Simple and Principled Uncertainty Estimation with Deterministic Deep Learning via Distance Awareness

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Introduction

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- Real world applications **need** efficient methods that reliably quantify a deep neural network's (DNN) predictive uncertainty.

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- Examples:
  - Object detection in autonomous driving
  - Ad click prediction in websites
  - Understanding in a conversational system (ChatGPT)
  - Domain-specific chatbot services (weather)

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GPs!

GPs need a previous feature extraction. We would like the DNN to be *distance aware*.

Notation

- Consider the data distribution $p^\star(y \mid \mathbf{x})$, where $y \in \{1, \dots, K\}$ and $x \in \mathcal{X} \subset \mathbb{R}^d$, where $\mathcal{X}$ is the data manifold with a suitable metric $\|\cdot\|_X$.

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- In practise, data is collected from a subset $\mathcal{X}_{IND} \subset \mathcal{X}$. As a result,

$$\begin{aligned} p^\star(y \mid \mathbf{x}) &= p^\star(y, \mathbf{x} \in \mathcal{X}_{IND} \mid \mathbf{x}) + p^\star(y, \mathbf{x} \notin \mathcal{X}_{IND} \mid \mathbf{x}) \\ &= p^\star(y \mid \mathbf{x}, \mathbf{x} \in \mathcal{X}_{IND}) \cdot p^\star(\mathbf{x} \in \mathcal{X}_{IND} \mid \mathbf{x}) \\ &\quad + p^\star(y \mid \mathbf{x}, \mathbf{x} \notin \mathcal{X}_{IND}) \cdot p^\star(\mathbf{x} \notin \mathcal{X}_{IND} \mid \mathbf{x}) \end{aligned}$$

  Models learn $p^\star(y \mid \mathbf{x}, \mathbf{x} \in \mathcal{X}_{IND})$.
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  However, $p^\star(y \mid \mathbf{x}, \mathbf{x} \notin \mathcal{X}_{IND})$ can be very different.
- In testing, models use a predictive $p(y \mid \mathbf{x})$ for any $\mathbf{x} \in \mathcal{X} = \mathcal{X}_{IND} \cup \mathcal{X}_{OOD}$. $\mathcal{X}_{OOD}$ can be very different even in a certain topic (user asking for earthquakes in a weather-themed chatbot)!

Towards the loss function

If the model predicts class y with confidence $\hat{p}$, we would like the model to be correct $\hat{p}$ of the times. In that case, the model is said to be **callibrated**. Formally, the model is calibrated if

$$\mathbb{P}(\hat{y} = y_{true} \mid \hat{p} = p) = p$$

We can take the expectation in the possible predicted confidences $\hat{p}$, leading to the Expected Calibration Error (ECE) [Guo et al., 2017]:

$$ECE = \mathbb{E}_{\hat{p}}\left[|P(\hat{y} = y_{true} \mid \hat{p} = p) - p|\right]$$

However, this loss function is not suitable for this case, since it is not uniquely minimized.

Towards the loss function

Definition

A scoring rule[1] is any extended real-valued function $\mathbf{S} : \mathcal{P} \times \Omega \to \mathbb{R}$ such that $\mathbf{S}(P, \cdot)$ is $\mathcal{P}$-quasi-integrable for all $P \in \mathcal{P}$.

$\mathbf{S}(P, y)$ represents the loss or penalty when the prediction $P \in \mathcal{P}$ is issued and the observation $y \in \Omega$ materializes.

[1] Wikipedia's link

Example: Brier's Score

An example of a strictly proper scoring rule is the **Brier's score**, defined as:

$$B(p, y) = \sum_{j=1}^{C} (y_j - p_j)^2,$$

where

- $y_j = 1$ if the the input belongs to class j-th and 0 otherwise,
- C is the number of classes and
- p_j is the probability assigned to class j.

