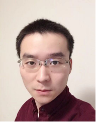
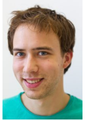
Doubly Stochastic Variational Inference for Neural Processes with Hierarchical Latent Variables

Q. Wang & Herke van Hoof





Amsterdam Machine Learning Lab

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  - formalization of a hierarchical $\mathcal{SP}$
  - plausible approximate inference method
- Competitive performance on extensive Uncertainty-aware Applications
  - high dimensional regressions on simulators/real-world dataset
  - classification and o.o.d. detection on image dataset

Outline of this Talk

1. Motivation for $\mathcal{SP}$s
2. Study of $\mathcal{SP}$s with LVMs
3. NP with Hierarchical Latent Variables
4. Experiments and Applications

Motivation for $\mathcal{SP}$s

Why Do We Need *Stochastic Processes*?

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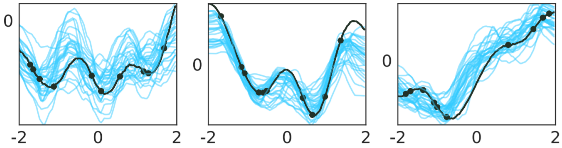

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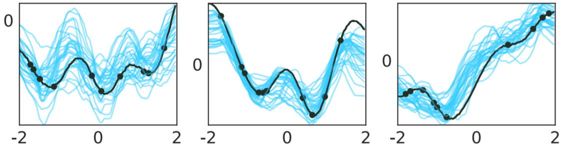

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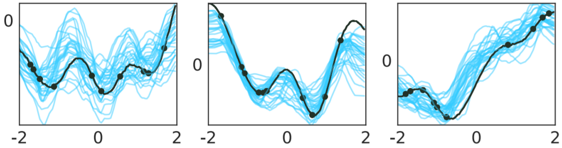

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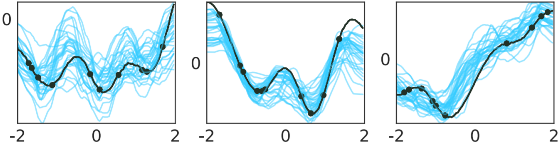

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- Quantify uncertainty in risk-sensitive applications : *e.g.* forecast $p(s_{t+1}|s_t, a_t)$ in autonomous driving [2] ;
- Model distributions instead of point estimates : working as a *generative model* for more realizations [3].

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- **Marginalization Consistency.** For any finite collection of random variables $\{y_1, y_2, \ldots, y_{N+M}\}$, the probability after *marginalization* over subset is unchanged.

$$\int \rho_{x_{1:N+M}}(y_{1:N+M}) dy_{N+1:N+M} = \rho_{x_{1:N}}(y_{1:N}) \tag{1.1}$$

- **Exchangeability Consistency.** Any random *permutation* over set of variables does not influence joint probability.

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With these two conditions, an exchangeable $\mathcal{SP}$ can be induced. (Refer to *Kolmogorov Extension Theorem*)

$\mathcal{SP}$s in Progress and Primary Concerns

Crucial properties for $\mathcal{SP}$s :

- Scalability in large-scale dataset:
- Flexibility in distributions:
- Extension to high dimensions:

Analysis on GPs/NPs :

- Gaussian Processes (GPs)
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  $\rightarrow$ more flexible with no explicit distributions

Study of $\mathcal{SP}$s with LVMs

Deep Latent Variable Model as $\mathcal{SP}$s

Here we present an implicit Latent Variable Model for $\mathcal{SP}$s :

- Generation paradigm with (potentially correlated) latent variables :

- Predictive distribution in $\mathcal{SP}$s : Let the *context* and *target input* be $\mathcal{C} = \{(x_i, y_i) | i = 1, 2, \ldots, N\}$ and x_T, the computation is

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NP family approximates $\mathcal{SP}$s in the form of LVMs :

- $\mathcal{GP}$ as an exchangeable $\mathcal{SP}$ with latent variables :

- NP as an exchangeable $\mathcal{SP}$ with a global latent variable :

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Remark

Some other models, such as Hierarchical $\mathcal{GP}$s [5] and Deep $\mathcal{GP}$s [6], [7] can also be expressed with LVMs.

Inference for Neural Processes

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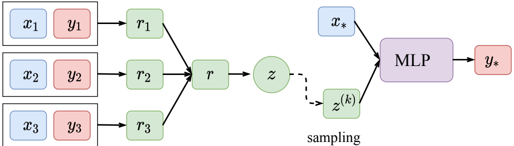

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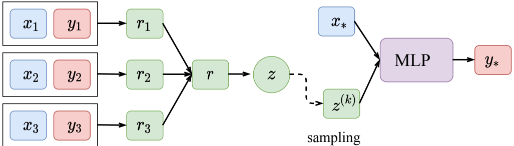
$$r_i = h_\theta(x_i, y_i), \quad r = \bigoplus_{i=1}^{N} r_i, \quad p_\theta(z_C|x_C, y_C) = \mathcal{N}(z_C|[f_\mu(r), f_\sigma(r)]) \tag{2.7}$$



NPs with Hierarchical Latent Variables

Extending NPs from A Hierarchical Bayes Perspective

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$$\rho_{x_{1:N+M}}(y_{1:N+M}) = \iint \prod_{i=1}^{N+M} p(y_i|z_G, z_i, x_i) p(z_i|x_i, z_G)p(z_G)dz_{1:N+M}dz_G \tag{3.1}$$

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Remark

DSVNP satisfies **Marginalization** and **Exchangeability Consistencies**, so it is a new exchangeable $\mathcal{SP}$.

