CSC 2541: Neural Net Training Dynamics

Lecture 8 - Implicit Regularization and Bayesian Inference

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University of Toronto, Winter 2021

Today

- Last week: the curse of stochasticity (slower convergence)
- This week: the blesssing of stochasticity (implicit regularization)
- Agenda
  - "Sharp and flat minima"
  - Disentangling implicit and explicit regularization
  - Explicit Bayesian inference
  - Implicit Bayesian inference
- This lecture will have lots of ideas that connect to each other, but no unifying message. This general topic is still messy!

Explicit and Implicit Regularization

How I'll use the terms in this course:

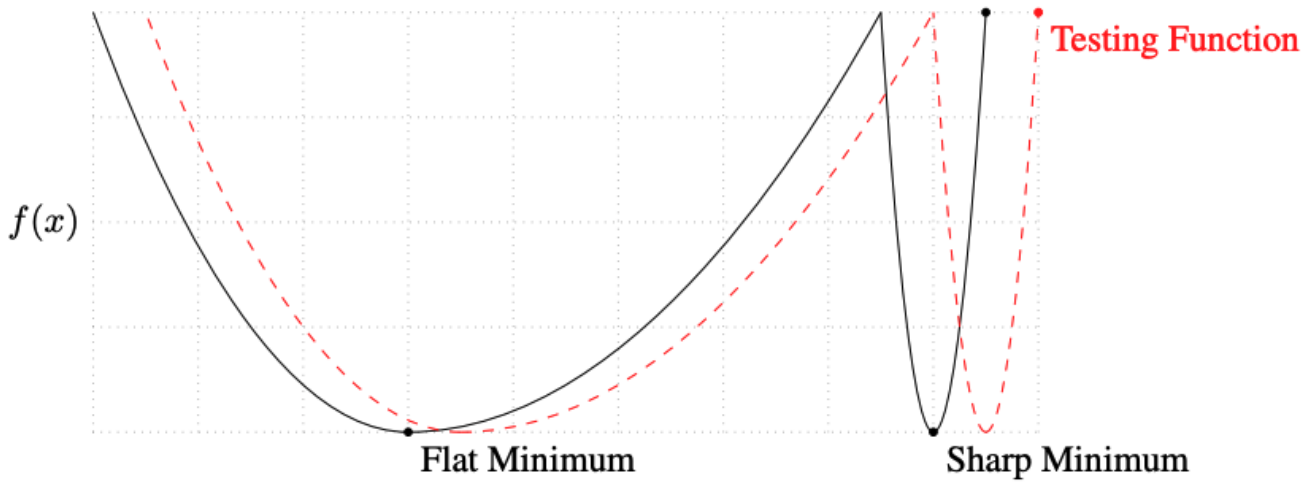
- Explicit regularization imposes an explicit penalty on the parameters of the model (typically some measure of complexity or sensitivity)
  - ℓ_2 regularization (traditional view — weight decay is more complicated, as we saw in Lecture 5)
  - dropout
  - batch norm (noisy statistics)
  - variational Bayes / MDL
- Implicit regularization occurs when the dynamics of training lead to certain minima rather than others
  - minimum norm solutions in linear regression (Lecture 1)
  - NTK dynamics (Lecture 6)
  - effects of gradient noise (still poorly understood)

Sharp and Flat Minima

Sharp and Flat Minima

Keskar et al., 2017. "On large batch training for machine learning: Generalization gap and sharp minima"

- Common observation: training with larger batch sizes often leads to worse test error, even if the model can fit all the training data
- **Claims:**
  - Training with larger batches leads to sharper minima
    - **Caution:** not necessarily "local minima". Could be a continuous manifold of minimizers.
  - Sharper minima generalize worse
- Sharpness quantified using the largest eigenvalues of $\mathbf{H}$