Towards the loss function

If the label y is sampled from a distribution Q, the expected score under $Q \in \mathcal{P}$ can be written as:

$$\mathbf{S}(P, Q) = \int \mathbf{s}(P, y) \; dQ(y).$$

Towards the loss function

If the label y is sampled from a distribution Q, the expected score under $Q \in \mathcal{P}$ can be written as:

$$\mathbf{S}(P, Q) = \int \mathbf{s}(P, y)\ dQ(y).$$

We can define a **divergence** of P from Q as:

$$d(P, Q) \triangleq \mathbf{S}(P, Q) - \mathbf{S}(Q, Q).$$

Towards the loss function

Definition

A scoring rule **S** is proper *relative to* $\mathcal{P}$ if

$$d(P, Q) \geq 0, \quad \forall P, Q \in \mathcal{P}.$$

Also, it is **strictly proper** [Gneiting and Raftery, 2007] if the above equation holds with equality if, and only if, $P = Q$.

Towards the loss function

Consider the vector of calibrated probabilities $\mathbf{C} = (C_1, \ldots, C_k)$ and let P be the output probabilities of a model. Using $\mathbf{C}$, the expected loss according a P.S.R. can be expressed [Kull and Flach, 2015] as:

$$\mathbb{E}\left[d(P, Y)\right] = \mathbb{E}[d(P, \mathbf{C})] + \mathbb{E}[d(\mathbf{C}, Y)]$$

Consequence: Each PSR is an upper bound of the calibration error, so minimizing a PSR implies minimizing the calibration error.

Towards the loss function

The problem of uncertainty quantification turns into constructing an optimal p to minimize the expected risk over $\mathcal{X}$:

$$\inf_{p \in \mathcal{P}} S(p, p^*) = \inf_{p \in \mathcal{P}} \mathop{\mathbb{E}}_{\mathbf{x} \in \mathcal{X}} \left[s(p, p^* | \mathbf{x}) \right]. \tag{1}$$

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However, this is not possible to solve since data only comes from $\mathcal{X}_{IND}$, OOD distribution is never learned, so generalization is not guaranteed. We then take a *Minimax* strategy (minimize the worst-case risk):

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$$\inf_{p \in \mathcal{P}} \left[\sup_{p^* \in \mathcal{P}^*} S(p, p^*) \right]. \tag{2}$$

Solution using Brier's Score

Under the classification task and using Brier's score, the solution to Eq. (2) is:

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, \mathbf{x} \in \mathcal{X}_{IND}) * p^*(\mathbf{x} \in \mathcal{X}_{IND} \mid \mathbf{x}) + p_{\texttt{uniform}}(y|\mathbf{x}, \mathbf{x} \notin \mathcal{X}_{IND}) * p^*(\mathbf{x} \notin \mathcal{X}_{IND} \mid \mathbf{x}).$$

Advantages:

- Intuitive!
- Verifies that there is the unique optimal solution to the problem in Eq. (2)

Disadvantage:

- We have to assume that the model can quantify $p^\star(\mathbf{x} \in \mathcal{X}_{IND} \mid \mathbf{x})$ well.

Input Distance Awareness

We need a notion of distance between a new example and $\mathcal{X}_{IND}$!

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Definition (Input Distance Awareness)

Consider a predictive distribution $p(y \mid \mathbf{x})$ trained on $\mathcal{X}_{IND}$. We say that it is **input distance aware** if:
Exists $u(\mathbf{x})$ a summary statistic of $p(y \mid \mathbf{x})$ such that:

1. quantifies model uncertainty (eg: predictive variance) and
2. reflects the distance between $\mathbf{x}$ and training data w.r.t. $\|\cdot\|_{\mathcal{X}}$

$$u(\mathbf{x}) = v(d(\mathbf{x}, \mathcal{X}_{IND})),$$

where v is a monotonic function and

$$d(\mathbf{x}, \mathcal{X}_{IND}) = \mathbb{E}_{x' \sim \mathcal{X}_{IND}} \|\mathbf{x} - \mathbf{x}'\|_X^2$$