Approximate Inference for DSVNP

Exact inference for this hierarchical LVM is mostly intractable, hence approximate inference is used here.

- Evidence Lower Bound for DSVNP :

- Generative (Black Lines) and Recognition Models (Blue/Pink Lines) in Graphs : Specify generative process with black line

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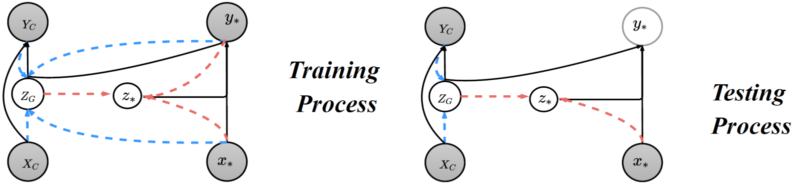

Training and Testing in Practice

Similar to that in NPs, DSVNP is trained in a SGVB way [8].

- Scalable training with random context points :

- Testing/Forecasting with priors and Monte Carlo estimates :

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Algorithm 1 Variational Inference for DSVNP in Training.

Input: Dataset $\mathcal{D} = \{x_C, y_C; x_T, y_T\}$, Maximum context points N_{max}, etc.
Output: Model parameters ϕ_1, ϕ_2 and θ.
for $i = 1$ **to** m **do**
  Draw some context number $N_C \sim U[1, N_{max}]$;
  Draw mini-batch pair instances $\{(x_C, y_C, x_T, y_T)_{bs}\}_{bs=1}^{B} \sim \mathcal{D}$;
  Feedforward instances to recognition model q_{ϕ_1};
  Feedforward latent variables to generative model p_θ;
  Update parameters by Optimizing Eq. (12):
    $\phi_1 \leftarrow \phi_1 + \alpha \nabla_{\phi_1} \mathcal{L}_{MC}$ ▷ $\phi_1 = [\phi_{1,1}, \phi_{1,2}]$
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- Testing/Forecasting with priors and Monte Carlo estimates :

$$p(y_*|x_C, y_C, x_*) \approx \frac{1}{KS} \sum_{k=1}^{K} \sum_{s=1}^{S} p_\theta(y_*|x_*, z_*^{(s)}, z_G^{(k)}) \tag{3.3}$$

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  Update parameters by Optimizing Eq. (12):
    $\phi_1 \leftarrow \phi_1 + \alpha \nabla_{\phi_1} \mathcal{L}_{MC}$ ▷ $\phi_1 = [\phi_{1,1}, \phi_{1,2}]$
    $\phi_2 \leftarrow \phi_2 + \alpha \nabla_{\phi_2} \mathcal{L}_{MC}$ ▷ $\phi_1 = [\phi_{2,1}, \phi_{2,2}]$
    $\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}_{MC}$
end for

- Testing/Forecasting with priors and Monte Carlo estimates :

$$p(y_*|x_C, y_C, x_*) \approx \frac{1}{KS} \sum_{k=1}^{K} \sum_{s=1}^{S} p_\theta(y_*|x_*, z_*^{(s)}, z_G^{(k)}) \tag{3.3}$$

using latent variables sampled in prior networks as $z_G^{(k)} \sim p_{\phi_{1,2}}(z_G|x_C, y_C)$ and $z_*^{(s)} \sim p_{\phi_{2,2}}(z_*|z_G^{(k)}, x_*)$.

Experiments and Applications

Toy Experiments

Discoveries in 1-D Simulation Experiments in terms of fitting errors and uncertainty quantification (UQ) :

- Episdemic uncertainty in a single curve :

- Interpolation in curves of a $\mathcal{SP}$:

- Extrapolation in curves of a $\mathcal{SP}$:

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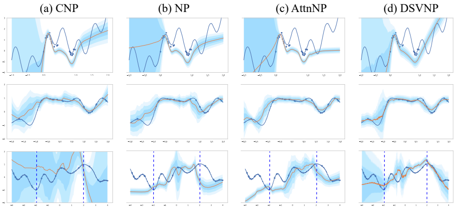

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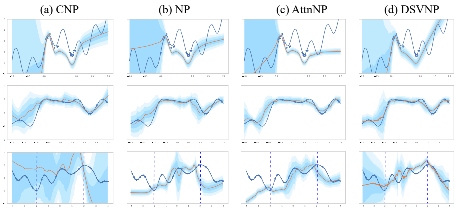

Table 2. Average Negative Log-likelihoods over all target points on realizations from Synthetic Stochastic Process. (Figures in brackets are variances.)