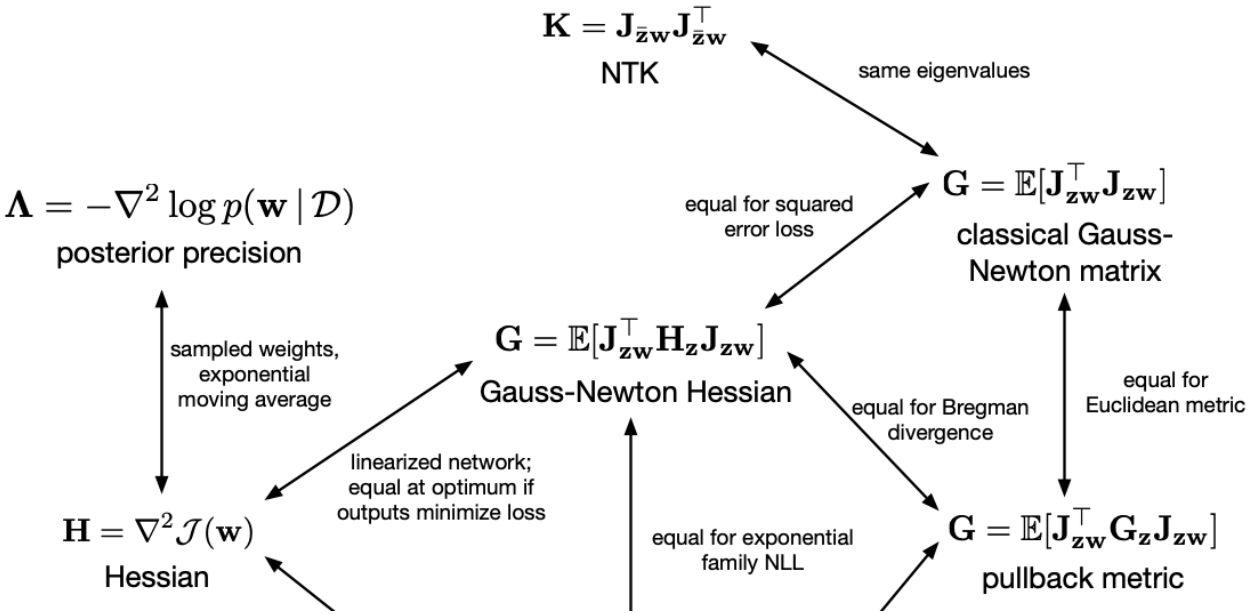


Sharp and Flat Minima

- The idea of sharp and flat minima is intuitive, but it's notoriously hard to fit everything together rigorously
- Dinh et al., 2017. "Sharp minima can generalize for deep nets"
  - We can easily reparameterize the network to an equivalent one with larger or smaller $\mathbf{H}$, so the size of $\mathbf{H}$ can't explain generalization
  - Note that some notions of sharpness don't have this problem
- Shallue et al., 2018. "Measuring the effects of data parallelism on neural network training"
  - Their experiments considered validation loss for a wide variety of tasks and architectures, and they never saw any degradation from large batches
  - They identify 2 frequent confounds in the literature
    - Batch norm creates an *explicit* regularizer which is stronger for smaller batch sizes
    - Some papers fix the number of *epochs*, so models with larger batches were trained for fewer iterations

Sharp and Flat Minima

- Another complication: $\mathbf{H}$ is related to lots of other matrices, so any apparent correlation between $\mathbf{H}$ and generalization might mean the *other* matrix explains generalization



- **Speculation:** the largest eigenvalue of $\mathbf{G} = \mathbb{E}[\mathbf{J}^\top \mathbf{J}]$ is the largest singular value of $\mathbf{J}$.
  - Smaller $\|\mathbf{J}\|_2$ implies less sensitivity to input perturbations (also consider adversarial robustness)
  - Bounded $\|\mathbf{J}\|_2$ implies a Lipschitz function, which was used in classical generalization bounds

Dropout

Dropout

- For a network to overfit, its computations need to be really precise. This suggests regularizing them by injecting noise into the computations, a strategy known as stochastic regularization.
- Dropout is a stochastic regularizer which randomly deactivates a subset of the units (i.e. sets their activations to zero).

$$h_i = \begin{cases} \phi(z_i) & \text{with probability } 1-\rho \\ 0 & \text{with probability } \rho, \end{cases}$$

where ρ is a hyperparameter.

