Projected Bayesian Neural Networks:

Avoiding weight-space pathologies by learning latent representations of neural network weights

ACML, Nov 17th, 2019

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CRCS Center for Research on Computation and Society
at Harvard John A. Paulson School of Engineering and Applied Sciences

HDSI | Harvard Data Science Initiative

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Joint work with my collaborators...


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Success of Deep Learning

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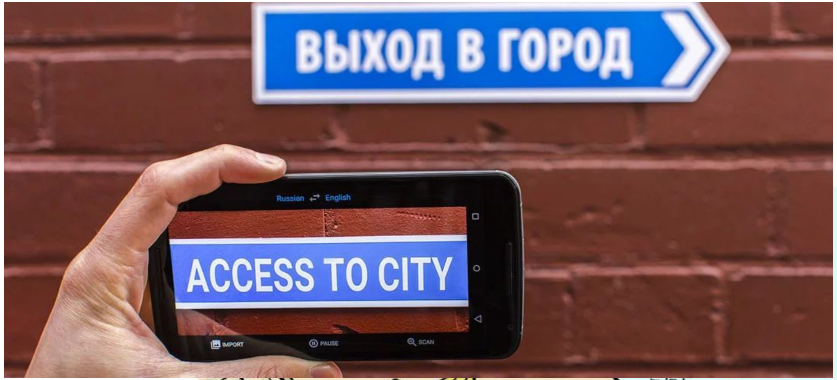
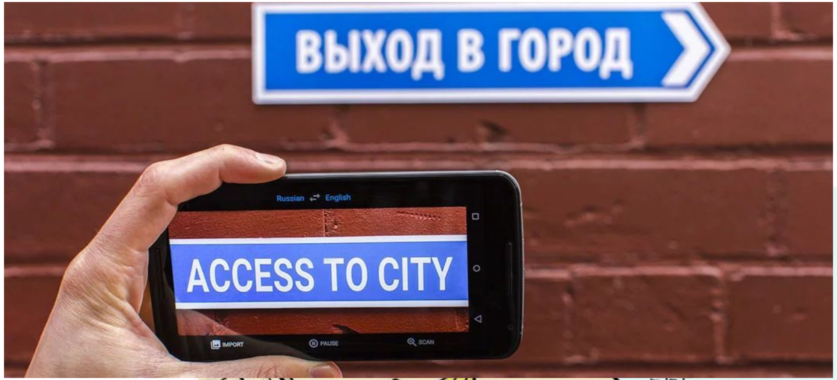
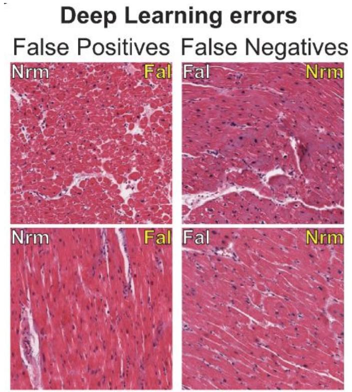


Success of Deep Learning



Huge amount of opportunities...

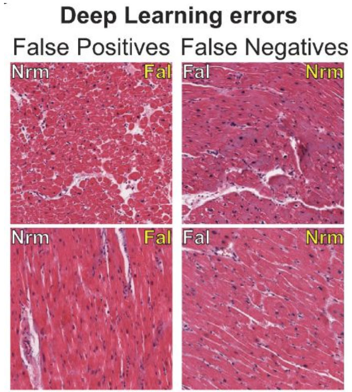
...but careful in high-stake decisions!



[Nirschi et.al, 2018]

[Eykholt et.al, 2018]

...but careful in high-stake decisions!



[Nirschi et.al, 2018]

[Eykholt et.al, 2018]

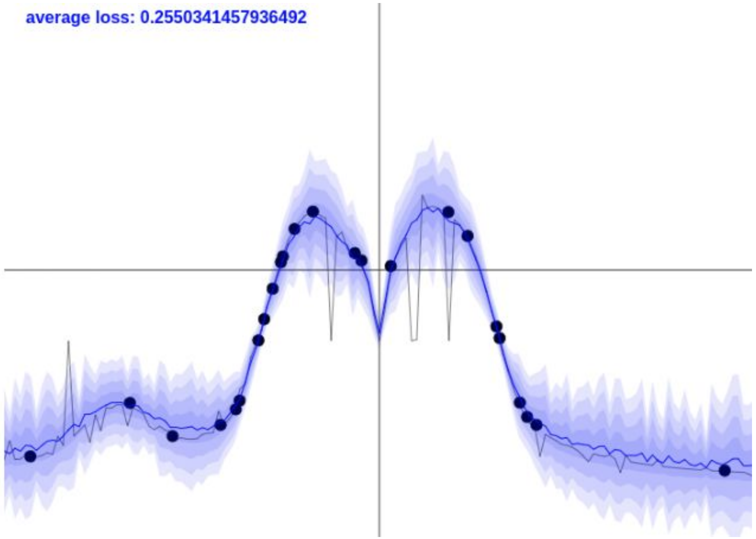
Our Goal: Quantify Uncertainty

With such uncertainty, we can:

