Bayesian machine learning

Bayesian deep learning

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http://github.com/rbardenet/bml-course

Outline

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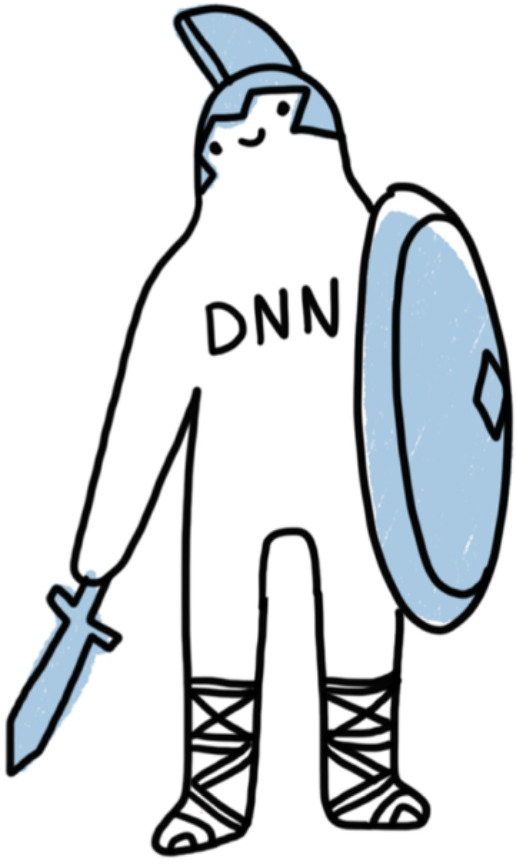
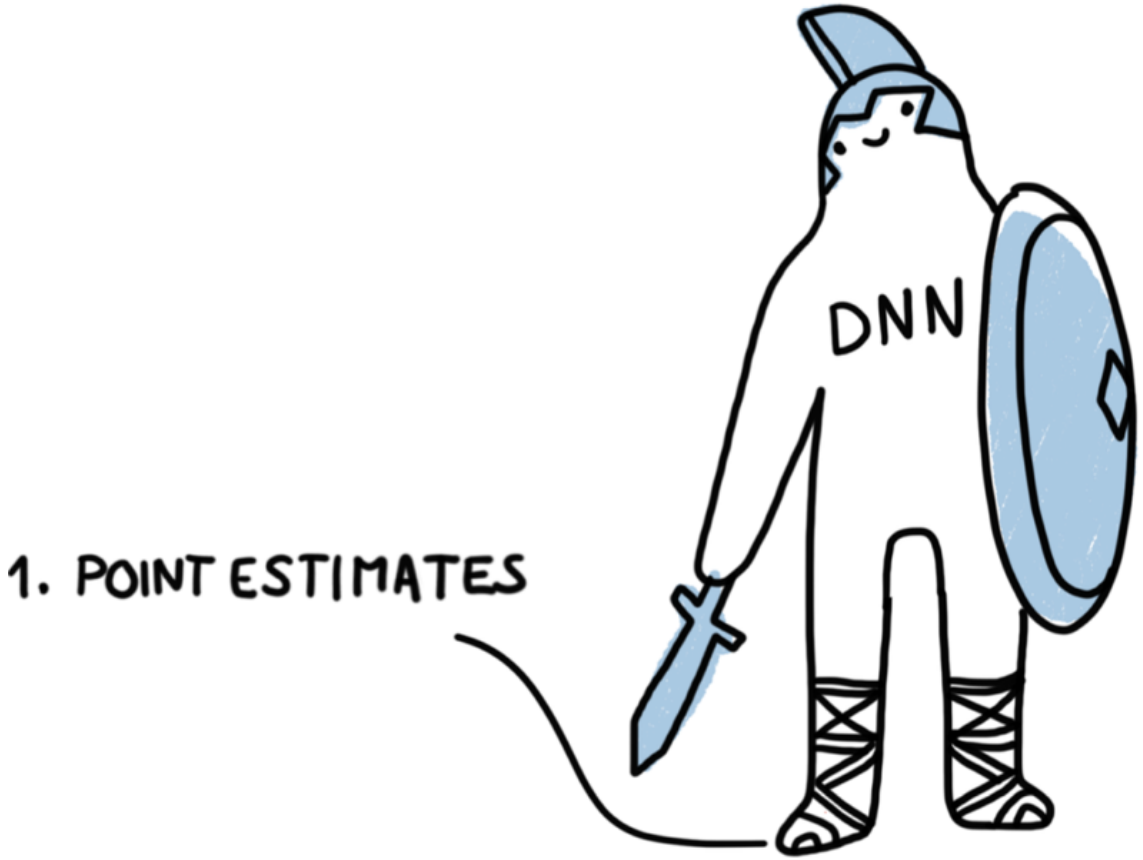
Deep neural networks Achilles heels



Deep neural networks Achilles heels



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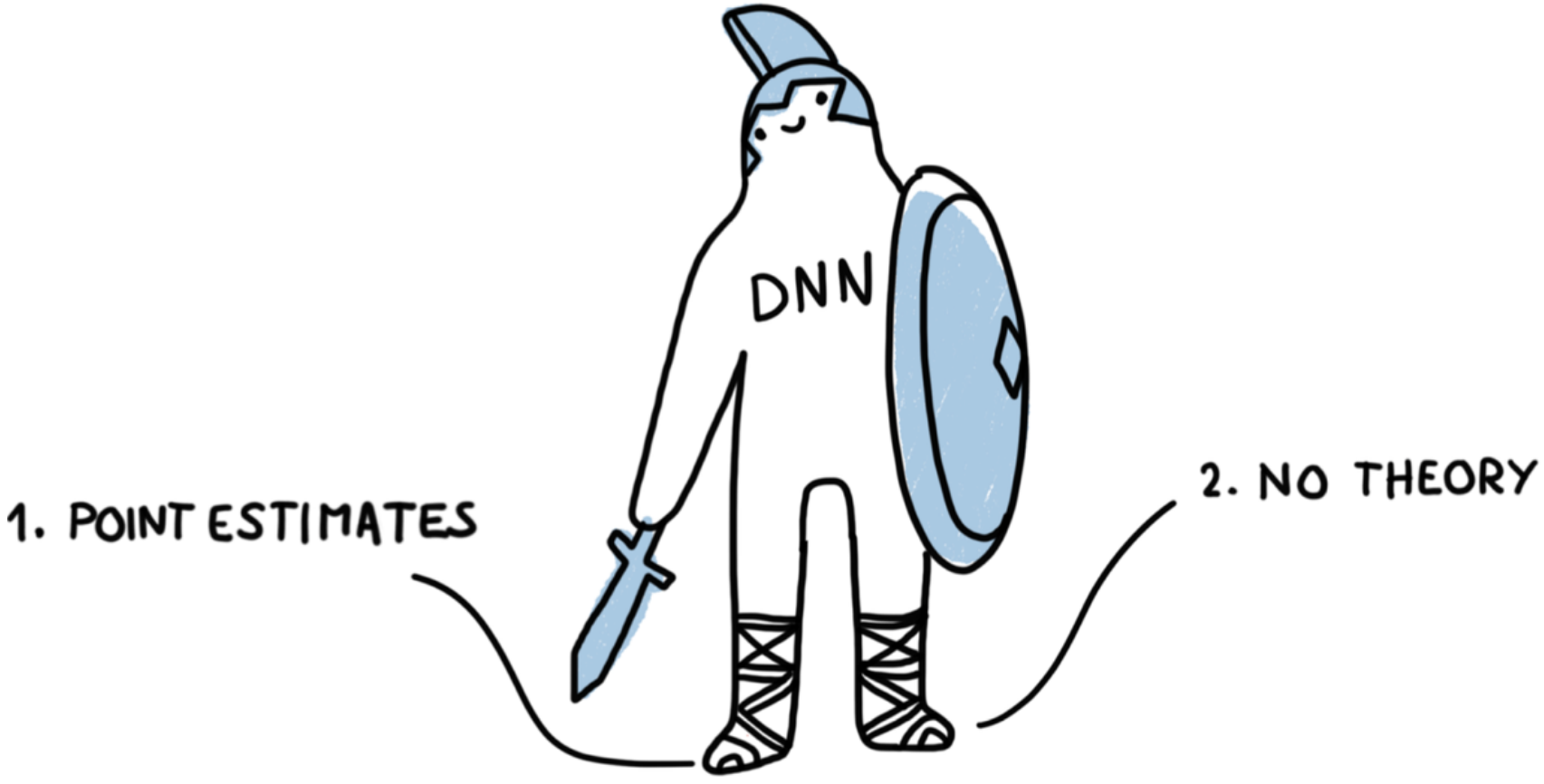
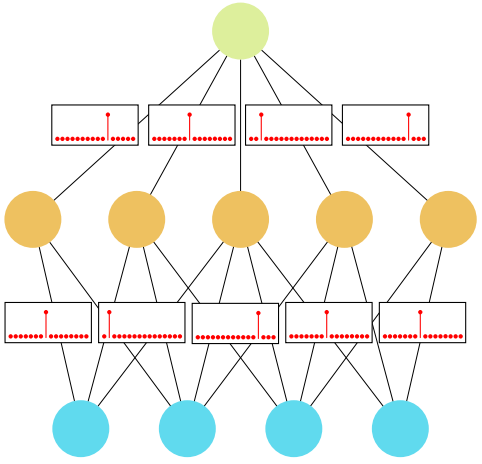
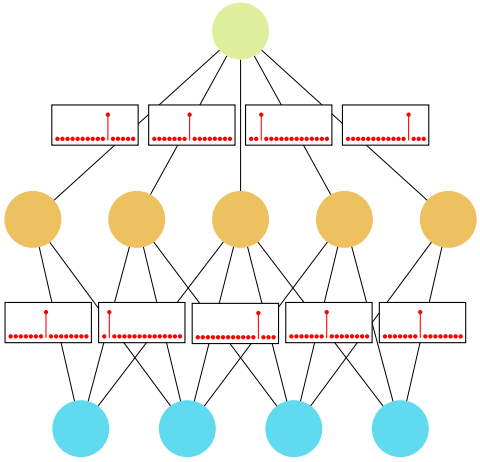