- Equivalently,

$$h_i = m_i \cdot \phi(z_i),$$

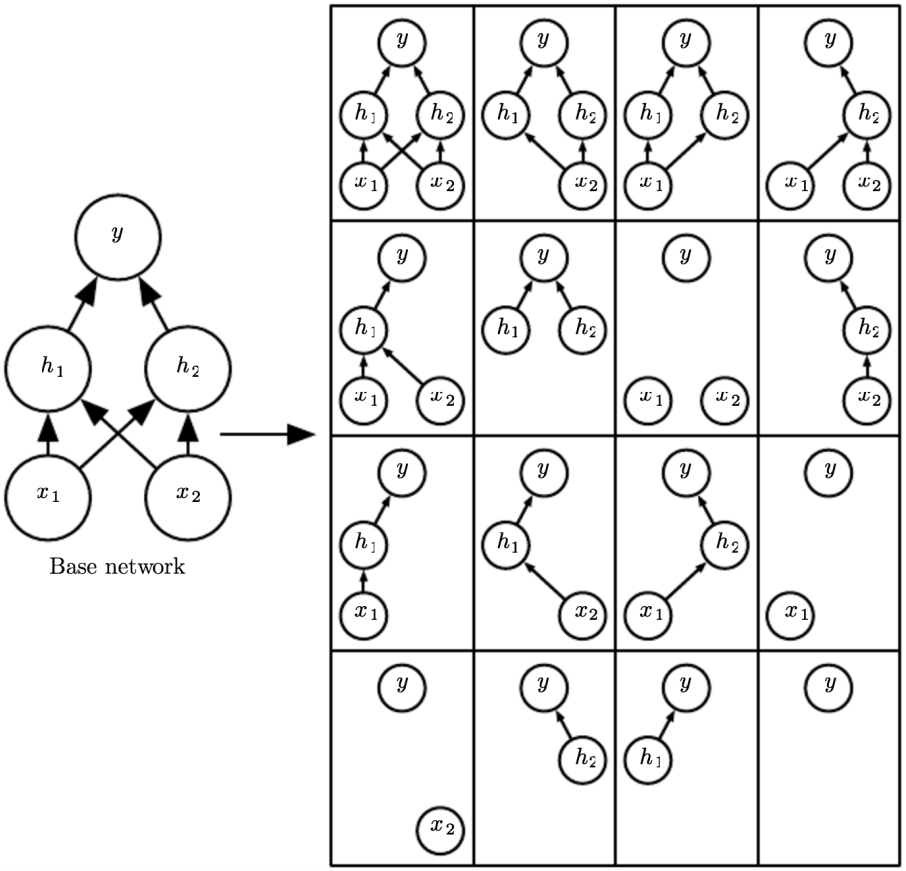
where m_i is a Bernoulli random variable, independent for each hidden unit.

- Backprop rule:

$$\overline{z_i} = \overline{h_i} \cdot m_i \cdot \phi'(z_i)$$

Dropout

- Dropout can be seen as training an ensemble of 2^D different architectures with shared weights (where D is the number of units):



— Goodfellow et al., *Deep Learning*

Dropout

Dropout at test time:

- Most principled thing to do: run the network lots of times independently with different dropout masks, and average the predictions.
  - Individual predictions are stochastic and may have high variance, but the averaging fixes this.
- In practice: don't do dropout at test time, but multiply the weights by $1 - \rho$
  - Since the weights are on $1 - \rho$ fraction of the time, this matches their expectation.

Dropout

- Dropout is traditionally viewed as an explicit regularizer. If the cost is the expectation with respect to the dropout mask, then:

$$\mathcal{J}_{\text{reg}}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \mathcal{R}(\mathbf{w})$$
$$\mathcal{J}(\mathbf{w}) = \mathbb{E}_{\mathbf{x},\mathbf{t}}[\mathcal{L}(\mathbf{t}, f(\mathbf{x}, \mathbf{w}))]$$
$$\mathcal{R}(\mathbf{w}) = \mathbb{E}_{\mathbf{x},\mathbf{t}}\left[\mathbb{E}_{\mathbf{m}}[\mathcal{L}(\mathbf{t}, f_{\text{drop}}(\mathbf{x}, \mathbf{w}; \mathbf{m}))] - \mathcal{L}(\mathbf{t}, f(\mathbf{x}, \mathbf{w}))\right]$$

- Here, $\mathbf{w}$ represents the "test time weights" (i.e. after multiplying by $1 - \rho$)
- $\mathcal{R}$ is the amount the training predictions were hurt as a result of the stochasticity
- The original dropout paper (Srivastava et al., 2014) derived $\mathcal{R}$ explicitly for linear regression. It's equivalent to an ℓ_2 penalty reweighted by the feature variance.