- Alert humans in unclear situations
- Diagnose ML systems (when and how does it fail)
- Get better predictive accuracy

Focus: Bayesian Neural Networks

Bayesian Neural Network (BNN)



[What my deep model does not know, post of Yarin Gal, 2015]

$$\mathcal{D} = \{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{N}$$

$$\boldsymbol{y} = f_{\boldsymbol{w}}(\boldsymbol{x}) + \boldsymbol{\epsilon}$$

$$\boldsymbol{w} \sim \mathcal{N}(0, \sigma_w^2 \mathbf{I}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma_\epsilon^2 \mathbf{I})$$

Quantities of interest:

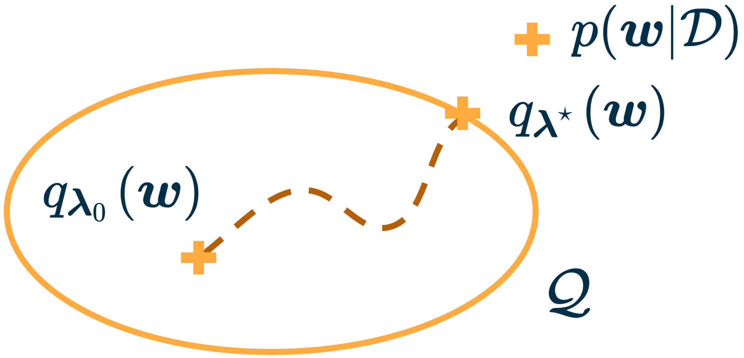
- Posterior of the weights $p(\boldsymbol{w}|\mathcal{D})$
- Predictive distribution

$$p(\mathbf{y}^\star|\mathbf{x}^\star, \mathcal{D}) = \int p(\mathbf{y}^\star|\mathbf{x}^\star, \boldsymbol{w}) p(\boldsymbol{w}|\mathcal{D}) d\boldsymbol{w}$$

Key challenge: $p(\boldsymbol{w}|\mathcal{D})$ intractable

Variational Inference: appealing for scalability

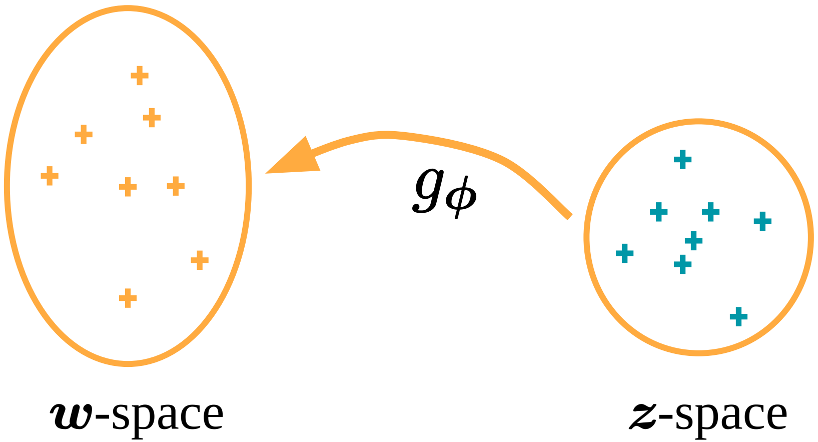
- Mean-field Approx. [Graves, 1993] [Blundell et.al, 2015]
- Structured Variational Approximations
  - Multivariate Gaussians [Louizos et.al, 2016; Sun et.al, 2017]
  - Hierarchical Variational Models [Ranganath et.al, 2016]
- Normalizing Flows and Transformations
  - Multiplicative Normalizing Flow [Louizos et. al, 2017]
  - Hypernetworks [Krueger et.al, 2017; Pawlowski et.al, 2017]



$q_{\boldsymbol{\lambda}}(\boldsymbol{w}) \in \mathcal{Q}$

Our Approach

Projected Bayesian NN (proj-BNN)



$$D_w \gg D_z$$

$$\mathcal{D} = \{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^N$$

$$\boldsymbol{y} = f_{\boldsymbol{w}}(\boldsymbol{x}) + \boldsymbol{\epsilon} \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma_\epsilon^2 \mathbf{I})$$

$$\boldsymbol{w} = g_{\boldsymbol{\phi}}(\boldsymbol{z}), \quad \boldsymbol{z} \sim p(\boldsymbol{z}), \quad \boldsymbol{\phi} \sim p(\boldsymbol{\phi}),$$

Quantities of interest:

- Posterior of the weights $p(z, \phi | \mathcal{D})$
- Predictive distribution

$$p(\mathbf{y}^\star | \mathbf{x}^\star, \mathcal{D}) = \int p(\mathbf{y}^\star | \mathbf{x}^\star, z, \phi) p(z, \phi | \mathcal{D}) d\boldsymbol{w}$$

How about inference?