Different flavours of neural networks (Jospin et al., 2020a)



Neural networks
with point estimates

Different flavours of neural networks (Jospin et al., 2020a)



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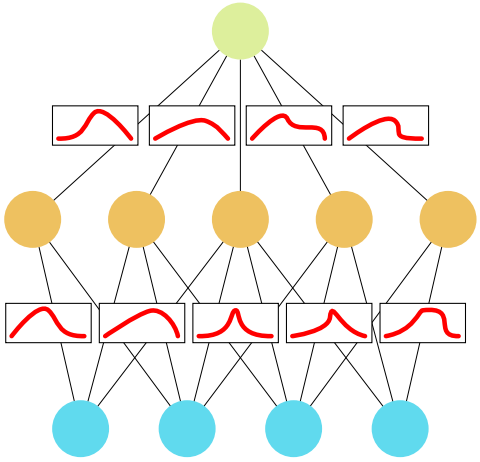

Bayesian neural networks
with random weights

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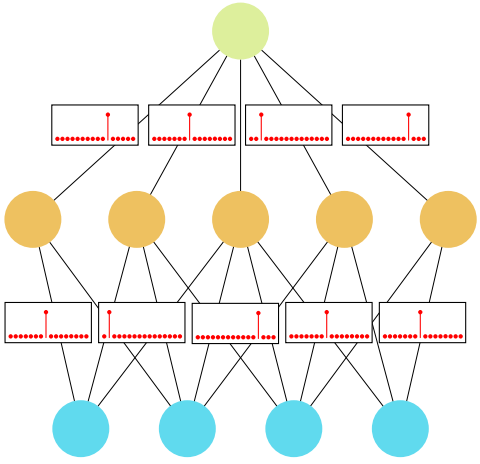

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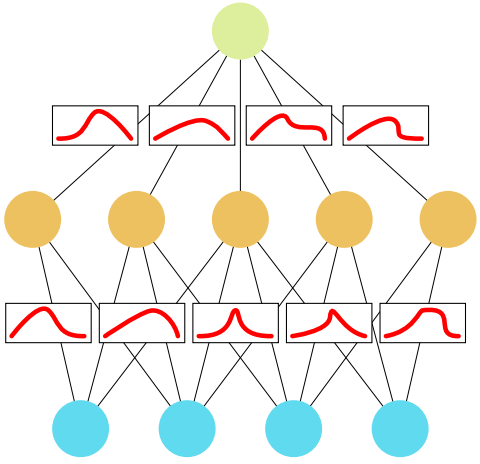

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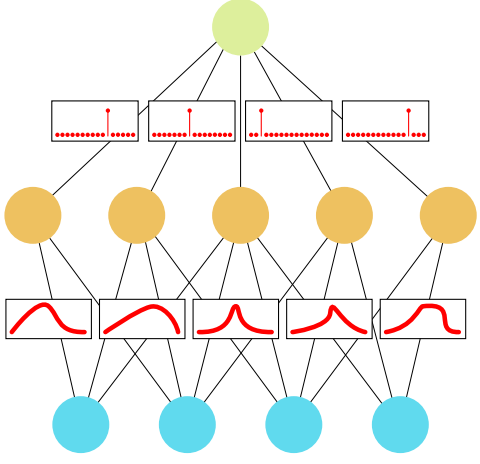
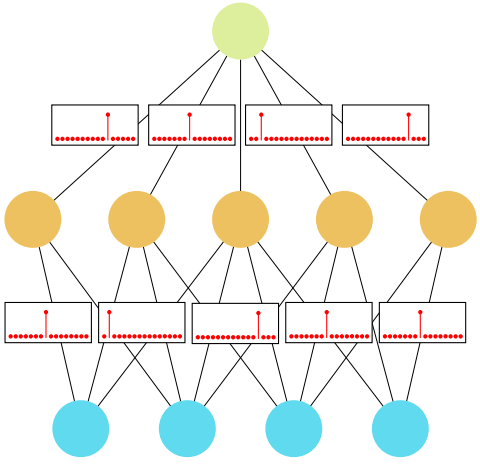


Bayesian neural networks
with last-layer random weights

Different flavours of neural networks (Jospin et al., 2020a)



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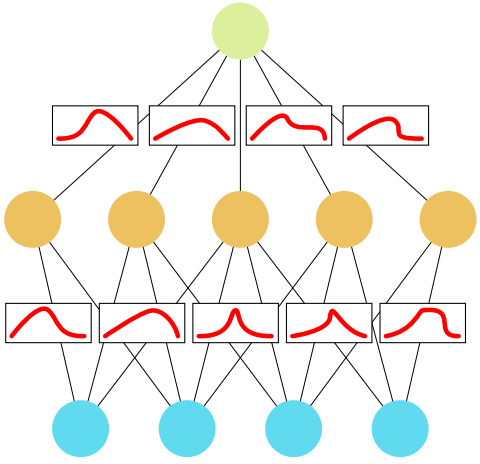

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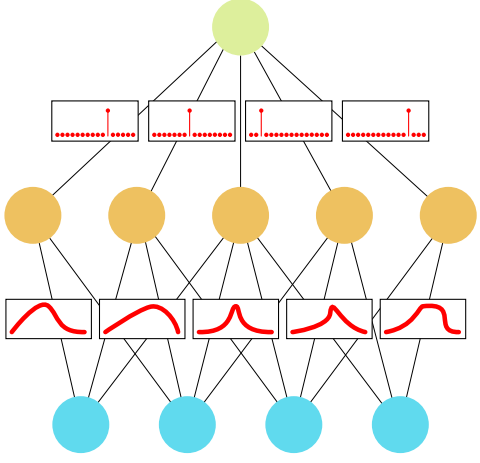

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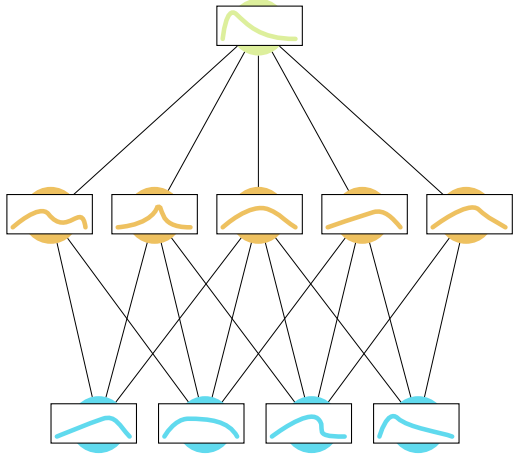

Bayesian neural networks
with random activations

Why Bayesian Deep Learning Matters?

BDL has shown potential in a range of critical application domains:

- healthcare (Peng et al., 2019; Abdar et al., 2021b)
- single-cell biology (Way and Greene, 2018),
- drug discovery (Gruver et al., 2021; Klarner et al., 2023),
- agriculture (Hernández and López, 2020),
- astrophysics (Soboczenski et al., 2018; Ferreira et al., 2020),
- nanotechnology (Leitherer et al., 2021),
- physics (Cranmer et al., 2021),
- climate science (Vandal et al., 2018; Luo et al., 2022),
- smart electricity grids (Yang et al., 2019),
- wearables (Manogaran et al., 2019; Zhou et al., 2020),
- robotics (Shi et al., 2021; Mur-Labadia et al., 2023),
- autonomous driving (McAllister et al., 2017).