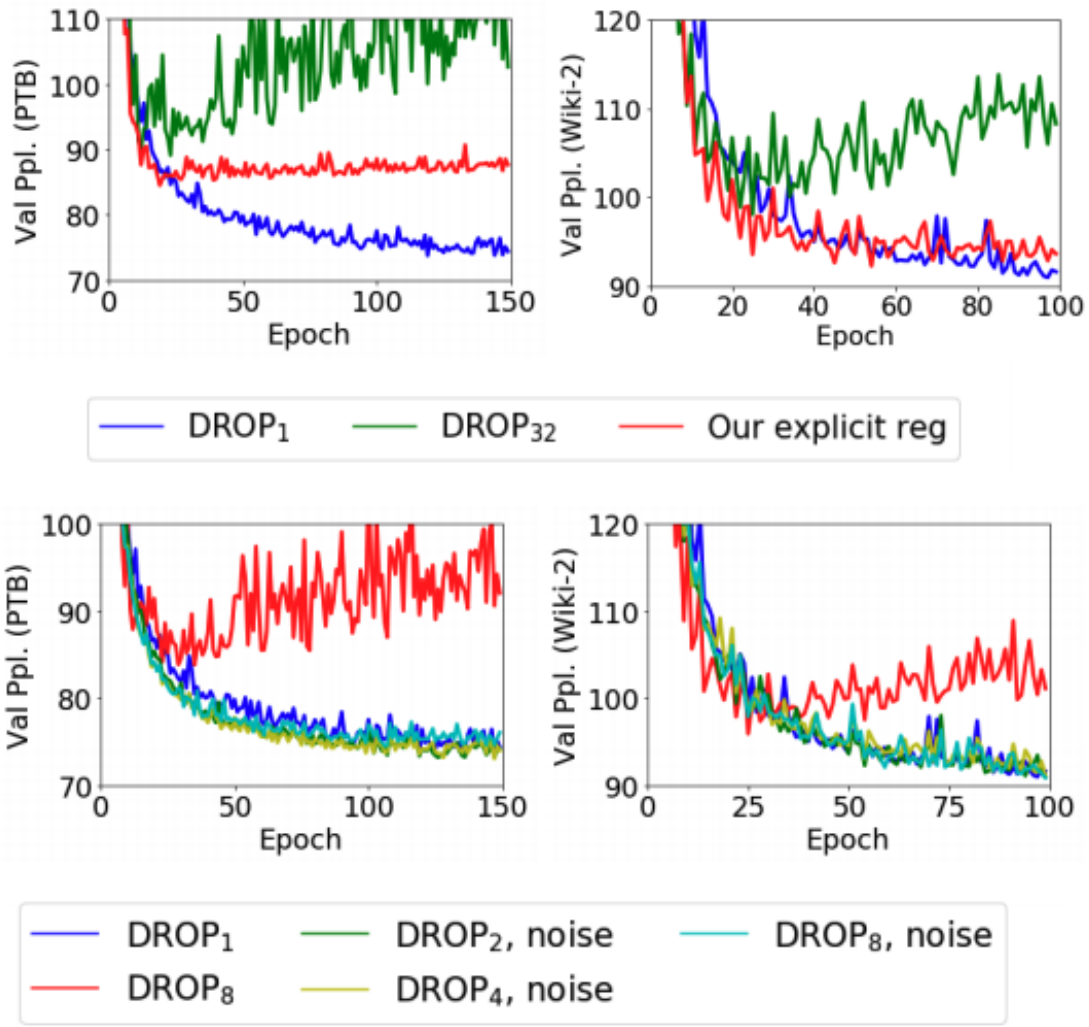
Dropout

Wei, Kakade, and Ma, 2020, "The implicit and explicit regularization effects of dropout"

- Since dropout samples the mask stochastically, it adds noise to the gradients
- This noise might have an implicit regularization effect, in addition to the explicit regularizer
- Disentangling the implicit and explicit effects
  - Sample K independent dropout masks for each gradient computation
  - This is still doing SGD on the same explicit objective
  - $K = 1$ is ordinary dropout training, and the dropout-induced gradient noise decays as $1/K$. So the implicit regularization effect vanishes as $K \to \infty$
- A further "knock-in" manipulation: compute the amount of gradient noise that was removed, inject it back in, and see if the algorithm behaves like ordinary dropout

