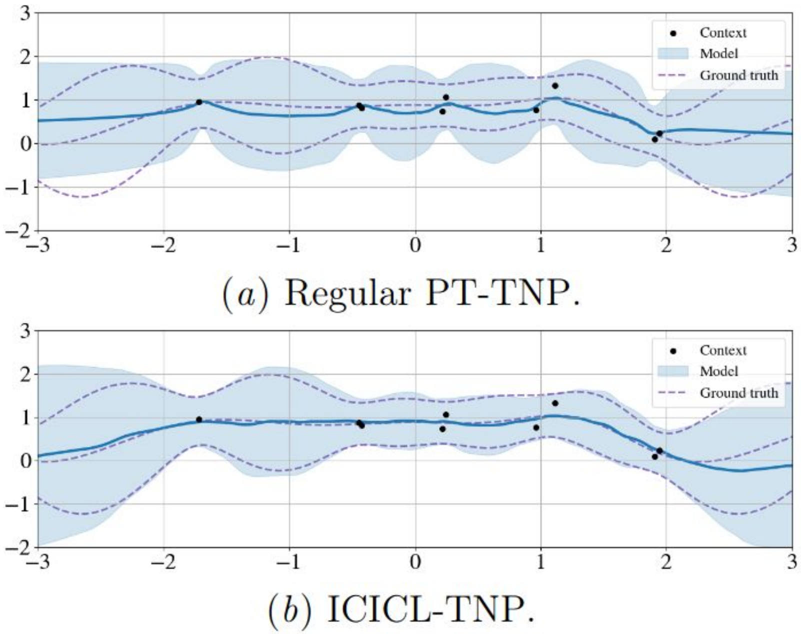
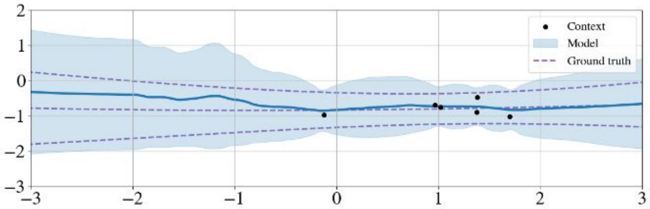
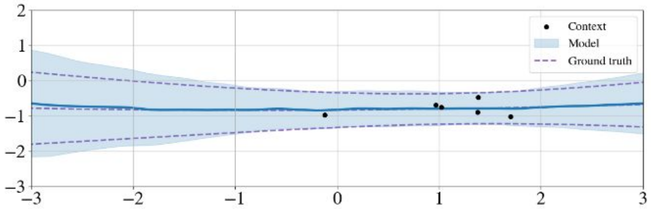


Figure 3: The difference between the predictive distributions when tested OOD of the regular PT-TNP and the ICICL-TNP when conditioning on three in-context datasets. The context datapoints come from a GP with a periodic kernel with $\ell = 6.08$.

Synthetic 1D Regression - OOD



(a) PT-TNP, RBF $\ell = 5.19$



(b) ICICL-TNP, RBF $\ell = 5.19$

Figure 13: A comparison between the predictive distribution when tested OOD of the PT-TNP (left) and the ICICL-TNP (right). In the top row the samples come from a GP with RBF kernel and $\ell = 5.19$. In the bottom row the samples come from a GP with periodic kernel and $\ell = 0.24$. The ICICL-TNP is conditioned on three in-context datasets.