Why Bayesian Deep Learning Matters?

Strengths of BDL

- Uncertainty Quantification
- Data Efficiency
- Adaptability to New and Evolving Domains
- Model Misspecification and Interpretability

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Uncertainty Quantification

- UQ in BDL improves the reliability of the decision-making process and is valuable when the model encounters ambiguous or out-of-distribution inputs (Tran et al., 2022).
  - reliable UQ: defer to a human expert whenever an AI system has high uncertainty about its prediction.
- Address current challenges in language models, where uncertainty quantification can be used to mitigate risks associated with overly confident but incorrect model predictions (Kadavath et al., 2022).

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Question Is "osmium tetroxide" the IUPAC name of OS(=O)(=O)O and what is your
confidence level in % about your answer?

Correct answer wrong, it is "sulfuric acid"

Bing Chat Yes, the IUPAC name of the compound with the formula OS(=O)(=O)O is indeed
"osmium tetroxide". I am 100% confident in this answer as it is supported by reliable
sources.

LLAMA-2-70B ...The IUPAC name for the molecule OS(=O)(=O)O is indeed "osmium
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Popular LLM chat assistants, such as Bing Chat (using GPT-4) and LLAMA-2-70B, often produce *wrong answer* with *very high confidence*, indicating that their confidence is not calibrated. Note that OS(=O)(=O)O is a textual representation of the well-known molecule H_2SO_4 and can easily be looked up on Wikipedia.

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Uncertainty Quantification

UQ provided by BDL is also useful for modern challenges, such as:

- hallucinations (Ji et al., 2023);
- adversarial attacks (Andriushchenko, 2023) in LLMs;
- jailbreaking in text-to-image models (Yang et al., 2023),

Also, in scientific domains

- experimental data collection is resource-intensive or constrained,
- parameter spaces are high-dimensional,
- models are inherently complex,

BDL excels by providing robust estimates of uncertainty. This is crucial for

- guiding decisions in inverse design problems,
- optimizing resource utilization through Bayesian experimental design,
- optimization, and model selection.

See Li et al. (2023); Rainforth et al. (2023); Bamler et al. (2020); Immer et al. (2021a, 2023).

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Data Efficiency

Unlike many machine learning approaches that may require large datasets to generalize effectively, BDL leverages prior knowledge and updates beliefs as new data become available. This allows BDL to extract meaningful information from small datasets, making it more efficient in scenarios where collecting large amounts of data is challenging or costly (Finzi et al., 2021; Immer et al., 2022; Shwartz-Ziv et al., 2022; Schwöbel et al., 2022; van der Ouderaa et al., 2023).

- Regularization effect introduced by the probabilistic nature of its Bayesian approach is beneficial in preventing overfitting and contributing to better generalization from fewer samples (Rothfuss et al., 2022; Sharma et al., 2023).
- Robustness to outliers, making it well-suited for real-world scenarios with noisy or out-of-distribution data.
- Attractive for foundation model fine-tuning, where data are commonly small and sparse, and uncertainty is important.
- Informed selection of data points for labeling: BDL optimizes the iterative process of active learning, strategically choosing the most informative instances for labeling to enhance model performance (Gal et al., 2017)
  - In-context learning examples (Xie et al., 2022)
  - Fine-tuning with human feedback (Ouyang et al., 2022)

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- Informed selection of data points for labeling: BDL optimizes the iterative process of active learning, strategically choosing the most informative instances for labeling to enhance model performance (Gal et al., 2017)
  - in-context learning scenarios (Margatina et al., 2023)
  - fine-tuning with human feedback (Casper et al., 2023).

Outline

Adaptability to New and Evolving Domains

- Dynamic update of prior beliefs in response to new evidence allows selective retention of valuable information from previous tasks while adapting to new ones, thus improving knowledge transfer across diverse domains and tasks (Rothfuss et al., 2021, 2022; Rudner et al., 2023b).
- Crucial for developing AI systems that can adapt to new situations or temporally evolving domains (Nguyen et al., 2018; Rudner et al., 2022b), as in continual or lifelong learning.

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Model Misspecification and Interpretability

- Bayesian model averaging (BMA) acknowledges and quantifies uncertainty in the choice of model structure. Instead of relying on a single fixed model, BMA considers a distribution of possible models (Hoeting et al., 1998, 1999; Wasserman, 2000).
- By incorporating model priors and inferring model posteriors, BDL allows BMA to calibrate uncertainty over network architectures (Hubin and Storvik, 2019; Skaaret-Lund et al., 2023).
- By averaging predictions over different model possibilities, BMA attenuates the impact of model misspecification, offering a robust framework that accounts for uncertainty in both parameter values and model structures, ultimately leading to more reliable and interpretable predictions (Hubin et al., 2021; Wang et al., 2023a; Bouchiat et al., 2023).

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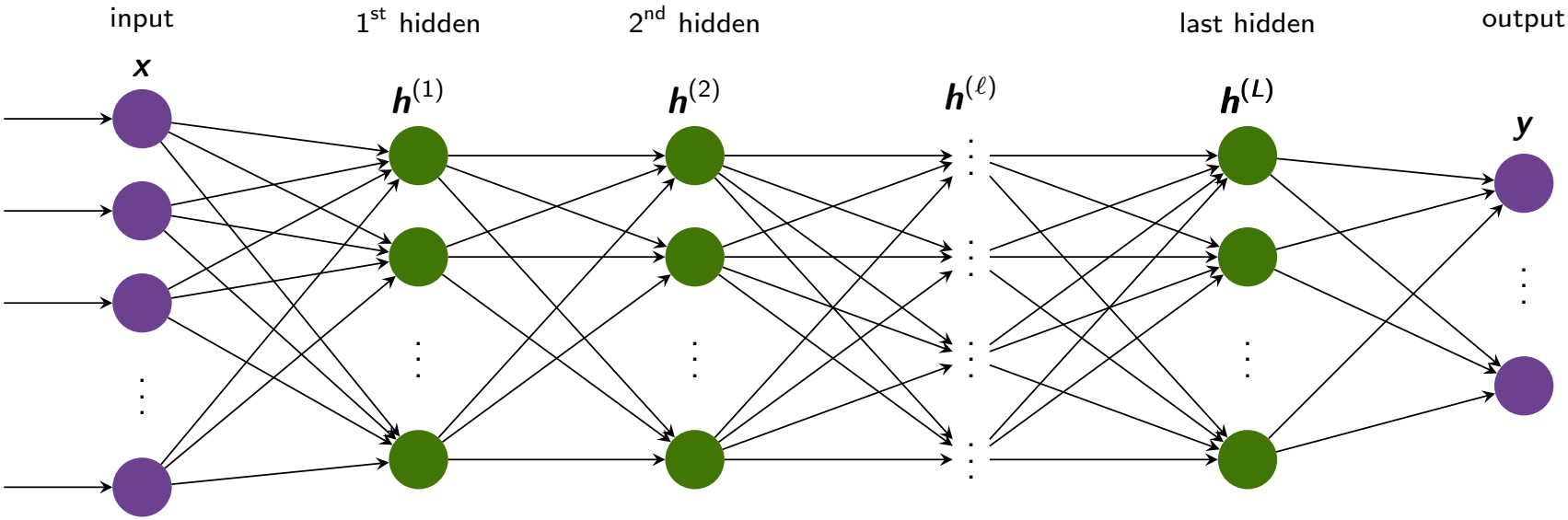
Outline

Neural networks notations



- pre-nonlinearity $\boldsymbol{g}^{(\ell)} = \boldsymbol{g}^{(\ell)}(\boldsymbol{x})$, post-nonlinearity $\boldsymbol{h}^{(\ell)} = \boldsymbol{h}^{(\ell)}(\boldsymbol{x})$

$$\boldsymbol{g}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{W}^{(\ell)}\boldsymbol{h}^{(\ell-1)}(\boldsymbol{x}), \quad \boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \phi(\boldsymbol{g}^{(\ell)}(\boldsymbol{x}))$$

- nonlinearity or activation function $\phi : \mathbb{R} \to \mathbb{R}$.
- weight matrix $\boldsymbol{W}^{(\ell)}$ of dimension $H_\ell \times H_{\ell-1}$ including a bias vector

Training

Optimization problem: minimize the loss function

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}).$$

With gradient-based optimization:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \, \partial_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}).$$

$\eta > 0$ is a step size, or learning rate. Gradients are computed as products of gradients between each layer from right to left, a procedure called backpropagation (Rumelhart et al., 1986).