Dropout

Wei et al., 2020



Variational Bayes and MDL

BNN Posterior Inference

- The cheapest and simplest way of training Bayesian neural nets is probably maximum a-posteriori (MAP) inference, which simply maximizes the posterior probability:

$$\begin{aligned}\mathbf{w}_{\text{MAP}} &= \arg\max_{\mathbf{w}} \log p(\mathbf{w} \mid \mathcal{D}) \\ &= \arg\max_{\mathbf{w}} \log p(\mathbf{w}, \mathcal{D}) \\ &= \arg\max_{\mathbf{w}} \overbrace{\sum_i \log p(\mathbf{t}^{(i)} \mid \mathbf{w}, \mathbf{x}^{(i)})}^{\text{likelihood}} + \overbrace{\log p(\mathbf{w})}^{\text{prior}}\end{aligned}$$

- With an i.i.d. Gaussian prior on the weights, the prior term is equivalent to ℓ_2 regularization (weight decay)
- To get uncertainty estimates, we can use the Laplace approximation to the posterior, which takes the second-order Taylor approximation to the log-likelihood around $\mathbf{w}_{\text{MAP}}$:

$$p(\mathbf{w} \mid \mathcal{D}) \approx \mathcal{N}(\mathbf{w}; \mathbf{w}_{\text{MAP}}, \bar{\mathbf{H}}^{-1})$$
$$\bar{\mathbf{H}} = N\mathbf{H} = -\nabla^2 \log p(\mathcal{D} \mid \mathbf{w})$$

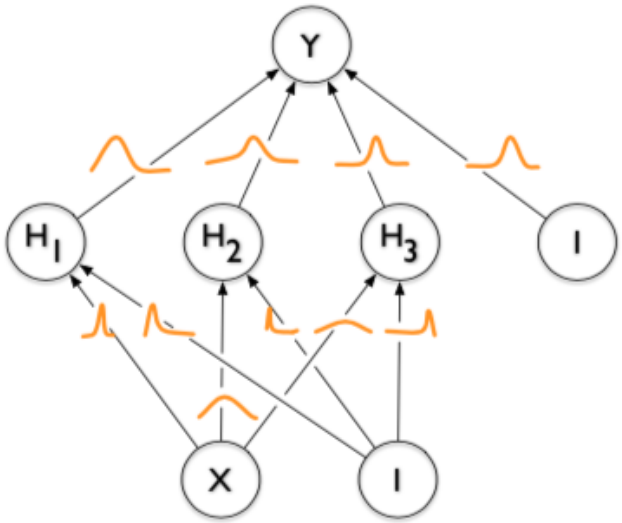
- This is like the Hessian of the training cost, up to a factor of N

Variational BNNs

- The problem with the Laplace approximation is that uncertainty isn't considered until training is finished
- Variational Bayes is a more accurate posterior inference method which accounts for uncertainty during training
- We approximate a complicated posterior distribution with a simpler variational approximation. E.g., assume a Gaussian posterior with diagonal covariance (i.e. fully factorized Gaussian):

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$
$$= \prod_{j=1}^{D} \mathcal{N}(\theta_j; \mu_j, \sigma_j)$$

- This means each weight of the network has its own mean and variance.



— Blundell et al., Weight uncertainty for neural networks

Posterior Inference: Variational Bayes

- The marginal likelihood is the probability of the observed data (targets given inputs), with all possible weights marginalized out:

$$\begin{aligned} p(\mathcal{D}) &= \int p(\mathbf{w})\, p(\mathcal{D} \mid \mathbf{w})\, \mathrm{d}\mathbf{w} \\ &= \int p(\mathbf{w})\, p(\{t^{(i)}\} \mid \{\mathbf{x}^{(i)}\}, \mathbf{w})\, \mathrm{d}\mathbf{w}. \end{aligned}$$

- Analogously to VAEs, we define a variational lower bound:

$$\log p(\mathcal{D}) \geq \mathcal{F}(q) = \mathbb{E}_{q(\mathbf{w})}[\log p(\mathcal{D} \mid \mathbf{w})] - \mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w}))$$

- Unlike with VAEs, $p(\mathcal{D})$ is fixed, and we are *only* maximizing $\mathcal{F}(q)$ with respect to the variational posterior q (i.e. a mean and standard deviation for each weight).