Synthetic 1D Regression - OOD

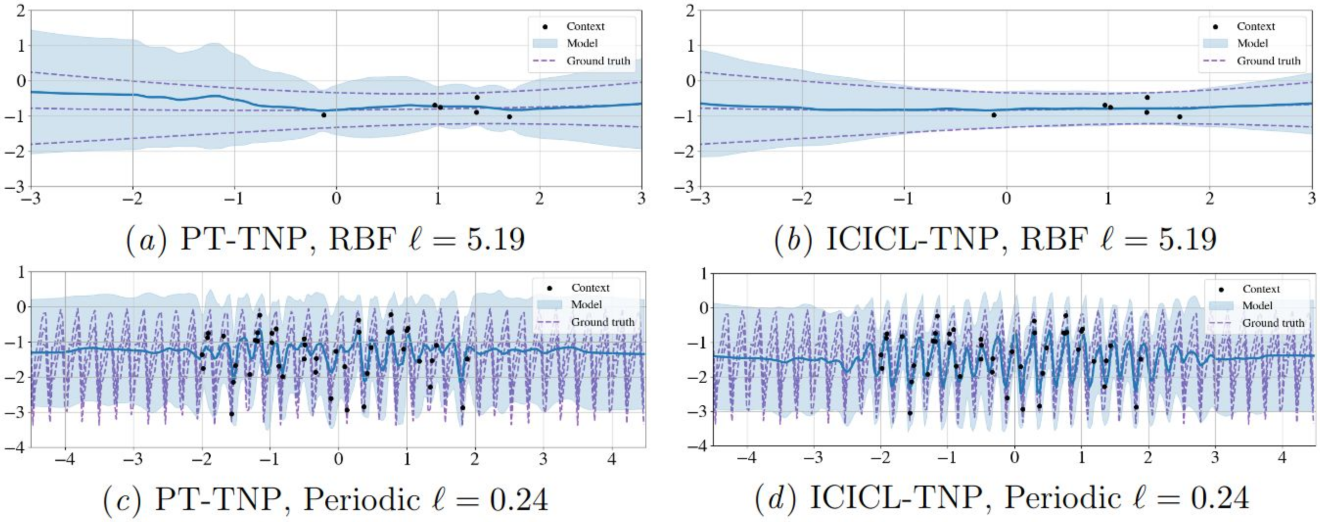
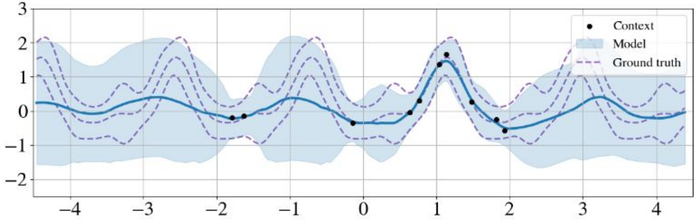
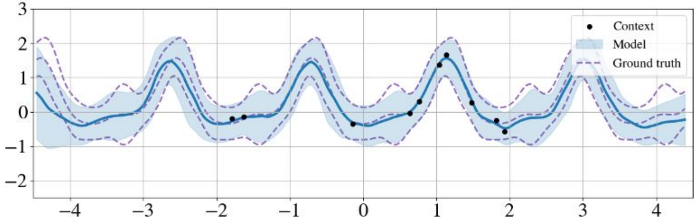


Figure 13: A comparison between the predictive distribution when tested OOD of the PT-TNP (left) and the ICICL-TNP (right). In the top row the samples come from a GP with RBF kernel and $\ell = 5.19$. In the bottom row the samples come from a GP with periodic kernel and $\ell = 0.24$. The ICICL-TNP is conditioned on three in-context datasets.