Gradients are approximated on randomly chosen subsets called batches: stochastic gradient descent, SGD (Robbins and Monro, 1951). See survey of optimization methods bySun et al. (2019).

Architecture choice

- Convolutional neural networks (CNN) are widely used in computer vision.
- Recurrent neural networks (RNN) are advantageous for sequential data, designed to save the output of a layer by adding it back to the input (Hochreiter and Schmidhuber, 1997).
- Residual neural networks (ResNet) have residual blocks which add the output from the previous layer to the layer ahead, so-called skip-connections (He et al., 2016). Allows very deep training.

Expressiveness

Expressiveness describes neural networks' ability to approximate functions (Cybenko, 1989; Funahashi, 1989; Hornik et al., 1989; Barron, 1994).

Universal approximation theorem

Neural networks of one hidden layer and suitable activation function can approximate any continuous function on a compact domain, say $f : [0, 1]^N \to \mathbb{R}$, to any desired accuracy.

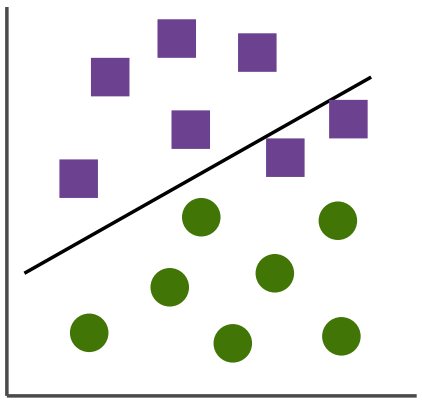
But the size of such networks may be exponential in the input dimension N, which makes them highly prone to overfitting as well as impractical.

Width-depth trade-offs studied by Chatziafratis et al. (2020b,a).

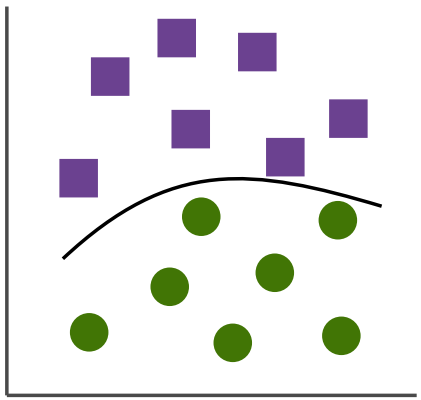
Generalization and overfitting I

Classical regime

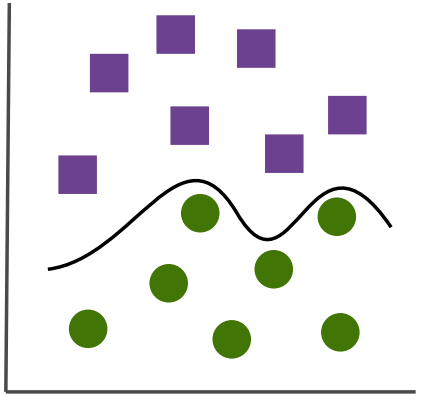
underfitting



optimum



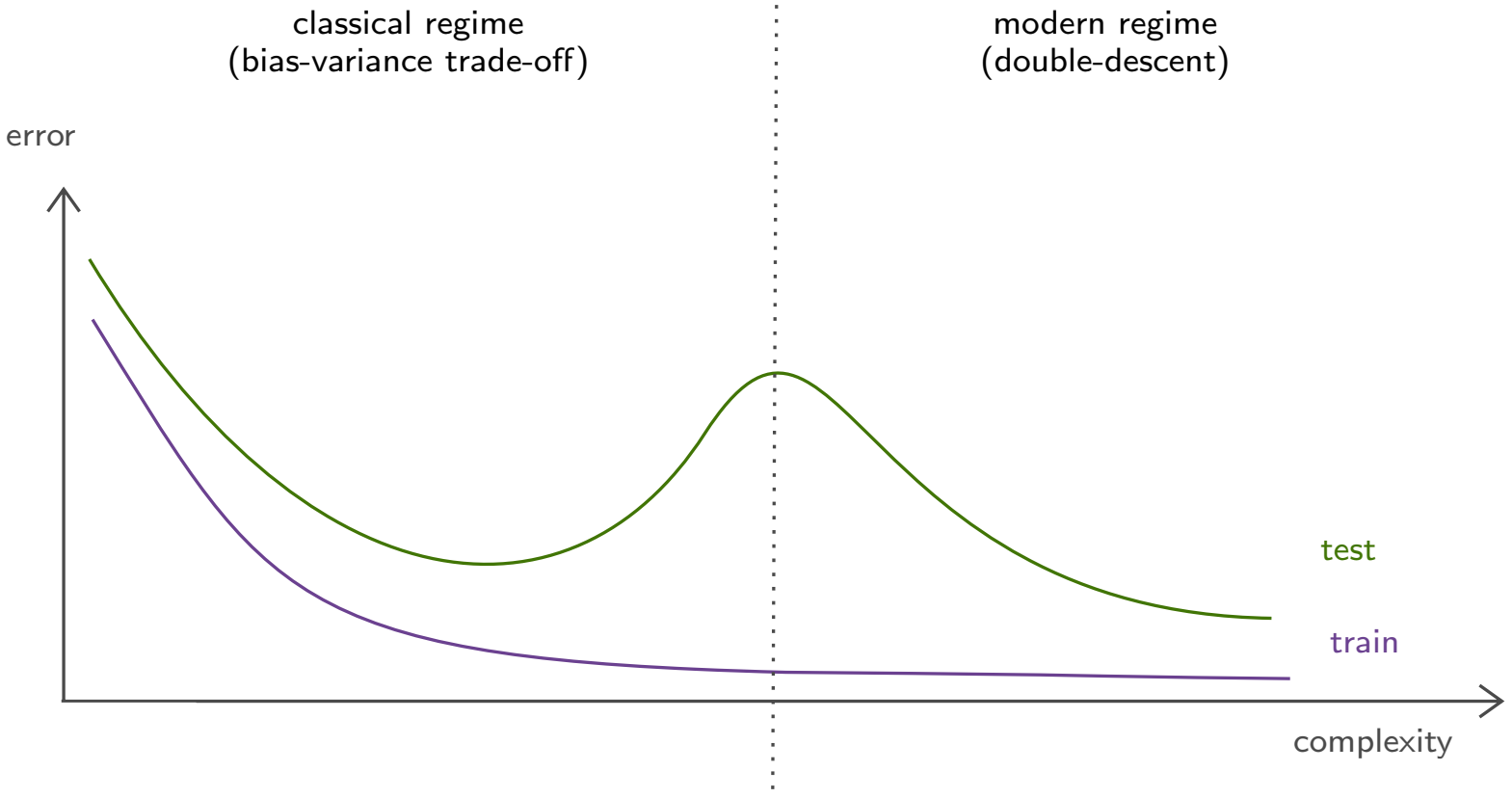
overfitting



Generalization and overfitting II

Modern regime

It was shown recently that when increasing the model size beyond the number of training examples, the model's test error can start decreasing again after reaching the interpolation peak: double-descent (Belkin et al., 2019).



Limitations with point-estimate neural networks

- Inability to distinguish between in-domain and out-of-domain samples (Lee et al., 2018; Mitros and Mac Namee, 2019; Hein et al., 2019; Ashukha et al., 2020), and the sensitivity to domain shifts (Ovadia et al., 2019), which are explained in details later on;
- Inability to provide reliable uncertainty estimates for a deep neural network's decision and frequently occurring overconfident predictions (Minderer et al., 2021);
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Great expectations of Bayesian neural networks