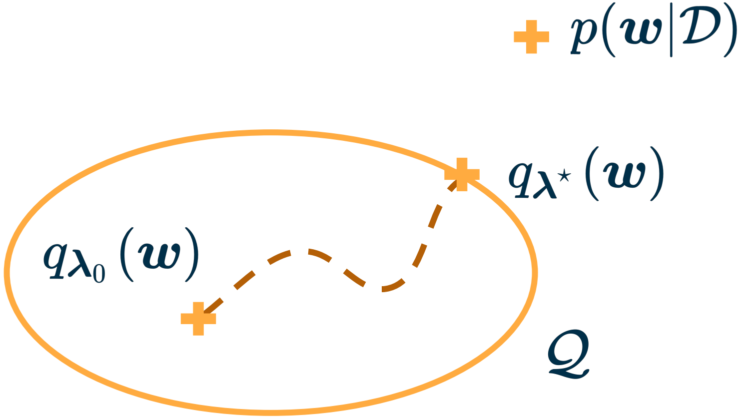
Objective: approximate $p(\boldsymbol{w}|\mathcal{D})$

$$q_{\boldsymbol{\lambda}}(\boldsymbol{w}) \in \mathcal{Q}$$

$$\underset{\boldsymbol{\lambda}^\star}{\operatorname{argmin}}\ D_{\mathrm{KL}}\Big(q_{\boldsymbol{\lambda}}(\boldsymbol{w})||p(\boldsymbol{w}|\mathcal{D})\Big)$$

$$\Updownarrow$$

$$\underset{\boldsymbol{\lambda}^\star}{\operatorname{argmax}}\ \mathcal{L}(\boldsymbol{\lambda}) = \mathbb{E}_q\Big[\log p\big(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{w}\big)\Big] - D_{\mathrm{KL}}\big(q_{\boldsymbol{\lambda}}(\boldsymbol{w})||p(\boldsymbol{w})\big)$$



Black-box VI [Ranganath et.al, 2013] + reparametrization trick [Kingma et.al, 2014; Rezende et.al, 2015]

How about inference?

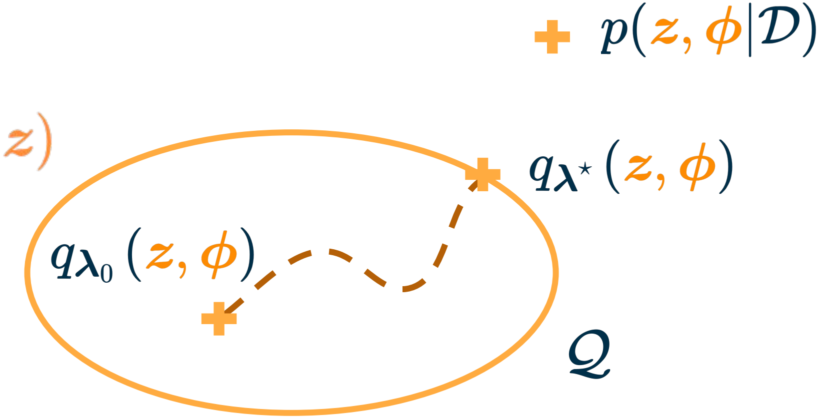
Objective: approximate $p(\boldsymbol{z}, \boldsymbol{\phi} | \mathcal{D})$

$$\boldsymbol{z} \sim q_{\boldsymbol{\lambda}_z}(\boldsymbol{z}), \quad \boldsymbol{\phi} \sim q_{\boldsymbol{\lambda}_\phi}(\boldsymbol{\phi}), \quad \boldsymbol{w} = g_{\boldsymbol{\phi}}(\boldsymbol{z})$$

$$\underset{\boldsymbol{\lambda}^\star}{\operatorname{argmin}}\ D_{\mathrm{KL}}\left(q_{\boldsymbol{\lambda}}(\boldsymbol{z}, \boldsymbol{\phi}) || p(\boldsymbol{z}, \boldsymbol{\phi} | \mathcal{D})\right)$$

$$\Updownarrow$$

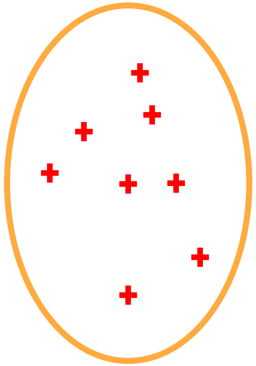
$$\underset{\boldsymbol{\lambda}^\star}{\operatorname{argmax}}\ \mathcal{L}(\boldsymbol{\lambda}) = \mathbb{E}_q\left[\log p(\boldsymbol{y} | \boldsymbol{x}, g_{\boldsymbol{\phi}}(\boldsymbol{z}))\right] - D_{\mathrm{KL}}\left(q_{\boldsymbol{\lambda}_z}(\boldsymbol{z}) || p(\boldsymbol{z})\right) - D_{\mathrm{KL}}\left(q_{\boldsymbol{\lambda}_\phi}(\boldsymbol{\phi}) || p(\boldsymbol{\phi})\right)$$