Synthetic 1D Regression - Incorrect In-context Conditioning

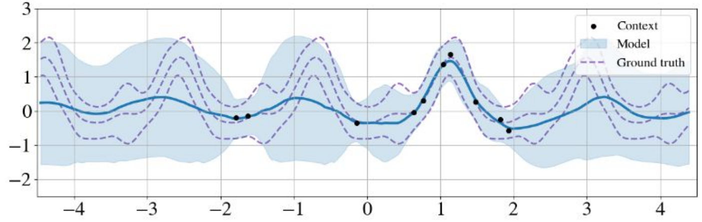


(a) No in-context datasets

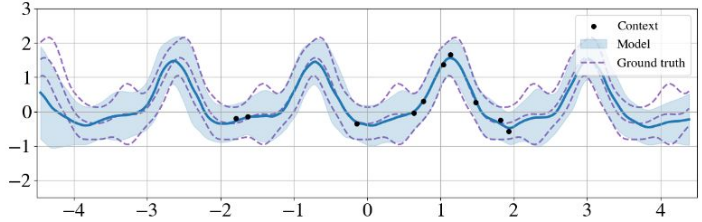


(b) Periodic kernel, $\ell = 1.85$

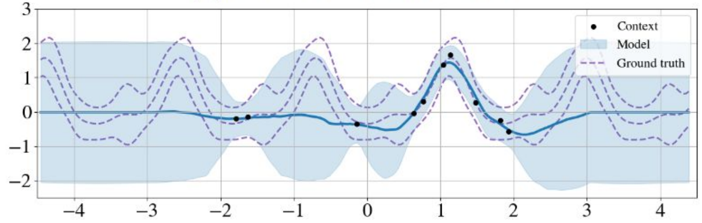
Synthetic 1D Regression - Incorrect In-context Conditioning



(a) No in-context datasets

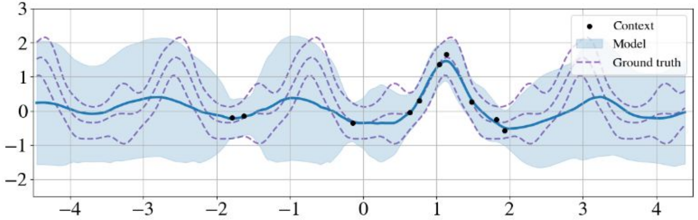


(b) Periodic kernel, $\ell = 1.85$

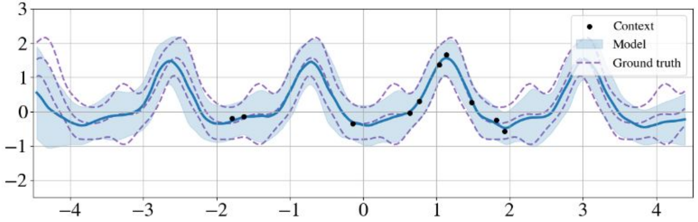


(c) RBF kernel, $\ell = 0.52$

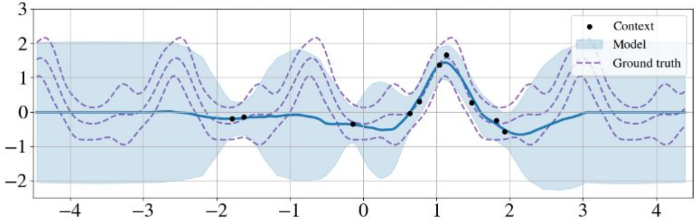
Synthetic 1D Regression - Incorrect In-context Conditioning



