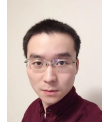
Doubly Stochastic Variational Inference for Neural Processes with Hierarchical Latent Variables

Q. Wang & Herke van Hoof



Amsterdam Machine Learning Lab

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Universiteit van Amsterdam

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- A novel exchangeable SP within a Hierarchical Bayesian Framework
  - formalization of a hierarchical 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 SPs
2. Study of SPs with LVMs
3. NP with Hierarchical Latent Variables
4. Experiments and Applications

Motivation for SPs

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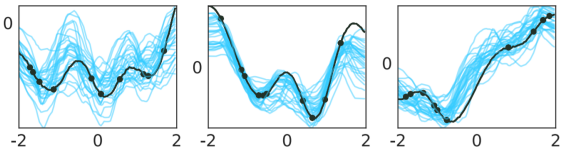

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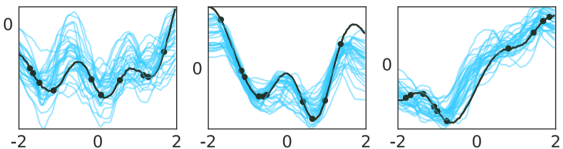

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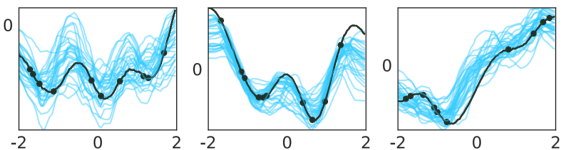

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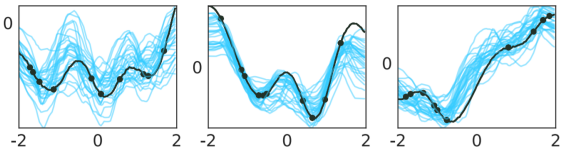

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- Quantify uncertainty in risk-sensitive applications : *e.g.* forecast $p(s_{t+1}|s_t; a_t)$ in autonomous driving [2] ;
- Model distributions instead of point estimates : working as a *generative model* for more realizations [3].

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

SPs in Progress and Primary Concerns

Crucial properties for SPs :

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

Analysis on GPs/NPs :

- Gaussian Processes (GPs)
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Study of SPs with LVMs

Deep Latent Variable Model as SPs

Here we present an implicit Latent Variable Model for SPs :

- Generation paradigm with (potentially correlated) latent variables :

- Predictive distribution in SPs : Let the *context* and *target input* be $C = f(x_i; y_i)ji = 1; 2; : : : ; Ng$ and x_T, the computation is

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$$p\ (z_T j x_C; y_C; x_T) = \frac{p(z_C; z_T)}{\int p(z_C; z_T) dz_C}; \tag{2.3}$$

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Gaussian Processes & Neural Processes

NP family approximates SPs in the form of LVMs :

- GP as an exchangeable SP with latent variables :

- NP as an exchangeable SP with a global latent variable :

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Remark

Some other models, such as Hierarchical GPs [5] and Deep GPs [6], [7] can also be expressed with LVMs.

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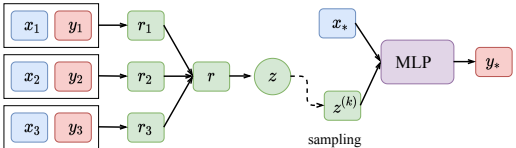

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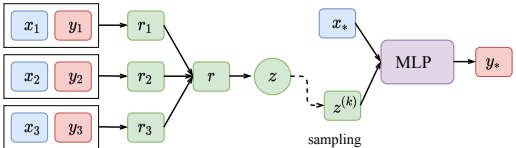
$$r_i = h(x_i, y_i); \quad r = \bigoplus_{i=1}^{M} r_i; \quad p(z_C|x_C, y_C) = N(z_C|[f(r), f(r)]) \tag{2.7}$$



NPs with Hierarchical Latent Variables

Extending NPs from A Hierarchical Bayes Perspective

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Remark

DSVNP satisfies **Marginalization** and **Exchangeability Consistencies**, so it is a new exchangeable 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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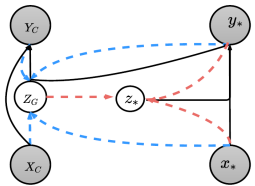
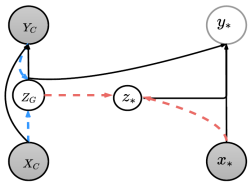


Training Process



Testing Process

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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using latent variables sampled in prior networks as $z_G^{(k)} \quad p\ _{1;2}(z_G jx_C; y_C)$ and $z^{(s)} \quad p\ _{2;2}(z\ jz_G^{(k)}; x\ )$.

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 SP:
- Extrapolation in curves of a SP:

Toy Experiments

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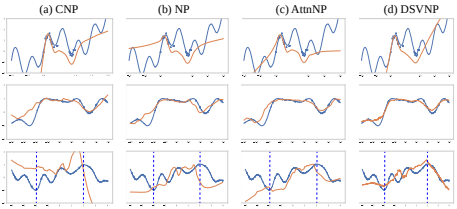

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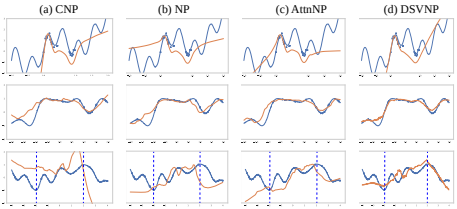

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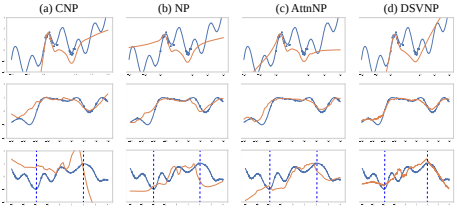

Multi-output Regression: Simulation/Real-world Dataset

Investigations on (1) system identification on cart-pole transitions [9]; (2) regression on real-world dataset :

- System identification :

- High-dim regression :

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Hierarchical latent variables advance performance signi cantly.

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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 SPs

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- More effective inference methods for our proposed hierarchical SPs
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- More explorations to Uncertainty-aware Decision-making Problems

Thanks for Your Listening

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