Example: Gaussian Processes

GPs with RBF kernel are input distance aware models:

- Predictive $p(y \mid \mathbf{x}) = softmax(g(\mathbf{x}))$
- Exists $u(\mathbf{x}^\star) = var(g(\mathbf{x}^\star)) = 1 - \mathbf{k}^{\star^T}\mathbf{V}\mathbf{k}^\star$, with

$$\mathbf{k}_i^\star = \exp\left(-\gamma \|\mathbf{x}^\star - \mathbf{x}_i\|_X^2\right)$$

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$$\mathbf{k}_i^\star = \exp\left(-\gamma \|\mathbf{x}^\star - \mathbf{x}_i\|_X^2\right)$$

In a typical DL model, the confidence in a class is computed in a dense layer as:

$$\text{logit}_k(\mathbf{x}) = h(\mathbf{x})^\top \beta_k.$$

The model decission is not based on its distance to training data $\mathcal{X}_{IND}$, but on its distance to the decission boundaries.

Conditions for IDA in Deep Learning

Consider a DL model $\mathit{logit}(\mathbf{x}) = g \circ h(\mathbf{x})$ where

- h creates a representation of $\mathbf{x}$ and
- g maps $h(\mathbf{x})$ to the label space.

To make this model distance aware we need:

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To make this model distance aware we need:

1. Make the output layer g distance aware, so it outputs an uncertainty metric reflecting distance in the representation space
2. Make the hidden mapping h *distance preserving*. Mathematically, that is fullfilling the bi-Lipschitz condition:

$$\underbrace{L_1 \, \|\mathbf{x}_1 - \mathbf{x}_2\|_X}_{\text{not unnecessarily invariant}} \leq \|h(\mathbf{x}_1) - h(\mathbf{x}_2)\|_H \leq \underbrace{L_2 \, \|\mathbf{x}_1 - \mathbf{x}_2\|_X}_{\text{robustness}},$$

where $0 < L_1 < 1 < L_2$. This condition encourages h to be approximately isometric.