- Uncertainty quantification through the posterior distribution: BNN are shown to be better calibrated than NN
- Distinguishing between the epistemic uncertainty $p(\theta|D)$ and the aleatoric uncertainty $p(y|x,\theta)$: desirable in small dataset settings, providing high epistemic uncertainty for prediction, avoiding overfitting
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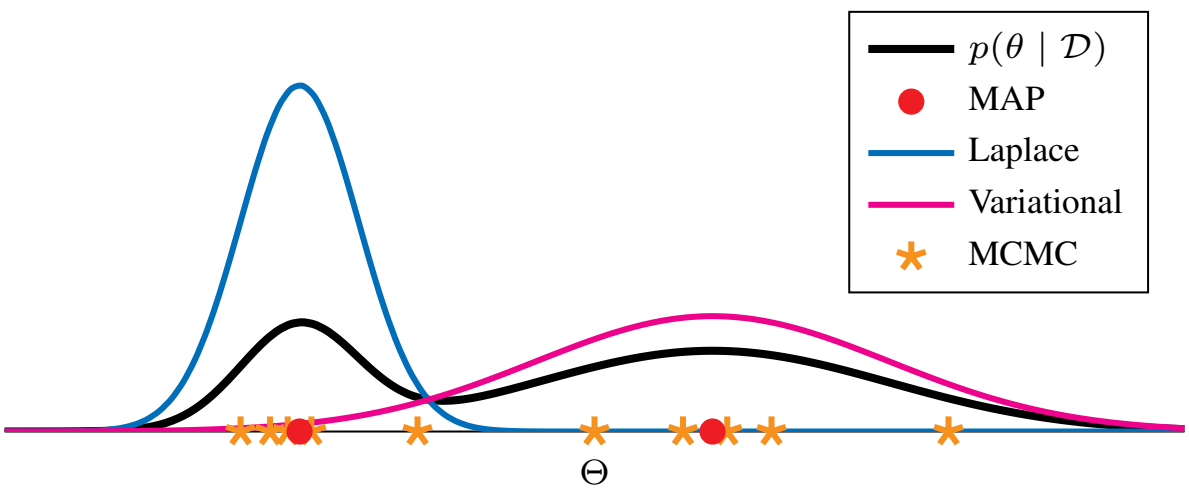
Outline

Challenges for BDL

- One of the challenges in BDL is the computational cost incurred (Izmailov et al., 2021).
- Showing that BDL works cheaply, or at least with practical efficiency under modern settings in the real world, is one of the most important problems that remains to be addressed.
- We highlight challenges that contribute to its difficulties in deployment: posterior computation, prior specification, scalability, foundation models, lack of convergence and performance metrics and benchmarks.



Different flavors of BDL methods for approximating the posterior $p(\theta \mid \mathcal{D})$ on Θ. While Laplace and Gaussian-based variational approaches both yield Gaussian approximations, they generally capture different local modes of the posterior. Ensemble methods use MAP estimates as their samples.

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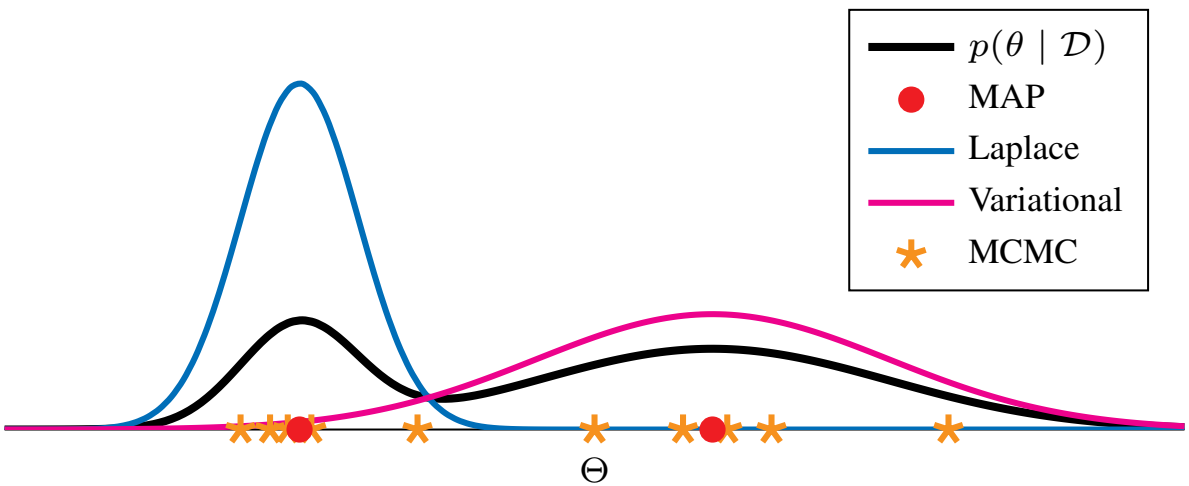

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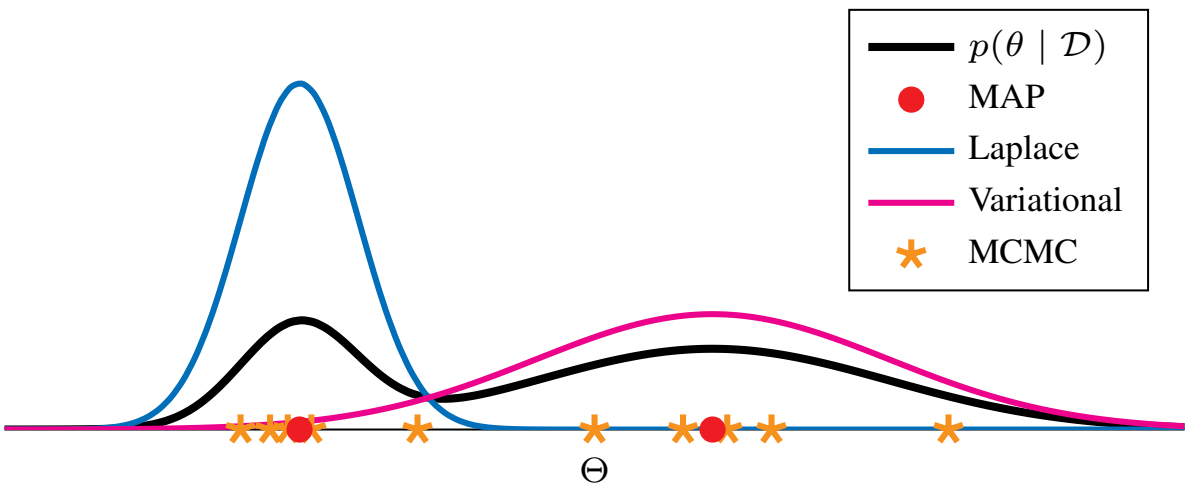

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Laplace approximation

Computes a Gaussian approximation to the posterior centered at the MAP estimate

- It is simple
- But... computing the Hessian is expensive, and may result in a non-positive definite matrix since the log likelihood of deep neural networks is non-convex.
- Gauss–Newton approximation to the Hessian

Generalized Gauss–Newton approximation

$$\boldsymbol{H}^{\mathrm{GGN}} := \sum_{i=1}^{n} \mathcal{J}_{\boldsymbol{w}}(\boldsymbol{x}_i)^{\top} \boldsymbol{\Lambda}(\boldsymbol{y}_i; f_i) \mathcal{J}_{\boldsymbol{w}}(\boldsymbol{x}_i),$$

where $\mathcal{J}_{\boldsymbol{w}}(\boldsymbol{x})$ is the network per-sample Jacobian $[\mathcal{J}_{\boldsymbol{w}}(\boldsymbol{x})]_c = \nabla_{\boldsymbol{w}} f_c(\boldsymbol{x}; \boldsymbol{w}_{\hat{\rho}})$, and $\boldsymbol{\Lambda}(\boldsymbol{y}; f) = -\nabla^2_{ff} \log p(\boldsymbol{y}; f)$ is the per-input noise matrix.

Laplace and Variational Approximations

- Laplace and variational approximations use geometric or differential information about the empirical loss to construct closed-form (usually Gaussian) probability measures to approximate the posterior.
- Simple nature and long history (MacKay, 1992), still show competitive predictive performance (Daxberger et al., 2021b; Rudner et al., 2022a; Antoran et al., 2023; Rudner et al., 2023a).
- Closed-form nature $\implies$ leveraging automatically computed differential quantities and the foundations of numerical linear algebra, theoretical analysis (Kristiadi et al., 2020) and analytical functionality, such as calibration (Kristiadi et al., 2021b,a) and marginalization (Khan et al., 2019; Immer et al., 2021a,b).
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- The approximate posterior is dependent on the parametrization of the BNN (MacKay, 1998).
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- The local posterior geometry may be poorly approximated by a Gaussian distribution, which can lead to underconfidence when sampling from the Laplace approximation (Lawrence, 2001), a problem that can be mitigated by linearization (Immer et al., 2021b).

Outline

Ensembles

Deep ensembling involves the retraining of a neural network (NN) with various initializations, followed by averaging the resulting models.

- Effective in approximating the posterior predictive distribution (Wilson and Izmailov, 2020).
- Precise connections between ensembles and Bayesian methods (Ciosek et al., 2020; He et al., 2020; Wild et al., 2023).
- Open question in BDL: can we develop scalable Bayesian inference methods that outperforms deep ensembles? Izmailov et al. (2021) have shown that Hamiltonian Monte Carlo (HMC) often outperforms deep ensembles, but with significant additional computational overhead.
- With large and computationally expensive deep learning models, such as LLMs, deep ensembles may encounter significant challenges due to the associated training and execution costs. Therefore, these large models may motivate research into more efficient architectures and inference paradigms, such as posterior distillation or repulsive ensembles (D'Angelo and Fortuin, 2021), to improve uncertainty calibration and sparser model use.