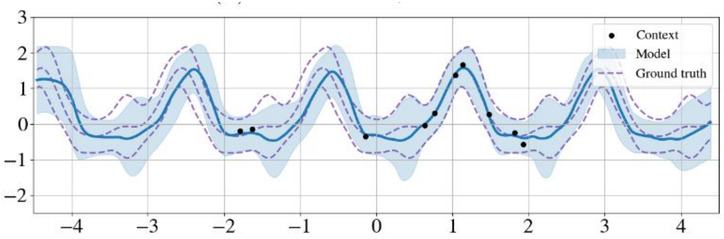
(a) No in-context datasets



(b) Periodic kernel, $\ell = 1.85$

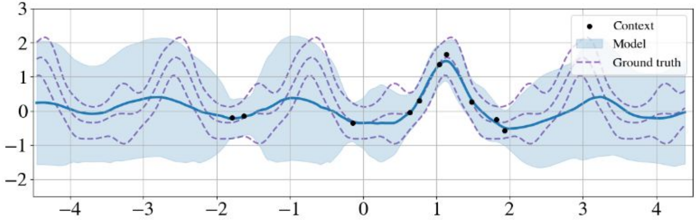


(c) RBF kernel, $\ell = 0.52$

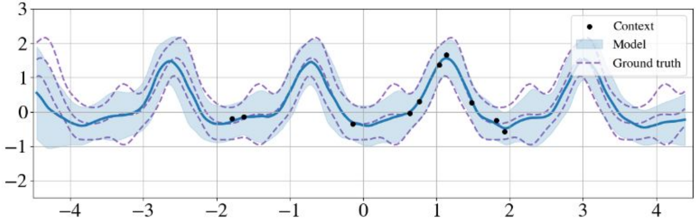


(d) Periodic kernel, $\ell = 1.76$

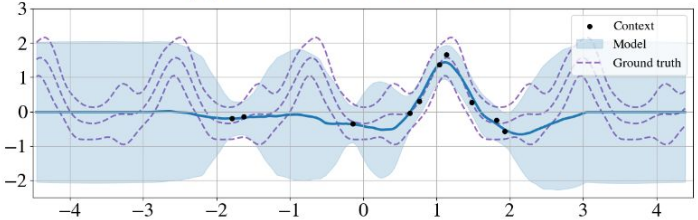
Synthetic 1D Regression - Incorrect In-context Conditioning



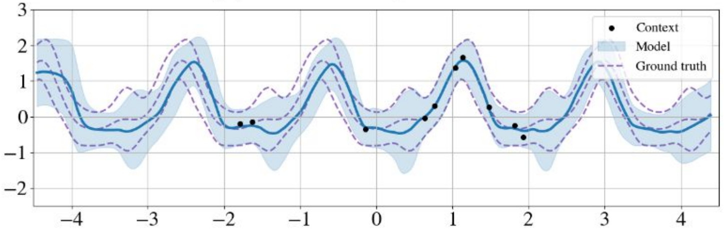
(a) No in-context datasets



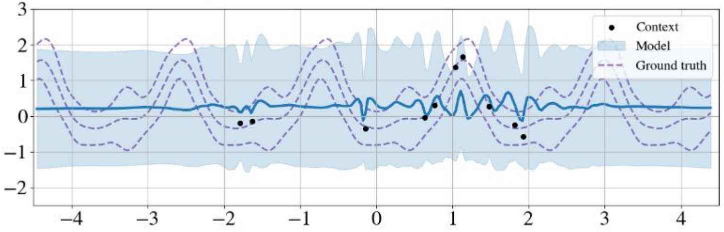
(b) Periodic kernel, $\ell = 1.85$



(c) RBF kernel, $\ell = 0.52$

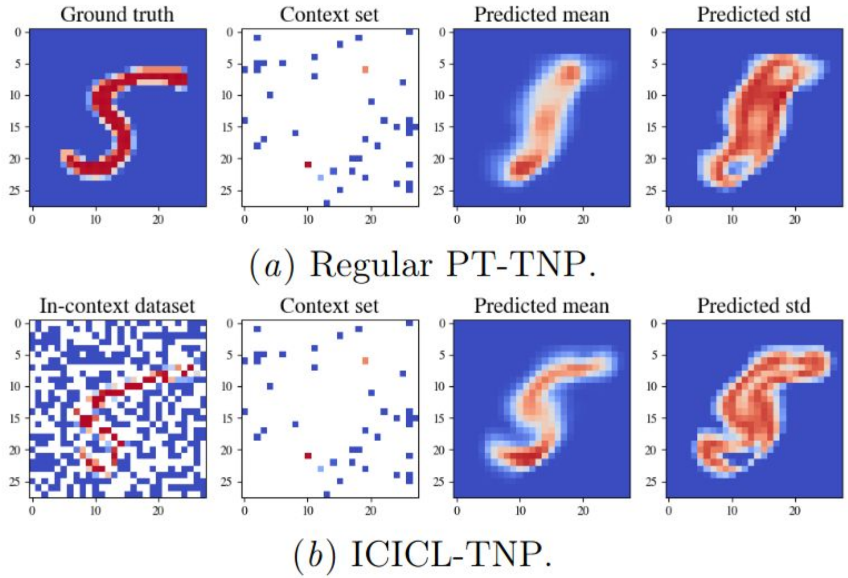


(d) Periodic kernel, $\ell = 1.76$



(e) Periodic kernel, $\ell = 0.28$

MNIST Image Completion



- $N = 784$ 2D pixel locations $x \in \mathbb{R}^2$
- Pixel values $y \in \mathbb{R}$

Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

MNIST Image Completion

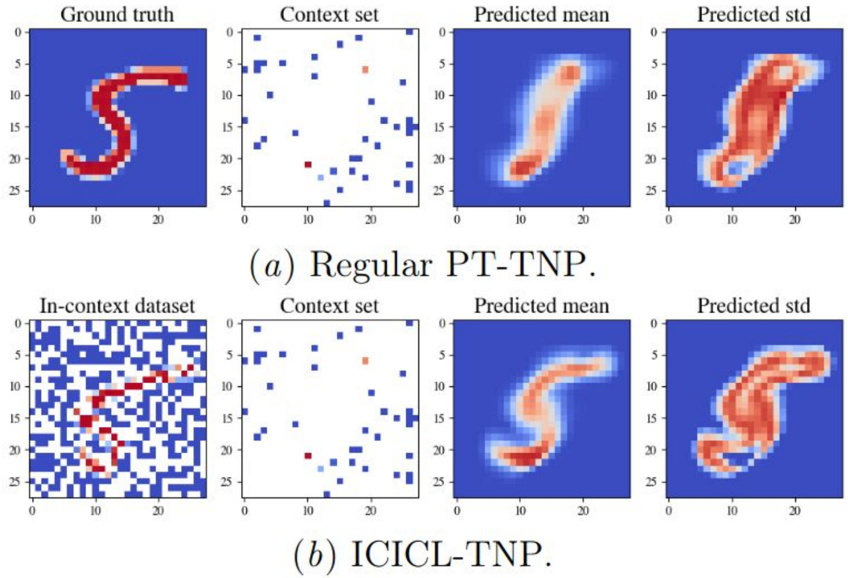


Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

- $N = 784$ 2D pixel locations $x \in \mathbb{R}^2$
- Pixel values $y \in \mathbb{R}$
- $N_c \sim \mathcal{U}_{\{N/100,\ldots,N/5\}}$ context points

MNIST Image Completion

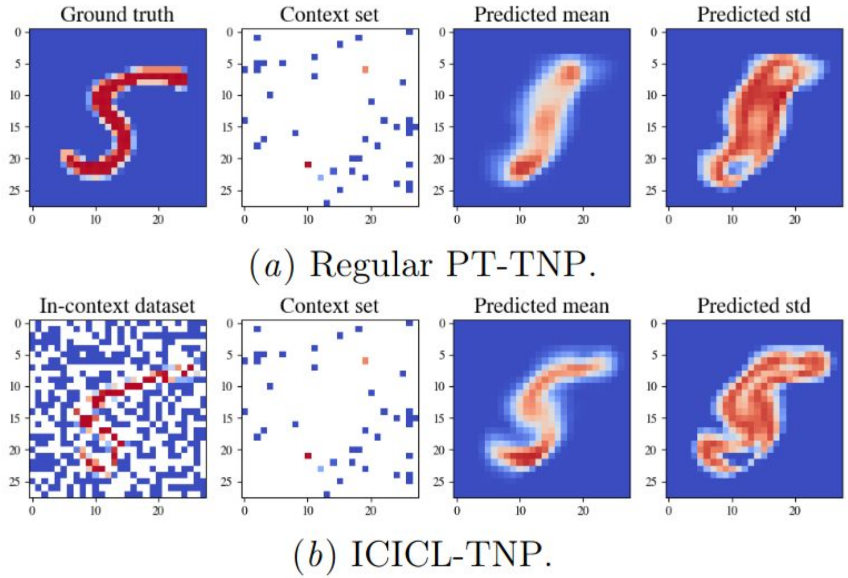


Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

- $N = 784$ 2D pixel locations $x \in \mathbb{R}^2$
- Pixel values $y \in \mathbb{R}$
- $N_c \sim \mathcal{U}_{\{N/100,\ldots,N/5\}}$ context points
- $N_{ic} \sim \mathcal{U}_{\{0,\ldots,3\}}$ in-context sets with $N_{ic,j} \sim \mathcal{U}_{\{N/100,\ldots,N/2\}}$