SNGP: Spectral-normalized Neural Gaussian Process

Visual description

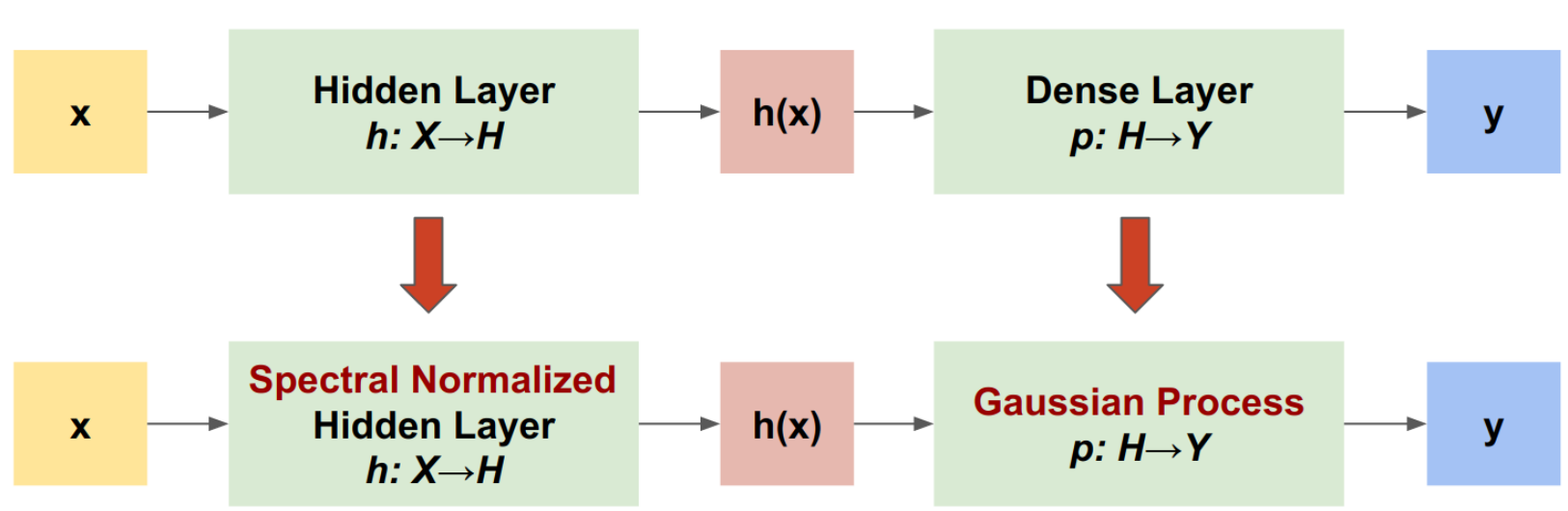

Figure 1: Visual description from the provided tutorial.

Distance-aware Output Layer

To make the output layer g distance aware, the model replaces the typical dense layer with a **GP with RBF Kernel**.

Specifically, given $\{\mathbf{x}_i, y_i\}_{i=1}^N$, we place the usual prior to the output layer $g_{N\times 1} = [g(h_1), \ldots, g(h_N)]^T$:

$$g_{N\times 1} \sim GP(\mathbf{0}, \mathbf{K}_{NN}), \quad \mathbf{K}_{i,j} = \exp(-\|h_i - h_j\|_2^2/2).$$

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As per usual with GPs, computing the exact posterior distribution is intractable.

Distance-aware Output Layer: Approximating GP Prior

The GP prior is approximated using **Random Fourier Features** (RFF)

$$\mathbf{g}_{N\times 1} \sim GP(\mathbf{0}, \mathbf{\Phi}\mathbf{\Phi}^\top), \qquad \mathbf{\Phi}_{i,D_L\times 1} = \sqrt{2/D_L} * \cos(-\mathbf{W}_L h_i + \mathbf{b}_L),$$

where $w_{ij} \sim \mathcal{N}(0,1)$ and $b_k \sim Uniform(0, 2\pi)$.

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where $w_{ij} \sim \mathcal{N}(0,1)$ and $b_k \sim Uniform(0, 2\pi)$.
As a result, for the k^{th} logit, this approximation can be written as a NN layer:

$$g_k(h_i) = \sqrt{2/D_L} * \cos(-\mathbf{W}_L h_i + \mathbf{b}_L)^\top \boldsymbol{\beta}_k,$$

where $\mathbf{W}$ is fixed and the prior of β_k is$\boldsymbol{\beta}^k_{D_L\times 1} \sim \mathcal{N}(0, \mathbf{I}_{D_L\times D_L})$.

Distance-aware Output Layer: Posterior Approximation

Consequence: We have reduced the infinite-dimensional GP to a Bayesian linear model, so we can apply one of the known posterior approximation methods.

Distance-aware Output Layer: Posterior Approximation

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Definition (Laplace approximation)

Laplace method approximates the posterior distribution $p(\beta \mid \mathcal{D})$ using a Gaussian distribution centered at the MAP estimate $\hat{\beta} = \arg\max_\beta p(\beta \mid \mathcal{D})$ and covariance matrix the inverse of the Hessian of the log posterior likelihood evaluated at $\hat{\beta}$, that is:

$$p(\beta_k \mid \mathcal{D}) \approx \mathcal{N}(\hat{\beta}_k, \hat{\mathbf{H}}_k^{-1}),$$

with $\hat{\mathbf{H}}_{k,(i,j)} = \frac{\partial^2}{\partial \beta_i \partial \beta_j} \log\, p(\beta_k|\mathcal{D})|_{\beta_k=\hat{\beta}_k}$

Distance-aware Output Layer: Results

The GP posterior can be learned:

- scalably,
- in closed form,
- with minimal modification to the training of a deterministic DNN,
- by the Bernstein-von-Mises theorem [Dehaene, 2019], the Laplace approximation ot the RFF posterior is asymptotically exact.