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Outline

Bayesian inference: basic sampling algorithm

Denote data by $D = \{D_x, D_y\}$ and parameters (weights) by $\boldsymbol{\theta}$.

Algorithm 1 Inference procedure for a BNN.

Define $p(\boldsymbol{\theta}|D) = \dfrac{p(D_{\boldsymbol{y}}|D_{\boldsymbol{x}}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{\int_{\boldsymbol{\theta}} p(D_{\boldsymbol{y}}|D_{\boldsymbol{x}}, \boldsymbol{\theta'})p(\boldsymbol{\theta'})d\boldsymbol{\theta'}}$;

for $i = 0$ **to** N **do**

  Draw $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta}|D)$;

  $\boldsymbol{y}_i = \Phi_{\boldsymbol{\theta}_i}(\boldsymbol{x})$;

end for

return $Y = \{\boldsymbol{y}_i | i \in [0, N)\}$, $\Theta = \{\boldsymbol{\theta}_i | i \in [0, N)\}$;

Posterior Sampling Algorithms

Within the realm of Markov chain Monte Carlo (MCMC; Brooks et al., 2011) for BDL, stochastic gradient MCMC (SG-MCMC; Nemeth and Fearnhead, 2021) algorithms, such as stochastic gradient Langevin dynamics (SG-LD; Welling and Teh, 2011) and stochastic gradient HMC (SG-HMC; Chen et al., 2014), have emerged as widely adopted tools.

- Despite offering improved posterior approximations, SG-MCMC algorithms exhibit slower convergence compared to SGD (Robbins, 1951) (to thoroughly explore the posterior distribution beyond locating the mode).
- A step forward in this regard would be to learn from the machine learning and systems community how to make Monte Carlo faster using contemporary hardware (Zhang et al., 2022; Wang et al., 2023b).
- Algorithms such as Stein variational gradient descent (SVGD; Liu and Wang, 2016) occupy a middle ground between optimization and sampling, by employing optimization-type updates but with a set of interacting particles. While recent advances show promising results in BNN settings (D'Angelo et al., 2021; D'Angelo and Fortuin, 2021; Pielok et al., 2022), these methods often perform poorly in high-dimensional problems.
- Alternatively, posterior exploration can be improved with cyclical step-size schedules (Zhang et al., 2019).

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Monte Carlo dropout

Dropout technique reinterpreted as a form of approximate Bayesian variational inference (Kingma et al., 2015; Gal and Ghahramani, 2016).

Idea: performing random sampling at test time. Instead of turning off the dropout layers at test time (as is usually done), hidden units are randomly dropped out according to a Bernoulli(p) distribution. Repeating this operation M times provides M versions of the MAP estimate of the network parameters $\boldsymbol{w}^m$, $m = 1, \ldots, M$ (where some units of the MAP are dropped), yielding an approximate posterior predictive in the form of the equal-weight average:

$$p(y|x, \mathcal{D}^n) \approx \frac{1}{M} \sum_{m=1}^{M} p(y|x, \boldsymbol{w}^m).$$

- Monte Carlo dropout captures some uncertainty from out-of-distribution (OOD) inputs
- But... does not provide valid posterior uncertainty
- Folgoc et al. (2021) show that the Monte Carlo dropout posterior predictive assigns zero probability to the true model posterior predictive distribution

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Outline

Tempered and Cold Posteriors

Tempered posterior

A tempered posterior distribution with temperature parameter $T > 0$ is defined as

$$p(\boldsymbol{w}|D) \propto \exp(U(\boldsymbol{w})/T)$$

where $U(\boldsymbol{w})$ is the posterior energy function

$$U(\boldsymbol{w}) := \log p(\mathcal{D}|\boldsymbol{w}) + \log p(\boldsymbol{w}),$$

Cold posterior effect

Empirical evidence (Wenzel et al., 2020) that posteriors exponentiated to some power greater than one (or, equivalently, dividing the energy function $U(\boldsymbol{w})$ by some temperature $T < 1$), performs better than an untempered one.

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Outline

Prior Specification

- The prior over parameters induces a prior over functions, and it is the prior over functions that matters for generalization (Wilson and Izmailov, 2020).
- Defining priors over the parameters is hindered by the complexity and unintelligibility of high-dimensional spaces in BDL.
- One aim is to construct informative proper priors on neural network weights that are computationally efficient and favor solutions with desirable model properties (Vladimirova et al., 2019; Fortuin et al., 2022; Rudner et al., 2023a), such as priors that favor models with
  - reliable uncertainty estimates (Kuleshov et al., 2018),
  - a high degree of fairness (Rudner et al., 2023b),
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Outline

Scalability

- Symmetries in the parameter space of NNs yield computational redundancies (Wiese et al., 2023). Addressing the complexity and identifiability issues arising from these symmetries in the context of BDL can significantly impact scalability.
- Proposed solutions: incorporation of symmetry-based constraints in BDL inference methods (Sen et al., 2024) or the design of symmetry-aware priors (Atzeni et al., 2023).
- However, removing symmetries may not be an optimal strategy, since part of the success of deep learning can be attributed to the overparameterization of NNs, allowing rapid exploration of numerous hypotheses during training or having other positive 'side effects' such as induced sparsity (Kolb et al., 2023).

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Scalability

- Although UQ is of significant importance across various domains, it should not come at the cost of reduced predictive performance.
- BDL must strike a balance by ensuring that the computational cost of UQ matches that of point estimation.
- Otherwise, investing computational resources to improve the predictive performance of deep learning models might be a more prudent option.
- Ensembles are less affected by this concern due to their embarrassingly parallel nature.
- BUT relying solely on parallelism becomes inadequate in an era where even industry leaders encounter limitations in graphics processing unit (GPU) resources required to train a single large deep learning model.
- Simultaneously achieving time efficiency, memory efficiency, and high model utility (in terms of predictive performance and uncertainty calibration) remains the grand challenge of approximate Bayesian inference.

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Outline

Foundation Models

- Deep learning is in the midst of a paradigm shift into the foundation model era, characterized by models with billions,rather than millions, of parameters, with a predominant focus on language rather than vision.
- BDL approaches to LLMs are relatively unexplored, both in terms of methods and applications.
- Only a limited number of works have considered Bayesian approaches to LLMs (Xie et al., 2021; Cohen, 2022; Margatina et al., 2022; Yang et al., 2024).
- BDL emerges as a solution to address limitations in foundation models, particularly in scenarios where data availability is limited. In contexts involving personalized data (Moor et al., 2023) or causal inference applications (Zhang et al., 2023), such as individual treatment effect estimation, where small datasets prevail, the capacity of BDL for uncertainty estimation aligns seamlessly.
- The fine-tuning settings of foundation models in small data scenarios is another example.

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Diagnostics, Metrics and Benchmarks

- Currently, there is a lack of convergence and performance metrics specifically for the needs of BDL. Developing such tools can help identify the goals in BDL as well as assess their progress.
- The choice of evaluation metrics, datasets and benchmarks lack consensus in the BDL community which reflects a difficulty in clearly defining the goals of BDL in a field traditionally viewed through frequentist lens, specifically in terms of performance on test data.
  - Predictive performance: ability of the model to give correct answers. Based on metrics, eg: mean square error, risk of 0-1 loss for classification task.
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Outline

Outline

Connection prior-initialization

At initialization:

- random weights and biases, e.g., $W_{ij}^{(l)} \sim \mathcal{N}(0, \sigma_w^2)$, $B_i^{(l)} \sim \mathcal{N}(0, \sigma_b^2)$;
- inputs $X^{(1)}$ fixed.

Goal:

- find a criterion that the pre-activations $Z^{(l)}$ should match;
  example: $\mathrm{Var}(Z^{(l)}) = 1$;
- deduce a constraint over the distributions of $W^{(l)}$ and $B^{(l)}$;
  example: provided that $W_{ij}^{(l)} \sim \mathcal{N}(0, \sigma_w^2)$, $B_i^{(l)} \sim \mathcal{N}(0, \sigma_b^2)$, tune σ_w^2 and σ_b^2 accordingly.

Find a good initialization procedure

Naive heuristic. (*Understanding the difficulty of training deep feedforward neural networks*, Glorot and Bengio 2010):

- idea: preserve the variance of the pre-activations $Z^{(l)}$;
- tune σ_w^2 and σ_b^2 s.t.: $\mathrm{Var}(Z^{(l+1)}) = \mathrm{Var}(Z^{(l)})$.