Black-box VI [Ranganath et.al, 2013] + reparametrization trick [Kingma et.al, 2014; Rezende et.al, 2015]

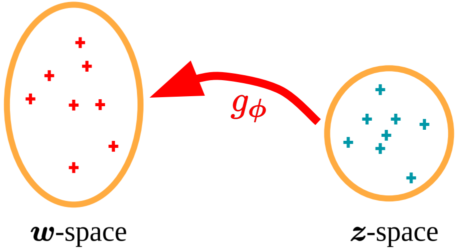
Smart-initialization Procedure

1. Characterize weight space



Sample multiple weight sets [Izmailov et.al, 2018]

2. Find point estimate g_ϕ



Train an autoencoder

3. Black-box VI (BBVI)

$$D_{\mathrm{KL}}\left(q_{\boldsymbol{\lambda}}(\boldsymbol{z},\boldsymbol{\phi})||p(\boldsymbol{z},\boldsymbol{\phi}|\mathcal{D})\right)$$

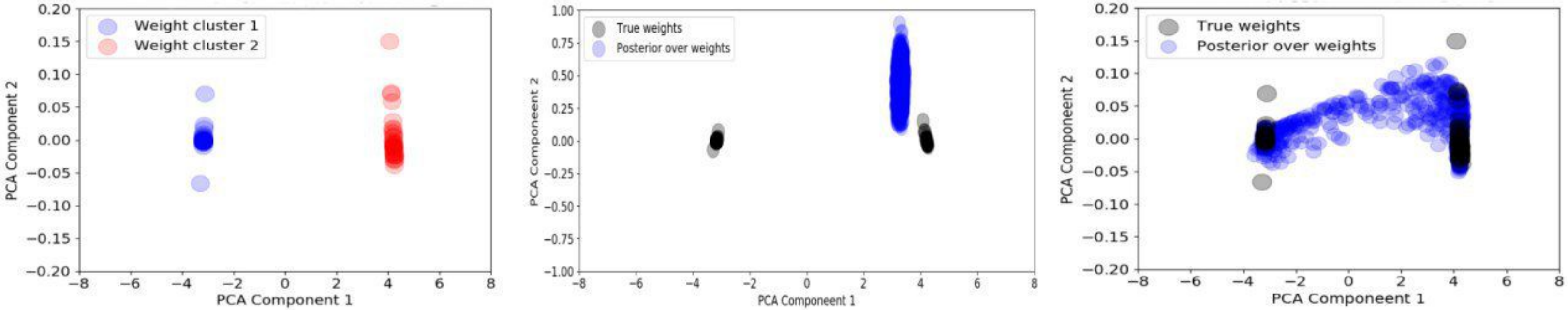
BBVI with smart initialization

Results

Results: Illustrative Toy Example

[Blundell et.al, 2015]

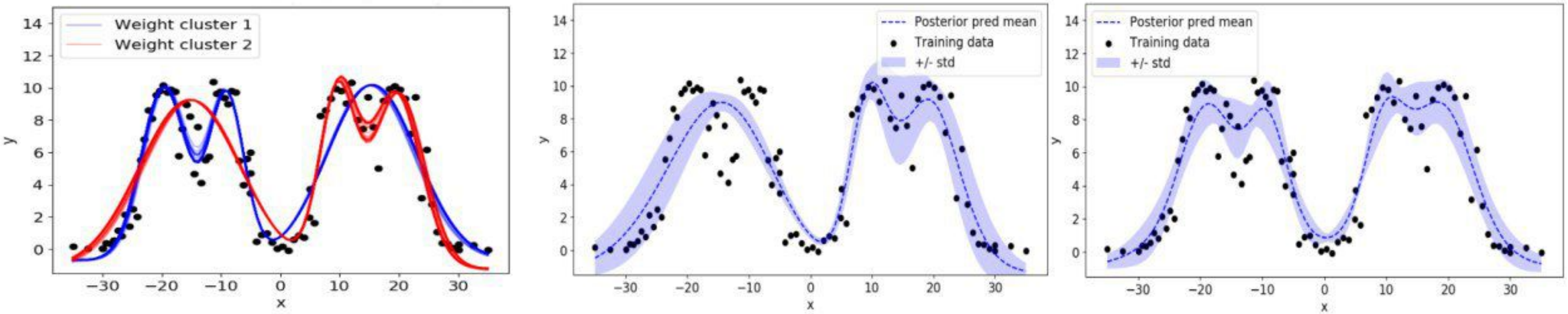
[Pradier et.al, 2018]