Distance-preserving Hidden Mapping

The last goal is to ensure that the hidden mapping h is *distance preserving* so that the distance in the hidden space $\|h(\mathbf{x}) - h(\mathbf{x}')\|_H$ has a meaningful correspondence to the distance in the input space $\|\mathbf{x} - \mathbf{x}'\|_X$.

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Note (Assumption)

The used models will be residual DL models (ResNets, Transformers), composed of residual blocks

$$h(\mathbf{x}) = h_{L-1} \circ \cdots \circ h_1(\mathbf{x}), \quad h_l(\mathbf{x}) = \mathbf{x} + f_l(\mathbf{x}). \tag{3}$$

Distance-preserving Hidden Mapping

Proposition

Let $h : \mathcal{X} \to \mathcal{H}$ be a hidden mapping with residual architecture (3). If for $0 < \alpha \leq 1$, all f_l are $\alpha-$Lipschitz, that is:

$$\|f_l(\mathbf{x}) - f_l(\mathbf{x}')\|_H \leq \alpha \|\mathbf{x} - \mathbf{x}'\|_X \text{ for all } (\mathbf{x}, \mathbf{x}') \in \mathcal{X},$$

then:

$$L_1 \cdot \|\mathbf{x} - \mathbf{x}'\|_X \leq \|h(\mathbf{x}) - h(\mathbf{x}')\|_H \leq L_2 \cdot \|\mathbf{x} - \mathbf{x}'\|_X,$$

where $L_1 = (1 - \alpha)^{L-1}$ and $L_2 = (1 + \alpha)^{L-1}$.

This result implies that if the previous conditions are fulfilled, h is distance preserving.

Distance-preserving Hidden Mapping

If $f_l(\mathbf{x}) = \sigma(\mathbf{W}_l\mathbf{x} + \mathbf{b}_l)$ is the residual block, since

$$\|f_l\|_{Lip} \leq \|\mathbf{W}_l\mathbf{x} + \mathbf{b}_l\|_{Lip} \leq \|\mathbf{W}_l\|_2,$$

it is sufficient to have $\|\mathbf{W}_l\|_2 \leq 1$ to ensure h is distance preserving.

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Definition (Spectral Normalization)

Let $\lambda = \|\mathbf{W}_l\|_2$ be the spectral norm of $\mathbf{W}_l$. Then, the spectral normalization is performed as:

$$\mathbf{W}_l = \begin{cases} c \cdot \mathbf{W}_l/\lambda & \text{if } c < \lambda \\ \mathbf{W}_l & \text{otherwise} \end{cases} \tag{4}$$

where $c > 0$ is a hyperparameter used as a threshold.

The hyperparameter is useful since it helps with the regularization of the model.

Method summary: Prediction

Algorithm 1 SNGP Prediction

1: **Input:** Testing example $\mathbf{x}$.

2: Compute Feature:

$$\mathbf{\Phi}_{D_L \times 1} = \sqrt{2/D_L} * \cos(\mathbf{W}_L h(\mathbf{x}) + \mathbf{b}_L),$$

