Implementation of a probabilistic Softmax for BNNs (Group 11)

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Based on the work proposed by J-A. Goulet & L. H. Nguyen

Tractable Approximate Gaussian Inference (TAGI)

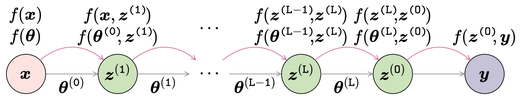
Parameters
$$\begin{cases} f(\boldsymbol{\theta}|\mathcal{D}) = \dfrac{f(\mathcal{D}|\boldsymbol{\theta})\, f(\boldsymbol{\theta})}{f(\mathcal{D})} \\ \quad = \mathcal{N}\left(\boldsymbol{\theta}; \boldsymbol{\mu}_{\theta|\mathcal{D}}, \boldsymbol{\sigma}^2_{\theta|\mathcal{D}}\mathbf{I}\right) \end{cases}$$

Hidden states
$$\begin{cases} f(\boldsymbol{z}|\mathcal{D}) = \mathcal{N}\left(\boldsymbol{z}; \boldsymbol{\mu}_{Z|\mathcal{D}}, \boldsymbol{\sigma}^2_{Z|\mathcal{D}}\mathbf{I}\right) \end{cases}$$

- Bayesian analytical inference { parameters, hidden states }
- Fast and scalable $\rightarrow \mathcal{O}(n)$
- End-to-end treatment of uncertainty
- No gradient backpropagation

Scalable analytical Bayesian inference in any neural network architecture

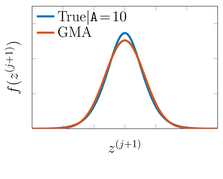
TAGI - Forward uncertainty propagation

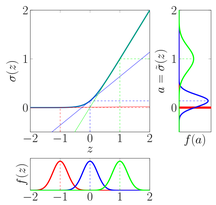


Challenge 1: GMA — Challenge 2: Locally Linearize

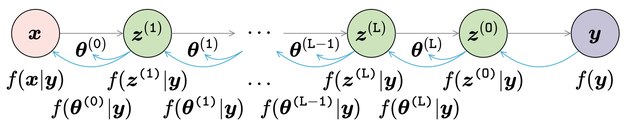
$$\begin{aligned} \boldsymbol{z}^{(1)} &= \boldsymbol{w}^{(0)}\boldsymbol{x} + \boldsymbol{b}^{(0)}, \\ \boldsymbol{a}^{(i)} &= \bar{\sigma}(\boldsymbol{z}^{(i)}), \\ \boldsymbol{z}^{(i)} &= \boldsymbol{w}^{(i)}\boldsymbol{a}^{(i-1)} + \boldsymbol{b}^{(i)}, \\ \boldsymbol{z}^{(0)} &= \boldsymbol{w}^{(L)}\boldsymbol{a}^{(L)} + \boldsymbol{w}^{(L)} \\ \boldsymbol{y} &= \boldsymbol{z}^{(0)} + \boldsymbol{v}. \end{aligned}$$

where $\boldsymbol{v}$ are the observation noise.





TAGI - Backward parameter and hidden state inference



First, given the observations $\boldsymbol{y}$, the output layer is updated as

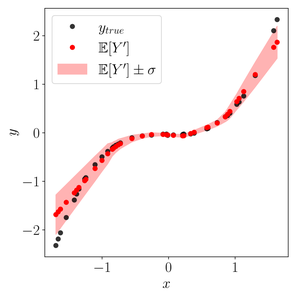
$$\begin{aligned} f\left(\boldsymbol{z}^{(0)} \mid \boldsymbol{y}\right) &= \mathcal{N}\left(\boldsymbol{z}^{(0)}; \boldsymbol{\mu}_{Z^{(0)}|y}, \boldsymbol{\Sigma}_{Z^{(0)}|y}\right) \\ \boldsymbol{\mu}_{Z^{(0)}|y} &= \boldsymbol{\mu}_{Z^{(0)}} + \boldsymbol{\Sigma}^{\top}_{YZ^{(0)}}\boldsymbol{\Sigma}^{-1}_{Y}\left(\boldsymbol{y} - \boldsymbol{\mu}_{Y}\right) \\ \boldsymbol{\Sigma}_{Z^{(0)}|y} &= \boldsymbol{\Sigma}_{Z^{(0)}} - \boldsymbol{\Sigma}^{\top}_{YZ^{(0)}}\boldsymbol{\Sigma}^{-1}_{Y}\boldsymbol{\Sigma}_{YZ^{(0)}}. \end{aligned}$$