(a) Projection of true weights

(b) BbB posterior over weights

(c) Proj-BNN posterior over weights

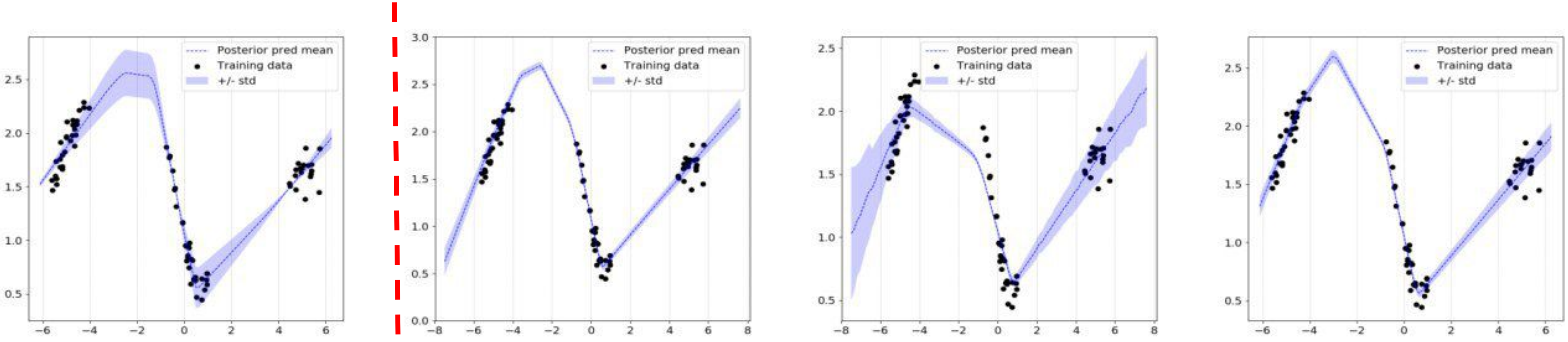


(d) Functions from true weights

(e) BbB posterior predictive

(f) Proj-BNN posterior predictive

Results: Uncertainty estimation

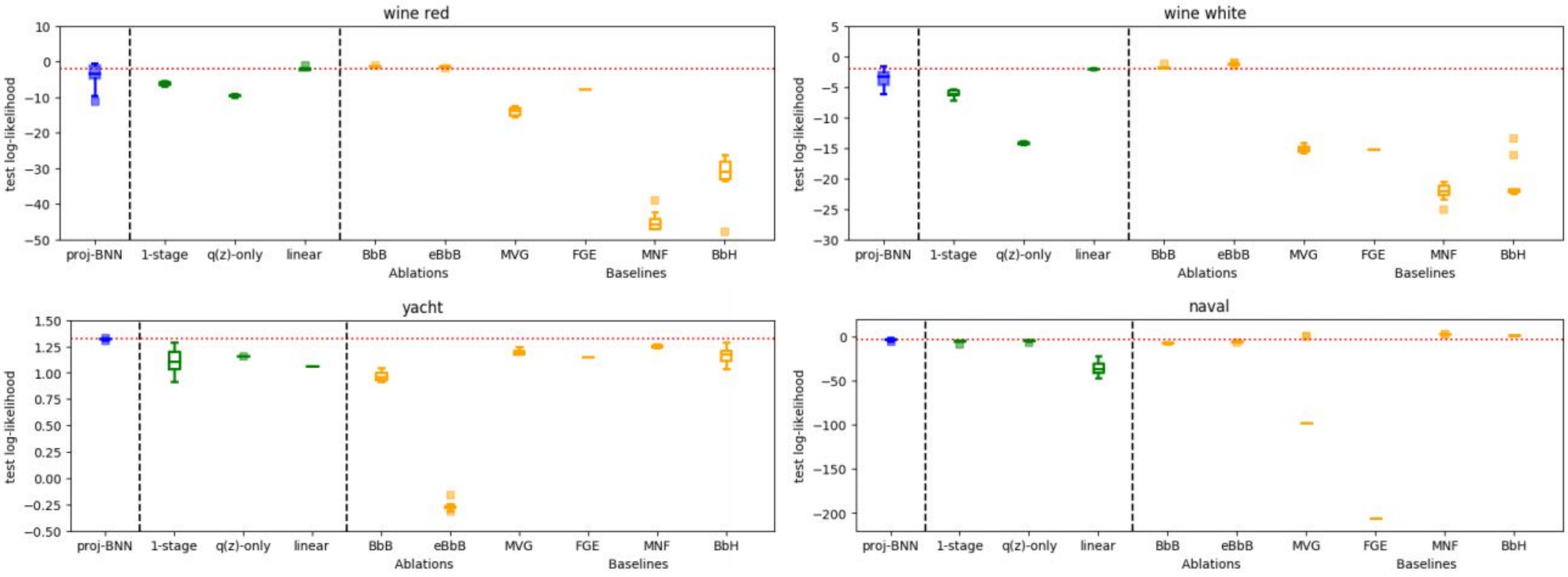


(a) Proj-BNN ($D_z = 2$) (b) BbB (c) MNF (d) MVG

- BbB: Bayes by Back Prop [Blundell et.al, 2015]
- MVG: Multivariate Gaussians [Louizos et.al, 2016]
- MNF: Multiplicative Normalizing Flow [Louizos et. al, 2017]