3: Compute Posterior Mean:

$$\text{logit}_k(\mathbf{x}) = \Phi^\top \boldsymbol{\beta}_k$$

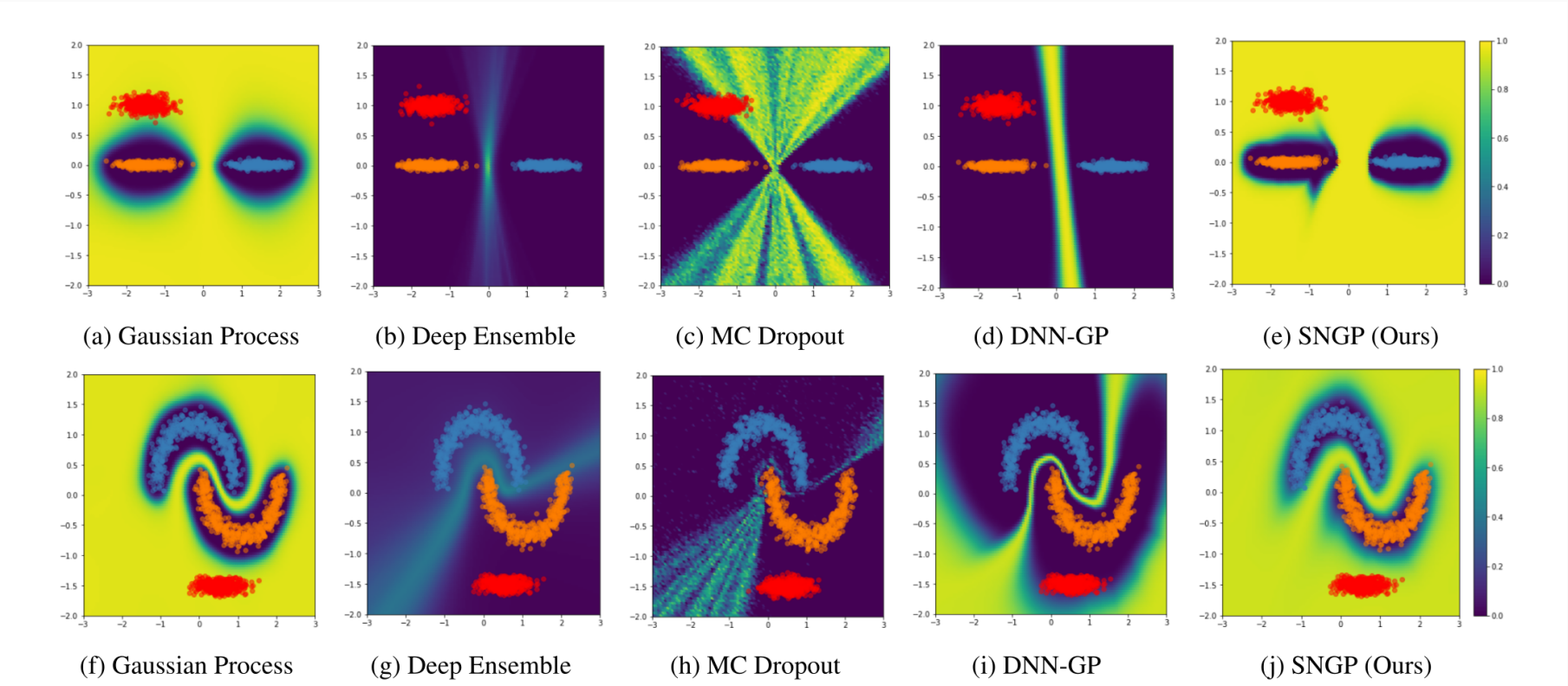
4: Compute Posterior Variance:

$$\text{var}_k(\mathbf{x}) = \Phi^\top \hat{\Sigma}_k \Phi.$$

5: Compute Predictive Distribution:

$$p(y|\mathbf{x}) = \int_{m \sim N(\text{logit}(\mathbf{x}), \text{var}(\mathbf{x}))} \text{softmax}(m)$$

Results



(a) Gaussian Process (b) Deep Ensemble (c) MC Dropout (d) DNN-GP (e) SNGP (Ours)

(f) Gaussian Process (g) Deep Ensemble (h) MC Dropout (i) DNN-GP (j) SNGP (Ours)