MNIST Image Completion

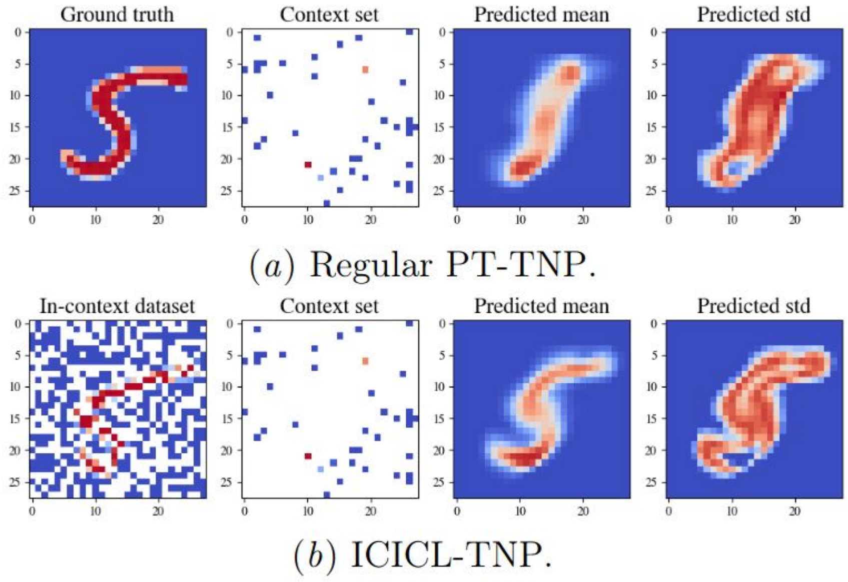


Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

- $N = 784$ 2D pixel locations $x \in \mathbb{R}^2$
- Pixel values $y \in \mathbb{R}$
- $N_c \sim \mathcal{U}_{\{N/100,\ldots,N/5\}}$ context points
- $N_{ic} \sim \mathcal{U}_{\{0,\ldots,3\}}$ in-context sets with $N_{ic,j} \sim \mathcal{U}_{\{N/100,\ldots,N/2\}}$
- $N_t = N - N_c$

MNIST Image Completion

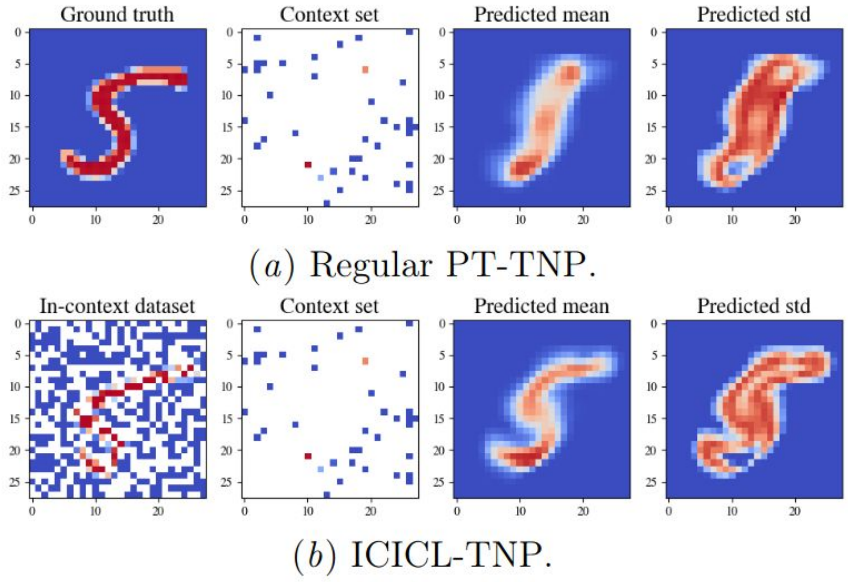


Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

- $N = 784$ 2D pixel locations $x \in \mathbb{R}^2$
- Pixel values $y \in \mathbb{R}$
- $N_c \sim \mathcal{U}_{\{N/100,\ldots,N/5\}}$ context points
- $N_{ic} \sim \mathcal{U}_{\{0,\ldots,3\}}$ in-context sets with $N_{ic,j} \sim \mathcal{U}_{\{N/100,\ldots,N/2\}}$
- $N_t = N - N_c$

(In-context datasets are drawn using the same class label as the context-dataset.)