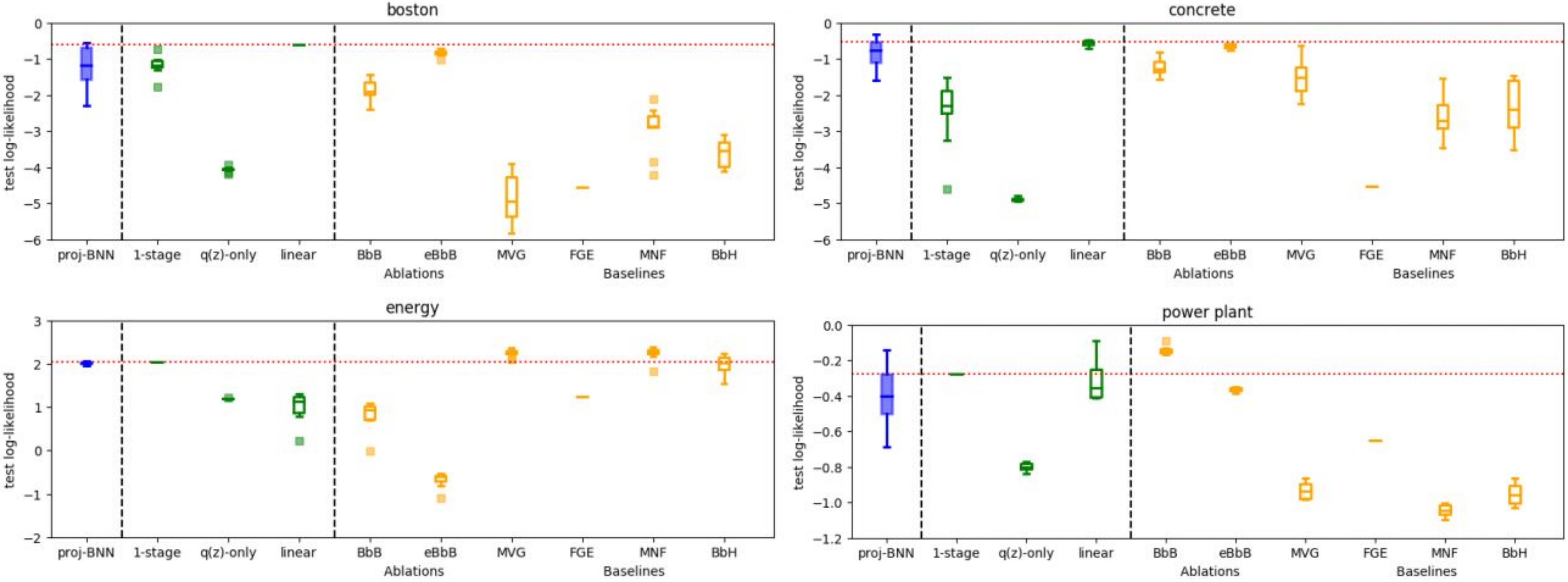
Results: Generalization

https://arxiv.org/abs/1811.07006



Results: Generalization

https://arxiv.org/abs/1811.07006



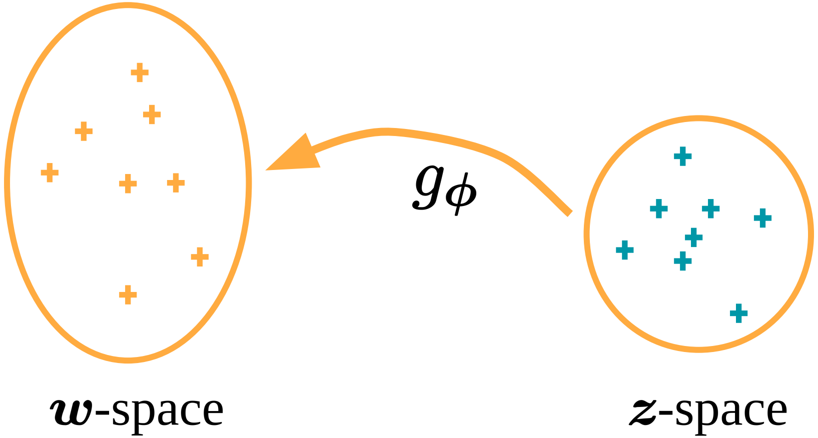
Conclusions

Contact: *melanie@seas.harvard.edu*

https://melaniefp.github.io/

In this talk...

- Alternative modeling for BNNs
- Better approximate inference



https://arxiv.org/abs/1811.07006

Thank you for listening!

Open questions

- Better evaluation of uncertainty?