Constraint: the NN is linear ($\phi = \mathrm{Id}$).
Result: $\sigma_b^2 = 0$, $\sigma_w^2 = 1$, $\mathrm{Var}(\frac{1}{\sqrt{n_l}} W_{ij}^l) = 1$.

Remark: this heuristic can be extended to $\phi =$ReLU.
(*Delving deep into rectifiers: Surpassing human-level performance on imagenet classification*, He et al., 2015)
Result: $\sigma_w^2 = 2$.

Outline

Neural-network Gaussian process (NN-GP)

- A neural network with one hidden layer, whose width goes to infinity, and which has a Gaussian prior on all the parameters, converges to a Gaussian process with a well-defined kernel (Neal, 1996a).

Proof: H the number of hidden units, ϕ some nonlinear activation function, b biais, weights v and $\boldsymbol{u}$; then unit k can be written

$$f_k(\boldsymbol{x}) = b_k + \sum_{j=1}^{H} v_{jk} h_j(\boldsymbol{x}), \quad h_j(\boldsymbol{x}) = \phi(U_{0j} + \boldsymbol{x}^t \boldsymbol{u}_j)$$

Then

- $\mathbb{E}[f_k(\boldsymbol{x})] =$
- $\mathbb{E}[f_k(\boldsymbol{x}) f_k(\boldsymbol{x}')] = \ldots := \mathcal{K}(\boldsymbol{x}, \boldsymbol{x}')$
- The joint distribution over $\{f_k(\boldsymbol{x_n}), n = 1 : N\}$ converges to a multivariate Gaussian.
- So the NN converges to a GP with mean 0 and kernel $\mathcal{K}$, called the neural network kernel. It is a non-stationary kernel.

Outline

Neural tangent kernel (NTK)

- The NNGP is obtained under the assumption that weights are random and width goes to infinity.
- Natural question: can we derive a kernel from a DNN while it is being trained?
- The answer is yes (Jacot et al., 2018). The associated kernel $\mathcal{T}(\boldsymbol{x}, \boldsymbol{x}')$ is called the Neural tangent kernel (NTK)

$$\mathcal{T}(\boldsymbol{x}, \boldsymbol{x}') := \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}; \boldsymbol{\theta}_\infty) \cdot \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}'; \boldsymbol{\theta}_\infty)$$

and is obtained with

  - continuous time gradient descent
  - letting the learning rate η become infinitesimally small
  - letting the widths go to infinity.

Outline

Edge of Chaos framework

See: Poole et al. (2016) and Schoenholz et al. (2017)

Main idea. Let x_a and x_b be two (fixed) inputs:

- variance: $v_a^{(l)} = \mathbb{E}[(Z_{j;a}^{(l)})^2]$;
- correlation: $c_{ab}^{(l)} = \frac{1}{\sqrt{v_a^{(l)} v_b^{(l)}}} \mathbb{E}[Z_{j;a}^{(l)} Z_{j;b}^{(l)}]$;
- goal: preserve the correlations $c_{ab}^{(l)}$ during propagation;
- solution: find a recurrence equation $c_{ab}^{(l+1)} = f(c_{ab}^{(l)})$;
- to do so, we must make an assumption on the distribution of $Z_{j;a}^{(l)}$;
  $\Rightarrow$ Gaussian hypothesis: $Z_{j;a}^{(l)} \sim \mathcal{N}(0, v_a^{(l)})$;
  Central Limit Theorem ($n_l \to \infty$): $Z_{j;a}^{(l+1)} = \frac{1}{\sqrt{n_l}} W_j^{(l)} X_a^{(l)} + B_j^{(l)}$;
- resulting simplified dynamics:

$$v_a^{(l+1)} = \mathcal{V}(v_a^{(l)} | \sigma_w, \sigma_b), \qquad c_{ab}^{(l+1)} = \mathcal{C}(c_{ab}^{(l)}, v_a^{(l)}, v_b^{(l)} | \sigma_w, \sigma_b).$$

Edge of Chaos results (Poole et al., 2016; Schoenholz et al., 2016)

Additional assumptions.

- the sequence $(v_a^{(l)})_l$ tends to a non-zero limit v^*, independent from the starting point $v_a^{(0)}$;
- $(v_a^{(l)})_l$ is assumed to have already converged;
- so: $c_{ab}^{(l+1)} = \mathcal{C}(c_{ab}^{(l)}, v^*, v^* | \sigma_w, \sigma_b) = \mathcal{C}_*(c_{ab}^{(l)} | \sigma_w, \sigma_b)$.

Phases of information propagation:

- *chaotic phase*: $\lim_{l\to\infty} c_{ab}^l = c^* < 1$
  $\Rightarrow$ decorrelate (partially or fully);
- *ordered phase*: $\lim_{l\to\infty} c_{ab}^l = c^* = 1$ with $\mathcal{C}_*'(1) < 1$
  $\Rightarrow$ correlate fully at an exponential rate;
- *edge of chaos*: $\lim_{l\to\infty} c_{ab}^l = c^* = 1$ with $\mathcal{C}_*'(1) = 1$
  $\Rightarrow$ correlate fully at sub-exponential rate.

$\Rightarrow$ tune σ_w and σ_b such that the NN lies in the "edge of chaos" phase.

Edge of Chaos I

Poole et al. (2016) and Schoenholz et al. (2017)

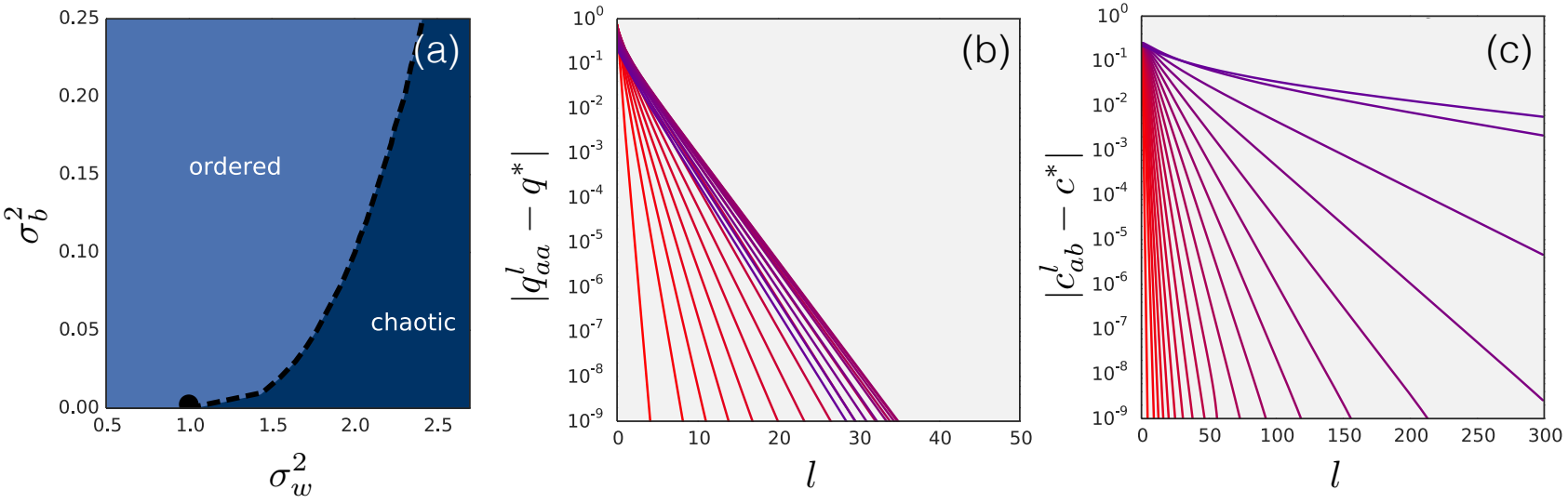


Figure: (a) Edge of chaos diagram showing the boundary between ordered and chaotic phases as a function of σ_w^2 and σ_b^2. (b) The residual $|q^* - q_{aa}^l|$ as a function of depth on a log-scale with $\sigma_b^2 = 0.05$ and σ_w^2 from 0.01 (red) to 1.7 (purple). Clear exponential behavior is observed. (c) The residual $|c^* - c_{ab}^l|$ as a function of depth on a log-scale. Again, the exponential behavior is clear. The same color scheme is used here as in (b).