Next, the hidden units and parameters of the layer i^{th} are updated using a layer-wise procedure as

$$\begin{aligned} f(\boldsymbol{z} \mid \boldsymbol{y}) &= \mathcal{N}\left(\boldsymbol{z}; \boldsymbol{\mu}_{Z|y}, \boldsymbol{\Sigma}_{Z|y}\right) \\ \boldsymbol{\mu}_{Z|y} &= \boldsymbol{\mu}_{Z} + \mathbf{J}_{Z}\left(\boldsymbol{\mu}_{Z^{+}|y} - \boldsymbol{\mu}_{Z^{+}}\right) \\ \boldsymbol{\Sigma}_{Z|y} &= \boldsymbol{\Sigma}_{Z} + \mathbf{J}_{Z}\left(\boldsymbol{\Sigma}_{Z^{+}|y} - \boldsymbol{\Sigma}_{Z^{+}}\right)\mathbf{J}^{\top}_{Z} \\ \mathbf{J}_{Z} &= \boldsymbol{\Sigma}_{ZZ^{+}}\boldsymbol{\Sigma}^{-1}_{Z^{+}}, \end{aligned} \qquad \begin{aligned} f(\boldsymbol{\theta} \mid \boldsymbol{y}) &= \mathcal{N}\left(\boldsymbol{\theta}; \boldsymbol{\mu}_{\theta|y}, \boldsymbol{\Sigma}_{\theta|y}\right) \\ \boldsymbol{\mu}_{\theta|y} &= \boldsymbol{\mu}_{\theta} + \mathbf{J}_{\theta}\left(\boldsymbol{\mu}_{Z^{+}|y} - \boldsymbol{\mu}_{Z^{+}}\right) \\ \boldsymbol{\Sigma}_{\theta|y} &= \boldsymbol{\Sigma}_{\theta} + \mathbf{J}_{\theta}\left(\boldsymbol{\Sigma}_{Z^{+}|y} - \boldsymbol{\Sigma}_{Z^{+}}\right)\mathbf{J}^{\top}_{\theta} \\ \mathbf{J}_{\theta} &= \boldsymbol{\Sigma}_{\theta Z^{+}}\boldsymbol{\Sigma}^{-1}_{Z^{+}}, \end{aligned}$$

where $\{\boldsymbol{\theta}^{+}, \boldsymbol{Z}^{+}\}$ is the short-hand notation of $\left\{\boldsymbol{\theta}^{(j+1)}, \boldsymbol{Z}^{(j+1)}\right\}$, and $\{\boldsymbol{\theta}, \boldsymbol{Z}\}$ is the short-hand notation of $\left\{\boldsymbol{\theta}^{(j)}, \boldsymbol{Z}^{(j)}\right\}$.

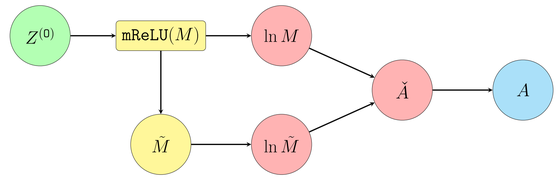
Regression toy example



- We re-implement the toy example presented by the authors using the numpy library in Python.
- This includes defining a fully connected neural network with one layer and 40 hidden units.
- The figure shows the output of the model on the test set with the epistemic uncertainty.

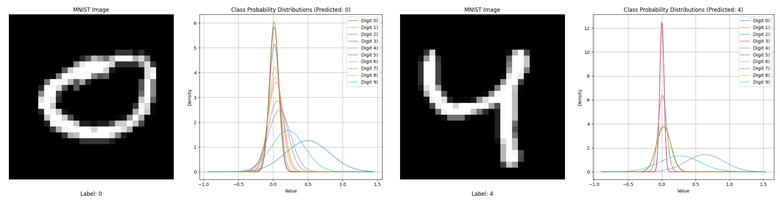
Remax - Probabilistic Softmax for uncertainty propagation

- TAGI cannot use directly the softmax function: $\texttt{softmax}(\boldsymbol{z}, i) = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$ since $\wedge/\wedge \neq \wedge$.
- J-A. Goulet & L. H. Nguyen propose probabilistic softmax by doing the division in log-transformed space.
- The random variable Z is Lognormal if $\ln Z$ is Normal and $\exp(Z)$ is Lognormal if Z is Normal.
- Probabilistic softmax does not work for Z with high variances; $Var(Z) \approx 1$.
- Alternative softmax function: $\texttt{remax}(\boldsymbol{z}, i) = \frac{\texttt{mReLU}(z_i)}{\sum_j \texttt{mReLU}(z_j)}$ where mReLU is a *Mixture Rectified Linear activation Unit*.
- We implement `remax` function in py/cuTAGI library using C++ and CUDA.



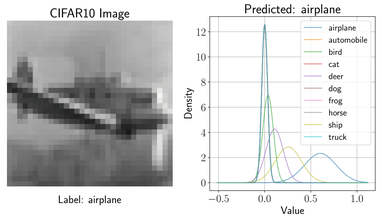
$$\begin{aligned} M &= \texttt{mReLU}(Z^{(0)}) &&= \texttt{mReLU}(\wedge) &&\approx \wedge \\ \tilde{M} &= \textstyle\sum_j (M_j) &&= \wedge + \wedge + \cdots + \wedge &&\approx \wedge \\ \ln M &= \ln(M) &&= \ln(\wedge) &&\approx \wedge \\ \ln \tilde{M} &= \ln(\tilde{M}) &&= \ln(\wedge) &&\approx \wedge \\ \check{A} &= \ln M - \ln \tilde{M} &&= \wedge - \wedge &&\approx \wedge \\ A &= \exp(\check{A}) &&= \exp(\wedge) &&\approx \wedge \end{aligned}$$

Epistemic uncertainty on classes using Remax

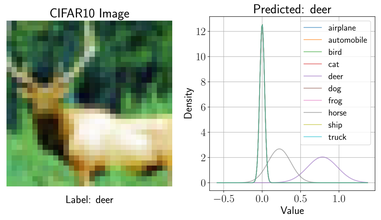


0 predicted on MNIST.