``Test log likelihood can be misleading”

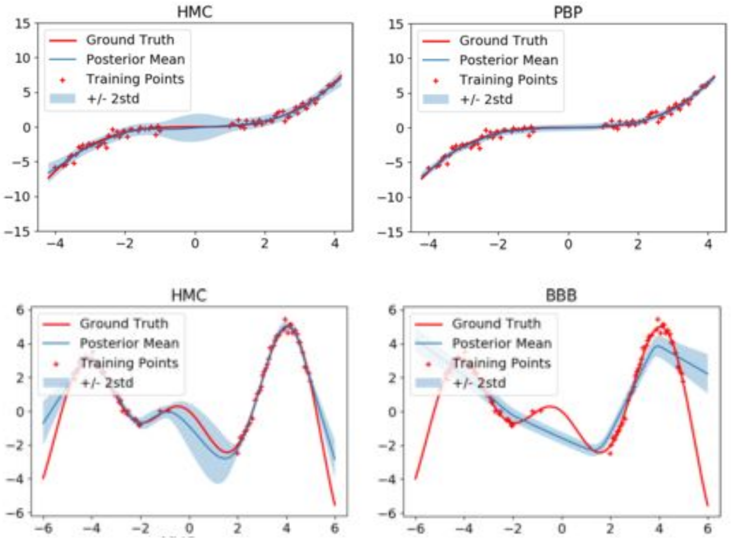
> Entangled sources of error: model, variational approx, optimization

- How does the topology in weight space looks like?

> Intuition misleading in high dimensions!

- How to exploit latent structure for interpretability?

[Yao et. al, ICML Workshop, 2019]



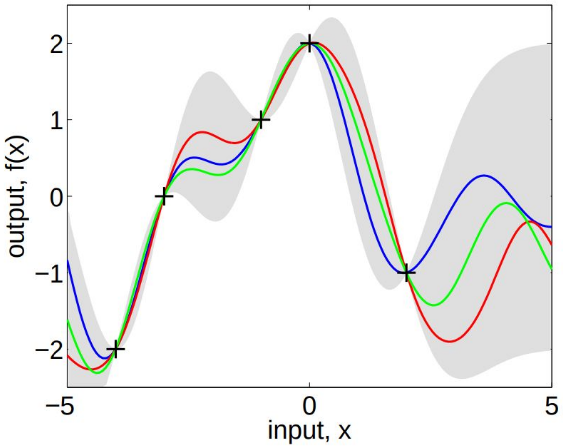
Related works on weight embeddings [Karaletsos et.al, 2018; Izmailov et.al, 2019]

Appendix

Uncertainty Estimation via GPs?

Gaussian Process (GP)

[Rasmussen et.al, 2016]



$$f(x) \sim \mathrm{GP}\left(m(x), k(x, x')\right)$$

Drawbacks of GPs

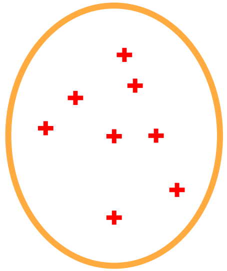
- Scalability
- Kernel learning is not trivial

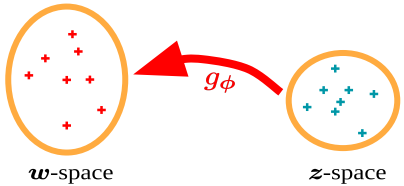
Alternative: Neural Networks with uncertainty

- Ensemble of Neural Networks
  [Lakshminarayanan et al., 2017; Pearce et.al, 2018]

- Bayesian Neural Networks
  [Buntine et al., 1991; MacKay, 1992; Neal, 1993]

Results: Generalization (Ablations)