MNIST Image Completion

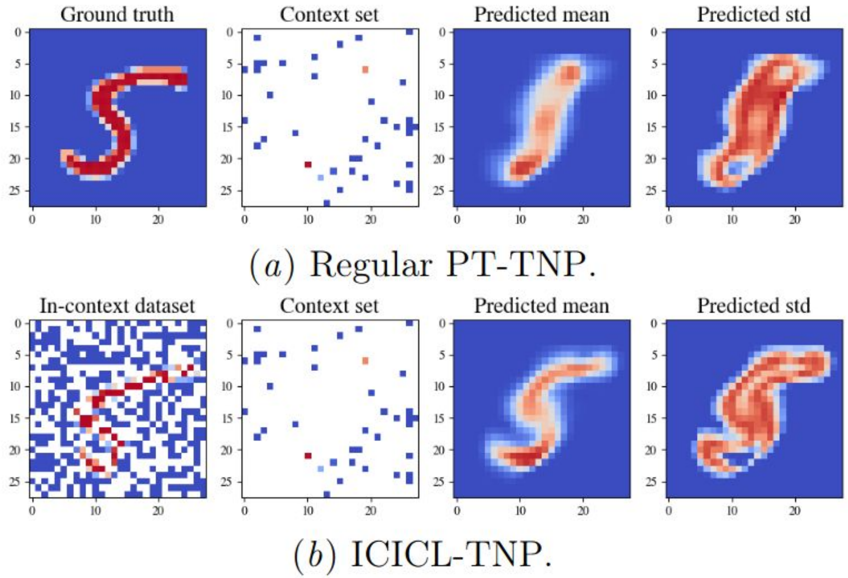


Figure 5: A comparison between the predictive distribution of the ICICL-TNP and the regular PT-TNP when conditioning on the context and in-context dataset shown.

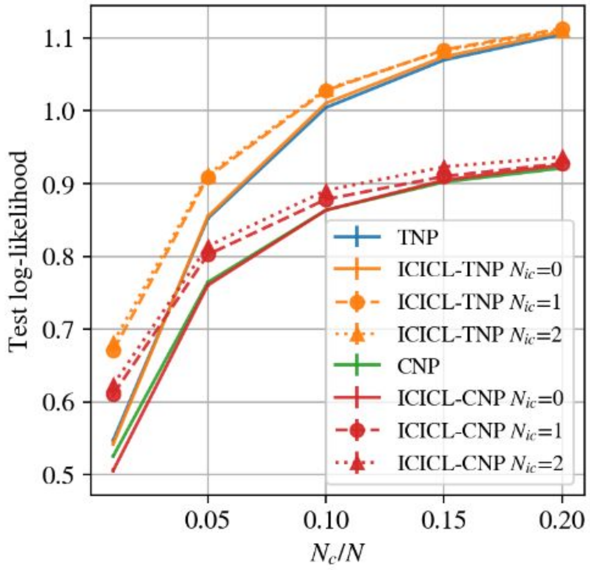
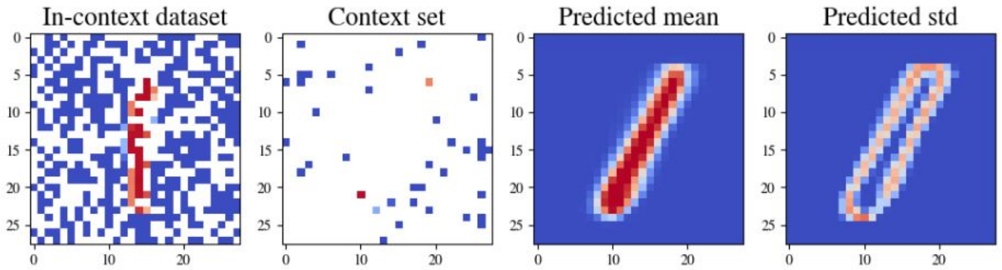