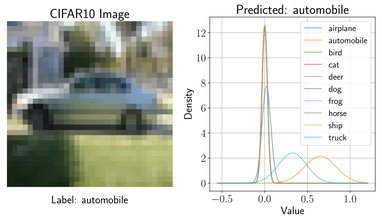
4 predicted on MNIST.



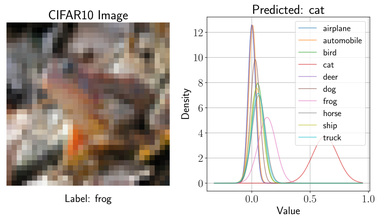
Correct prediction on CIFAR10.



Correct prediction on CIFAR10.



Correct prediction on CIFAR10.



Wrong prediction on CIFAR10.

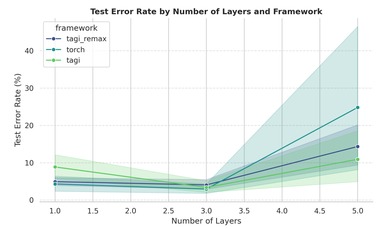
Key Results: TAGI-HRC vs. TAGI-Remax vs. Torch

Framework	Avg. Training Error	Avg. Test Error
Torch	10.05	10.69
TAGI-HRC	7.07	**7.73**
TAGI-Remax	7.14	**7.78**

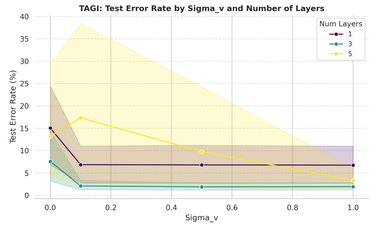
Important Findings

- **Batch Size:** TAGI excels with smaller batches, while Torch performs better with larger batches.
- **Network Depth:** TAGI maintains stability as depth increases, unlike Torch, which struggles without batch normalization.
- **Effect of σ_v:** Higher σ_v values enhance TAGI's performance, especially in deeper networks.
- **Capacity Effect:** TAGI benefits more from increasing neurons/channels, showing improved generalization, while Torch fails to utilize additional capacity effectively.
- **Comparison of Implementations:** TAGI-HRC achieves better error rates overall, while TAGI-Remax shows higher stability but less frequent best-case performance.
- **Batch Normalization:** TAGI performs well even without batch normalization, handling deeper architectures (5+ layers) where Torch often diverges.

Ablation Study: Performance Comparisons and Capacity Effects



Test Error vs Network Depth: TAGI maintains low error rates, while Torch degrades significantly.



Impact of σ_v: Higher σ_v values improve TAGI's test error.

Framework	Small Batch (16) With BN	Small Batch (16) W.o BN	Large Batch (512) With BN	Large Batch (512) W.o BN
Torch	**1.35**	31.20	**1.06**	16.22
TAGI-HRC	1.97	**1.74**	4.11	15.99
TAGI-Remax	12.05	7.30	5.75	**5.43**

Framework	Small (32) Neurons/layer	Large (512) Neurons/layer
Torch	7.03	7.32
TAGI-HRC	13.58	**8.98**
TAGI-Remax	9.25	**6.91**

py/cuTAGI – Open-source Bayesian deep-learning framework

cuTAGI

`github.com/lhnguyen102/cuTAGI`

`pip install pytagi`

- **Performance-Oriented Kernels** written in C++/CUDA from scratch, with pybind11 for a seamless integration. It allows running on CPU & CUDA devices through a Python API.
- **Broad Architecture Support** of the basic DNN layer including *Linear*, *CNNs*, *Transposed CNNs*, *LSTM*, *Average pooling*, *Batch* and *Layer normalization*, enabling the building of mainstream architectures such as *Autoencoders*, *Transformers*, *Diffusion Models*, and *GANs*.
- **Model Building and Execution** currently supports sequential model building, with plans to introduce Eager Execution
- **Open Platform** providing access to its entire codebase.

TAGI-related references

- *Analytically tractable hidden-states inference in Bayesian neural networks* (Nguyen and Goulet. Journal-to-conference track, ICLR 2024)
- *Analytically tractable heteroscedastic uncertainty quantification in Bayesian neural networks for regression tasks* (Deka, Nguyen & Goulet. Neurocomputing, 2024)
- *Tractable approximate Gaussian inference for Bayesian neural networks* (Goulet, Nguyen, & Amiri, JMLR, 2021)