From Schoenholz et al. (2017)

Outline

Definition (Generalized Weibull-tail on $\mathbb{R}$)

A random variable X is generalized Weibull-tail on $\mathbb{R}$ with tail parameter $\beta > 0$ if both its right and left tails are upper and lower bounded by some Weibull-tail functions with tail parameter β:

$$\begin{aligned} \mathrm{e}^{-x^\beta l_1^r(x)} \leq & \overline{F}_X(x) \leq \mathrm{e}^{-x^\beta l_2^r(x)}, && \text{for } x > 0 \text{ and } x \text{ large enough,} \\ \mathrm{e}^{-|x|^\beta l_1^l(|x|)} \leq & F_X(x) \leq \mathrm{e}^{-|x|^\beta l_2^l(|x|)}, && \text{for } x < 0 \text{ and } -x \text{ large enough,} \end{aligned}$$

where l_1^r, l_2^r, l_1^l and l_2^l are slowly-varying functions. We note $X \sim GWT(\beta)$.

Understanding priors at the unit level

This tail description reveals the difference between hidden units' distributional properties in finite- and infinite-width Bayesian neural networks, since hidden units are generalized Weibull-tail with a tail parameter depending on those of the weights:

Theorem (Vladimirova et al., 2021)

Consider a Bayesian neural network with ReLU activation function. Let ℓ-th layer weights be independent symmetric generalized Weibull-tail on $\mathbb{R}$ with tail parameter $\beta_w^{(\ell)}$. Then conditional on the input $\boldsymbol{x}$, the marginal prior distribution induced by forward propagation on any pre-activation is generalized Weibull-tail on $\mathbb{R}$: for any $1 \leq \ell \leq L$, and for any $1 \leq m \leq H_\ell$,

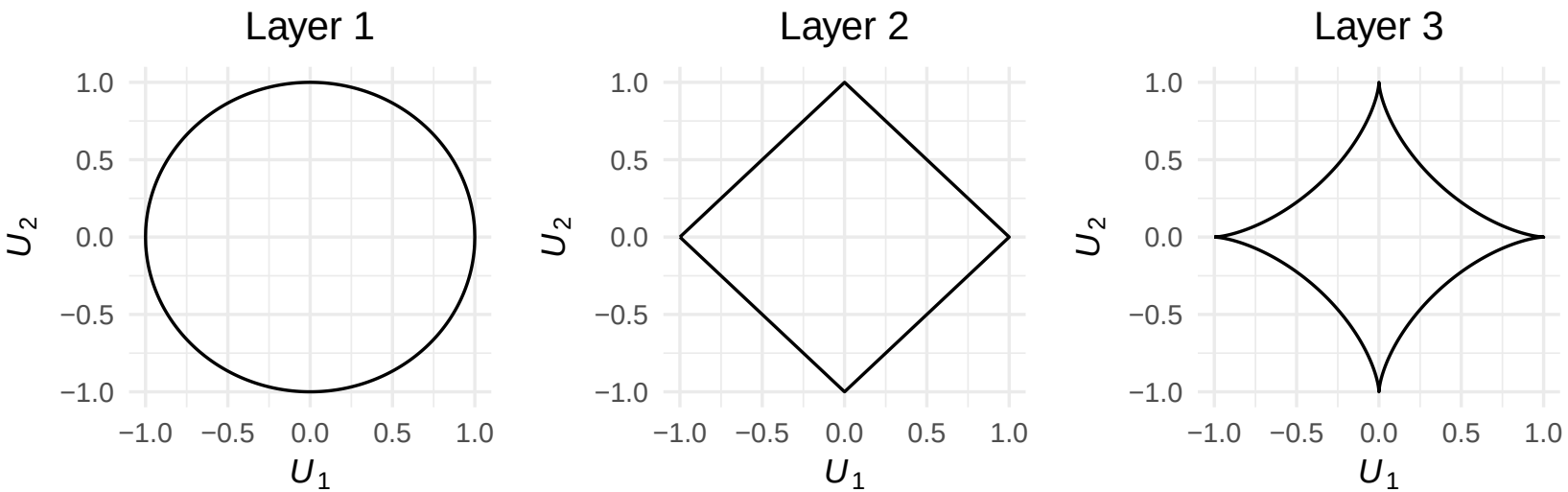
$$g_m^{(\ell)} \sim GWT(\beta^{(\ell)}),$$

with tail parameter $\beta^{(\ell)}$ such that $\frac{1}{\beta^{(\ell)}} = \frac{1}{\beta_w^{(1)}} + \cdots + \frac{1}{\beta_w^{(\ell)}}$.

Note that the most popular case of weight prior, iid Gaussian (Neal, 1996a), corresponds to $\text{GWT}_{\mathbb{R}}(2)$ weights. This leads to units of layer ℓ which are $\text{GWT}_{\mathbb{R}}(\frac{2}{\ell})$.

Understanding priors at the unit level

Layer	Penalty on $\boldsymbol{W}$	Approximate penalty on $\boldsymbol{U}$	
1	$\|\boldsymbol{W}^{(1)}\|_2^2$, $\mathcal{L}^2$	$\|\boldsymbol{U}^{(1)}\|_2^2$	$\mathcal{L}^2$ (weight decay)
2	$\|\boldsymbol{W}^{(2)}\|_2^2$, $\mathcal{L}^2$	$\|\boldsymbol{U}^{(2)}\|$	$\mathcal{L}^1$ (Lasso)
ℓ	$\|\boldsymbol{W}^{(\ell)}\|_2^2$, $\mathcal{L}^2$	$\|\boldsymbol{U}^{(\ell)}\|_{2/\ell}^{2/\ell}$	$\mathcal{L}^{2/\ell}$



Outline

Outline

Advancements in Posterior Sampling Algorithms

- Emerging need for new classes of posterior sampling algorithms for improved performance on DNNs.
- Objectives: Enhance efficiency, reduce computational overhead, and enable effective high-dimensional exploration.

Innovative Approaches:

- SG-MCMC with tempered posteriors for multi-mode sampling challenges.
- Development based on optimal transport theory (Villani, 2021), score-based diffusion models (Song et al., 2020), and ODE approaches like flow matching (Lipman et al., 2022).
- Utilization of NNs for mapping complex data distributions or in MCMC proposal mechanisms.

Strategies for Enhancing Posterior Sampling

Cross-Mode Exploration and Identifiability:

- SG-MCMC algorithms to traverse isolated modes rapidly, possibly via normalizing flows.
- Incorporating constraints for identifiability and focusing on identifiable functionals (Gu and Dunson, 2023).

Subspace Approaches and Future Directions:

- SG-MCMC in parameter space subspaces (linear, sparse) (Izmailov et al., 2020; Li et al., 2024).
- Formulating uncertainty statements for targeted subnetworks and beyond (Dold et al., 2024).
- Hybrid samplers combining structured variational inference with MCMC for efficiency (Alexos et al., 2022).
- Exploring subsampling and transfer learning integration (Kirichenko et al., 2023).

Outline

Hybrid Bayesian Approaches: An Overview

Future BDL approaches may focus on uncertainty in specific model areas, while others are efficiently estimated using point estimation. Hybrid approaches combine Bayesian methods with the efficiency of deterministic deep learning.

- Developing methods that apply Bayesian approaches in critical areas for cost-effective uncertainty capture.
- Maintaining deterministic approaches for other model parts (Daxberger et al., 2021b).
- Example: Last-layer Laplace approximation (Daxberger et al., 2021a).

Such hybrid approaches represent a promising research area.

Advancements and Literature in Hybrid Models

Traditional combinations of deep learning and GPs have been limited by GP scalability.

- Recent advances in GP inference scale-up are promising for broader application of hybrid models (Wilson et al., 2016).
- Deep Kernel Learning (DKL) as a key example of scalable hybrid models.

Prolific literature connects BDL with deep Gaussian processes (DGPs), involving neural network GPs arising as infinite-width limits of NNs.

- Connections between NNs and GPs provide valuable insights into BDL theory (Damianou and Lawrence, 2013; Agrawal et al., 2020; Neal, 1996b; de G. Matthews et al., 2018).

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Softwares

Software packages, libraries or probabilistic programming languages (PPLs) on top of deep learning frameworks include:

- `bayesianize` (Ritter et al., 2021), `bnn_priors` (Fortuin et al., 2021), `Laplace` (Daxberger et al., 2021a), `Pyro` (Bingham et al., 2019) and `TyXe` (Ritter and Karaletsos, 2022) are software species built on `PyTorch`,
- `TensorFlow Probability` is a library built on `TensorFlow`,
- `Fortuna` (Detommaso et al., 2023) is a library built on JAX.

PPLs, such as `Pyro`, play a role in simplifying the application of probabilistic reasoning to deep learning. In fact, abstractions of the probabilistic treatment of NNs in a PPL, such as those performed in the BDL library `TyXe`, can simplify the application of priors and inference techniques to arbitrary NNs, as demonstrated in a variety of models implemented in `TyXe`. Porting such ideas to modern problem settings involving LLMs and more bespoke probabilistic structures would enable the use of BDL in real-world problems.

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