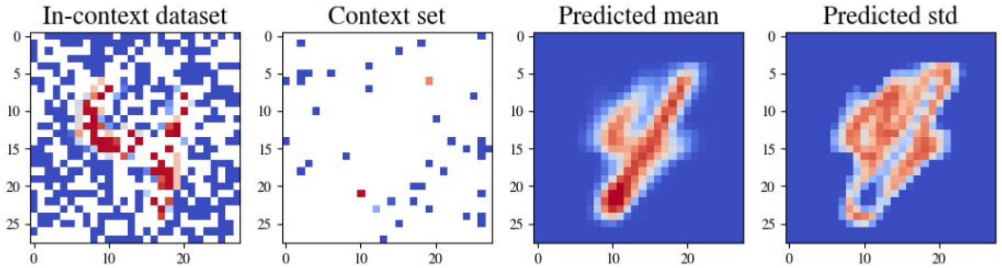
Figure 4: A comparison between the predictive performance of the ICICL-TNP, regular PT-TNP, ICICL-CNP and CNP as the proportion of context datapoints N_c/N varies in the MNIST inpainting experiment.

MNIST Image Completion

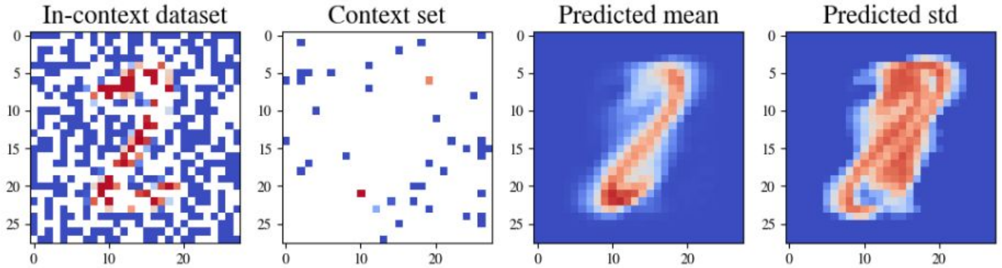
(Notice high uncertainty for 4 and 2, where the context set is less compatible with the label of the in-context dataset.)



(b) In-context dataset label: 1



(c) In-context dataset label: 4



(d) In-context dataset label: 2

Environmental Data

Regression on spatio-temporal data for surface air temperature.

In-context datasets are obtained from the same location but at different times.

Model	**Test Log-Likelihood**
PT-TNP	1.15 ± 0.01
ICICL-TNP (0)	1.15 ± 0.01
ICICL-TNP (1)	1.18 ± 0.01
ICICL-TNP (2)	1.19 ± 0.01

Table 3: Comparison of the test log-likelihood on the environmental data for the PT-TNP and ICICL-TNP with varying number of in-context datasets (indicated within brackets).

Environmental Data

Another baseline: also allow PT-TNP to train on the in-context sets (but just stick that data in with the main context).

Model	Test Log-Likelihood
PT-TNP	1.15 ± 0.01
PT-TNP-merged (0)	1.14 ± 0.01
PT-TNP-merged (1)	1.15 ± 0.01
PT-TNP-merged (2)	1.14 ± 0.01
ICICL-TNP (0)	1.15 ± 0.01
ICICL-TNP (1)	1.18 ± 0.01
ICICL-TNP (2)	1.19 ± 0.01

Table 5: Comparison of the test log-likelihood on the environmental data for the PT-TNP and ICICL-TNP with varying number of in-context datasets (indicated within brackets). As an additional baseline, we also consider the PT-TNP-merged where the in-context datasets are merged into the context datasets.

(This doesn't help.)

Weaknesses

- More experiments?
  - Larger-scaled
  - (Though the experiments in this paper seem to match standard experiments in other NP papers…)

- Include the PT-TNP-merged baseline in all experiments.
  - (Or some other method to let PT-TNP use the in-context data, even if badly.)

- ICICL relies on identifying in-context datasets drawn from the same stochastic process as the context dataset. This is often not possible.

References

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Appendix: Attentive Neural Process (ANP)