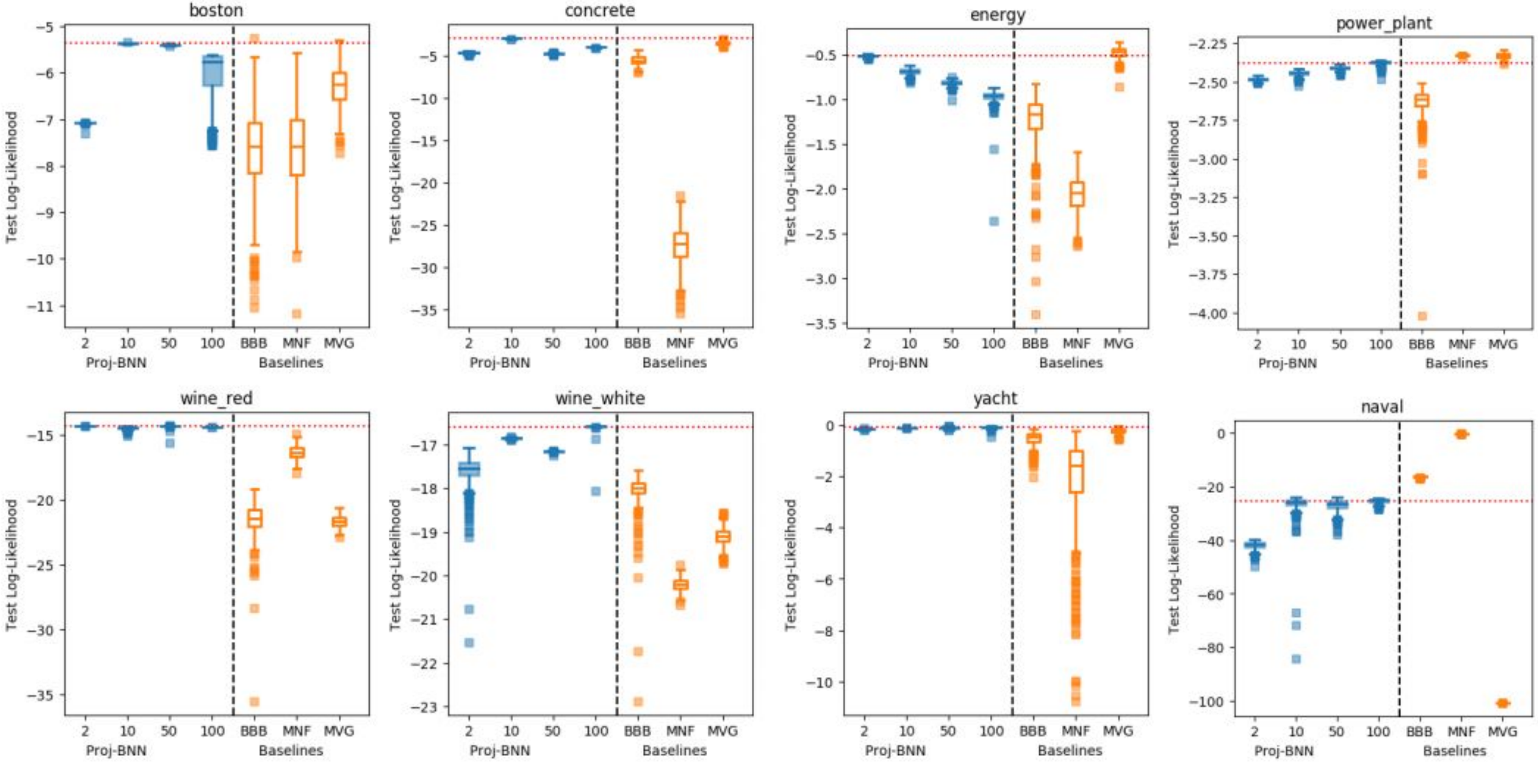


$$D_{\mathrm{KL}}\Big(q_{\boldsymbol{\lambda}}(\boldsymbol{z},\boldsymbol{\phi})\,||\,p(\boldsymbol{z},\boldsymbol{\phi}|\mathcal{D})\Big)$$

	1. Characterize w-space	2. Find point estimate g_ϕ	3. Black-box VI (BBVI)
1-stage	✗	✗	✓
linear	✓	linear	✓
q(z) only	✓	✓	$q_{\boldsymbol{\lambda}_z}(\boldsymbol{z})$

Cross-validation of latent dimension

https://arxiv.org/abs/1811.07006



Prediction-constrained Autoencoder

$$\{\boldsymbol{\theta}^\star, \boldsymbol{\phi}^\star\} = \operatorname*{argmin}_{\boldsymbol{\theta},\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}) = \min_{\boldsymbol{\theta},\boldsymbol{\phi}} \left\{ \frac{1}{R} \sum_{r=1}^{R} \left(\mathbf{w_c}^{(r)} - g_{\boldsymbol{\phi}} \left(f_{\boldsymbol{\theta}} \left(\mathbf{w_c}^{(r)} \right) \right) + \gamma^{(r)} \right)^2 \right.$$
$$\left. + \, \beta \, \mathbb{E}_{(x,y)\sim\mathcal{D}} \left[\frac{1}{R} \sum_{r=1}^{R} \log p \big(y | x, g_{\boldsymbol{\phi}} \left(f_{\boldsymbol{\theta}} \left(\mathbf{w_c}^{(r)} \right) \right) \big) \right] \right\},$$

My research: probabilistic models for societal needs

Highly driven by real-world application, with special emphasis on…

A) Latent Representation Learning

M. F. Pradier, B. Reis, L. Jukofsky, F. Milletti, T. Ohtomo, F. Perez-Cruz, and O. Puig. **Case-control Indian Buffet Process identifies biomarkers of response to Codrituzumab**. *BMC Cancer*. 2019.

I. Valera, M. F. Pradier, M. Lomeli, and Z. Ghahramani. **General Latent Feature Models for Heterogeneous Datasets**. *In submission to Journal of Machine Learning Research*. 2018.

M. F. Pradier, W. Pan, M. Yau, R. Singh, and F. Doshi-Velez. **Hierarchical Stick-breaking Paintbox**. *BNP@NeurIPS Workshop*. Montreal (Canada), December 2018.

B) Uncertainty Quantification

M. F. Pradier, W. Pan, J. Yao, S. Ghosh, and F. Doshi-Velez. **Projected BNNs: Avoiding Pathologies in Weight Space by projecting Neural Network Weights**. Arxiv. 2019.

B. Coker, M. F. Pradier, and F. Doshi-Velez. **Poisson Process Radial Basis Function Networks.** (Arxiv coming soon)

W. Yang, L. Lorch, M. A. Graule, S. Srinivasan, A. Suresh, J. Yao, M. F. Pradier, and F. Doshi-Velez. **Output-Constrained Bayesian Neural Networks**. *ICML Workshop on Generalization*. 2019.