PREDICTION	CNP	NP	ATTNNP	DSVNP
INTER	-0.802 (1E-6)	-0.958 (2E-5)	**-1.149 (8E-6)**	-0.975 (2E-5)
EXTRA	**1.764 (1E-1)**	8.192 (7E1)	8.091 (7E2)	**4.203 (9E0)**

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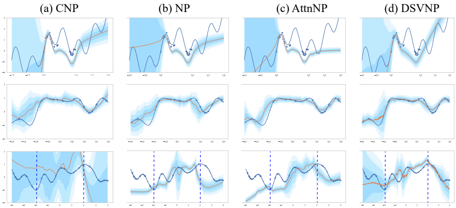

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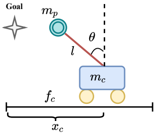

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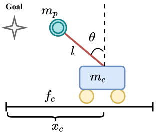

Table 3. Predictive Negative Log-Likelihoods and Mean Square Errors on Cart-Pole State Transition Testing Dataset. (Figures in brackets are variances.)

METRICS	CNP	NP	ATTNNP	DSVNP
NLL	-2.014 (9E-4)	-1.537 (1E-3)	-1.821 (7E-3)	**-2.145 (9E-4)**
MSE	0.096 (3E-4)	0.074 (2E-4)	0.067 (1E-4)	**0.036 (2.1E-5)**

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  Hierarchical latent variables advance performance significantly.

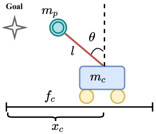

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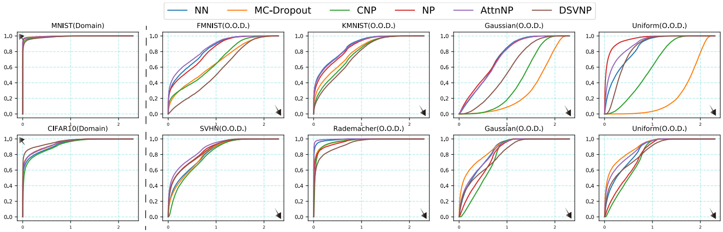
Table 4. Predictive MSEs on Multi-Output Dataset. CNP's results are for target points. D records (input,output) dimensions, and N is the number of samples. MC-Dropout runs 50 stochastic forward propagation and average results for prediction in each data point. (Figures in brackets are variances.)

Dataset	N	D	MC-Dropout	CNP	NP	AttnNP	DSVNP
Sarcos	48933	(21,7)	1.215(3E-3)	1.437(2.9E-2)	1.285(1.2E-1)	1.362(8.4E-2)	**0.839(1.5E-2)**
WQ	1060	(16,14)	0.007(9.6E-8)	0.015(2.4E-5)	0.007(5.2E-6)	0.01(8.5E-6)	**0.006(1.6E-6)**
SCM20D	8966	(61,16)	0.017(2.4E-7)	0.037(6.7E-5)	0.015(7.1E-8)	0.015(8.1E-7)	**0.007(2.3E-7)**

Classification with Uncertainty Quantification

Observations in image classification and out of distribution detection (based on cumulative distribution of entropies) :



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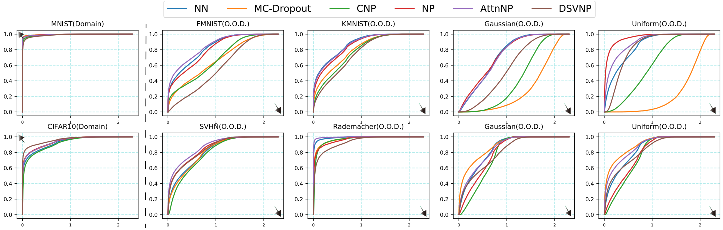

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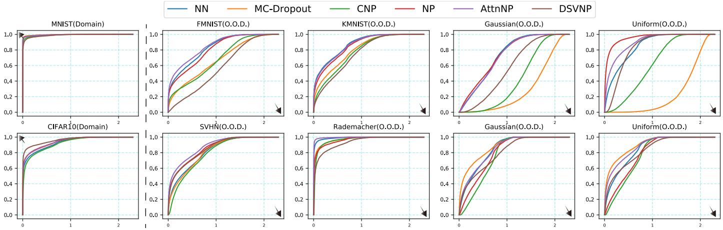

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- CIFAR10: DSVNP(86.3%) ≻ MC/CNP ≻ AttnNP/NP ≻ NN (Classification Performance) ; DSVNP → best entropy distributions in domain dataset and most robust to Rademacher noise.

Future Works

Some Challenging and Promising Directions

- More effective inference methods for our proposed hierarchical $\mathcal{SP}$s

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- More explorations to Uncertainty-aware Decision-making Problems

Thanks for Your Listening

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