Results: OOD metrics

To evaluate the model performance in OOD detection in this task, the **model's uncertainty estimate** is used as a predictive score for OOD classification.

$$u(\mathbf{x}) = \frac{K}{K + \sum_{i=1}^{K} \exp(\text{logit}_i(h(\mathbf{x}))}. \tag{5}$$

Results: OOD Evaluation

1. Generate the dataset adequately: merge two datasets (in-distribution and OOD) in one and add a new label (in/out distribution) to each item.
2. Compute the logits given by the linear model representing the GP.
3. Then, using this logits, we compute an uncertainty metric $u(\mathbf{x})$ for each datapoint as in Equation (5).
4. Create a **new binary classification problem**: OOD class as the positive class (label 1), and we take $u(\mathbf{x})$ to be the *model's* probability of this class.
5. We compute the metrics using this probabilities and the created labels.

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Extra slides

Definition of quasi-integrable

Consider

- a sample space Ω,
- a σ-algebra $\mathcal{A}$ of subsets of Ω and
- a convex class $\mathcal{F}$ of probability measures on $(\Omega, \mathcal{A})$.

Definition

A function defined on Ω and taking values in the extended real line, $\overline{\mathbb{R}} = [-\infty, \infty]$, is $\mathcal{F}$-quasi-integrable if it is measurable with respect to $\mathcal{A}$ and is quasi-integrable with respect to all $F \in \mathcal{F}$.

Method summary: Training

Algorithm 2 SNGP Training

1: **Input:**
Minibatches $\{D_i\}_{i=1}^{N}$ for $D_i = \{y_m, \mathbf{x}_m\}_{m=1}^{M}$.

2: **Initialize:**

$$\hat{\Sigma} = \mathbf{I}, \mathbf{W}_L \overset{iid}{\sim} N(0,1), \mathbf{b}_L \overset{iid}{\sim} U(0, 2\pi)$$

3: **for** train_step $= 1$ **to** max_step **do**
4: SGD update $\left\{\beta, \{\mathbf{W}_l\}_{l=1}^{L-1}, \{\mathbf{b}_l\}_{l=1}^{L-1}\right\}$
5: Spectral Normalization $\{\mathbf{W}_l\}_{l=1}^{L-1}$ (4).
6: **if** final_epoch **then**
7: Update precision matrix $\{\hat{\Sigma}_k^{-1}\}_{k=1}^{K}$ (6).
8: **end if**
9: **end for**
10: Compute posterior covariance $\hat{\Sigma}_k = inv(\hat{\Sigma}_k^{-1})$.

Implementation: Posterior precision matrix

Under the linear-model formulation of the RFF posterior, the precision matrix has the following expression:

$$\hat{\Sigma}_k^{-1} = \mathbf{I} + \sum_{i=1}^{N} \hat{p}_{i,k}(1 - \hat{p}_{i,k})\Phi_i \Phi_i^T, \tag{6}$$

where $\hat{p}_{i,k}$ is the model prediction $softmax(\hat{g}_i)$ under the MAP estimates $\hat{\beta}$.

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where $\hat{p}_{i,k}$ is the model prediction $softmax(\hat{g}_i)$ under the MAP estimates $\hat{\beta}$.

When using minibatches of size M, the posterior mean $\hat{\beta}$ is updating via SGD with respect to the log posterior $-\log p(\beta \mid \mathcal{D})$ and the posterior precision matrix is *cheaply* updated as

$$\hat{\Sigma}_{k,t}^{-1} = (1 - m) * \hat{\Sigma}_{k,t-1}^{-1} + m * \sum_{i=1}^{M} \hat{p}_{i,k}(1 - \hat{p}_{i,k})\Phi_i \Phi_i^\top,$$

where m is a small scaling coefficient. This computation is only performed **once at the final epoch**.

Implementation: Spectral Normalization

The spectral norm is approximated by using the **power iteration** method.

Thank you for your attention