Bayesian deep learning

Bayesian inference for deep neural networks :)

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As I read papers in more details, I will add more details to the slides. Slides for today are created based on Part 1 and 3 of the 2020 ICML tutorial on bayesian deep learning.

The posterior predictive is a bayes model average

In many machine learning applications, we care a lot of about predicting a quantity. This includes both classification and regression problems.

This is most naturally* captured by the following integral:

$$p(y|\, x, D) = \int p(y|\, x, \theta) p(\theta|\, D)\, d\theta$$

where $p(\theta|\, D)$ is the posterior over the parameter vector given observed data $D = \{(x^{(i)}, y^{(i)})\}$.

Interpretation. Rather than finding one solution, average across several solutions

Other names: **marginalization** over θ

$$p(y|\, x, D) = \int p(y, \theta|\, x, D)\, d\theta$$

How about MAP and MLE?

If we want to approximate the posterior by **a point estimate**, then one can argue that we should use the MAP. When the prior is uniform, then we have the MLE.

$$p(\theta|\, D) = \delta_{\hat{\theta}_{\mathrm{MAL}}}(\theta) = \begin{cases} \infty & \text{if } \theta = \hat{\theta}_{\mathrm{MAP}} \\ 0 & \text{otherwise} \end{cases}$$

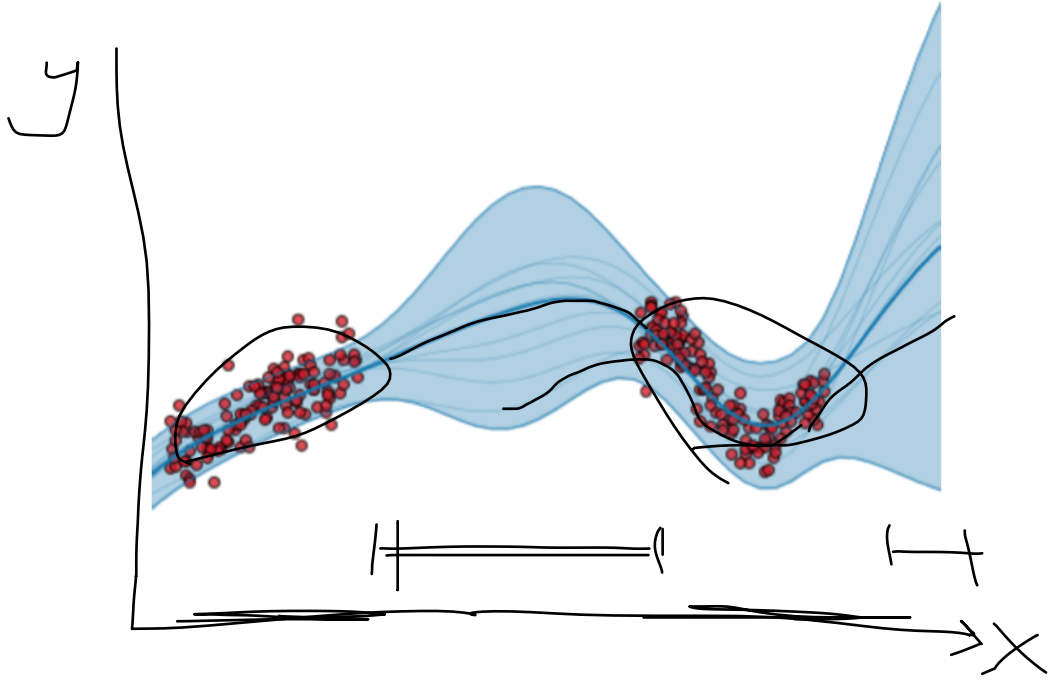
If we do this approximation, then the posterior predictive becomes

$$\begin{aligned} p(y|\, x, D) &= \int p(y|\, x, \theta)\, p(\theta|\, D)\, d\theta \\ &= \int p(y|\, x, \theta)\, \delta(\hat{\theta}_{\mathrm{MAP}})\, d\theta \\ &= p(y|\, x, \hat{\theta}_{\mathrm{MAP}}). \end{aligned}$$

Why is bayes model average particularly important for NNs?

Posterior is diffused, so point estimation would give different result (in terms of the predictive distribution) compared to doing the integral (which is arguably the correct thing to do?)

- Otherwise, underestimation of epistemic uncertainty
- High variance problem ("variance" as in bias-variance tradeoff) $\rightarrow$ bad generalization



Also: Architecture agnostic! Empirically leads to *better* performance than MLE training!

Methods (a very limited overview) - up to 2020

Challenge:

- Lots of parameters (e.g., intractable for standard MCMC methods) (i.e., $|\boldsymbol{\theta}|$ is large)

Rough idea:

- Learn approximate posterior

- Efficiently generate samples from the posterior

By year

- ICML 2015: Bayes by Backprop: factored Gaussian prior over parameters; finding approximate posterior by optimizing evidence lower bound using SGD

does dropout induce more bias

- ICML 2016: MC Dropout: similar to ensemble? average across dropout

- NeurIPS 2017: Deep Ensembles: retrain model multiple times to find different SGD solutions

- UAI 2018: Subspace inference: approximate posterior in lower dimensional space

- NeurIPS 2019: Stochastic Weighted Average (Gaussian): model SGD iterates

- 11, 14, 20: Stochastic MCMC

few-shot context