Posterior Inference: Variational Bayes

$$\log p(\mathcal{D}) \geq \mathcal{F}(q) = \mathbb{E}_{q(\mathbf{w})}[\log p(\mathcal{D} \mid \mathbf{w})] - \mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w}))$$

- Same as for VAEs, the gap equals the KL divergence from the true posterior:

$$\mathcal{F}(q) = \log p(\mathcal{D}) - \mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w} \mid \mathcal{D})).$$

  Hence, maximizing $\mathcal{F}(q)$ is equivalent to approximating the posterior.

Posterior Inference: Variational Bayes

- Likelihood term:

$$\mathbb{E}_{q(\mathbf{w})}[\log p(\mathcal{D} \mid \mathbf{w})] = \mathbb{E}_{q(\mathbf{w})}\left[\sum_{i=1}^{N} \log p(t^{(i)} \mid \mathbf{x}^{(i)}, \mathbf{w})\right]$$

  This is just the usual likelihood term (e.g. minus classification cross-entropy), except that $\mathbf{w}$ is sampled from q.

- KL term:

$$\mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w}))$$

  This term encourages q to match the prior, i.e. each dimension to be close to $\mathcal{N}(0, \eta^{1/2})$.

- Without the KL term, the optimal q would be a point mass on $\mathbf{w}_{\mathrm{ML}}$, the maximum likelihood weights.
  - Hence, the KL term encourages q to be more spread out (i.e. more stochasticity in the weights).

Posterior Inference: Variational Bayes

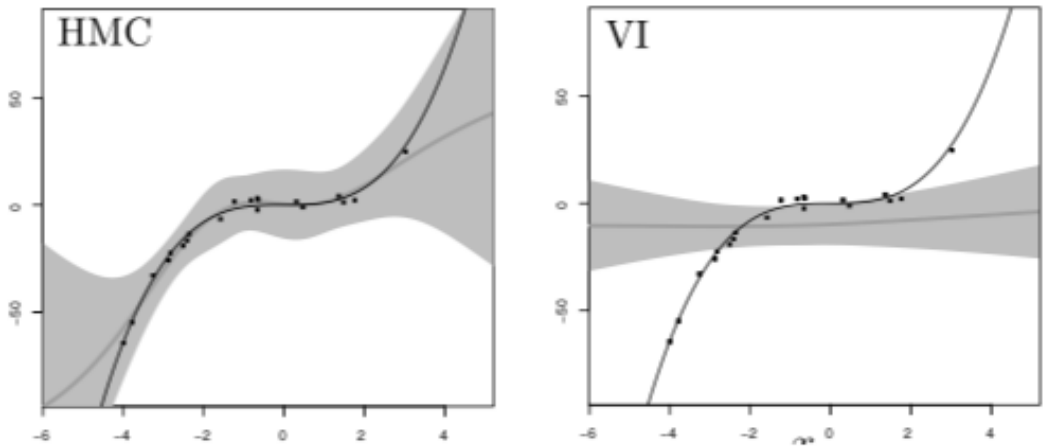
- We can train a variational BNN using the same reparameterization trick as from VAEs.

$$\theta_j = \mu_j + \sigma_j \epsilon_j,$$

  where $\epsilon_j \sim \mathcal{N}(0, 1)$.
- Then the ϵ_j are sampled at the beginning, independent of the μ_j, σ_j, so we have a deterministic computation graph we can do backprop on.
- If all the σ_j are 0, then $\theta_j = \mu_j$, and this reduces to ordinary backprop for a deterministic neural net.
- Hence, variational inference injects stochasticity into the computations. This acts like a regularizer, just like with dropout.
  - The difference is that it's stochastic activations, rather than stochastic weights.
  - See Kingma et al., "Variational dropout and the local reparameterization trick", for the precise connections between variational BNNs and dropout.

Posterior Inference: Variational Bayes

- Bad news: variational BNNs aren't a good match to Bayesian posterior uncertainty.
- The BNN posterior distribution is complicated and high dimensional, and it's really hard to approximate it accurately with fully factorized Gaussians.

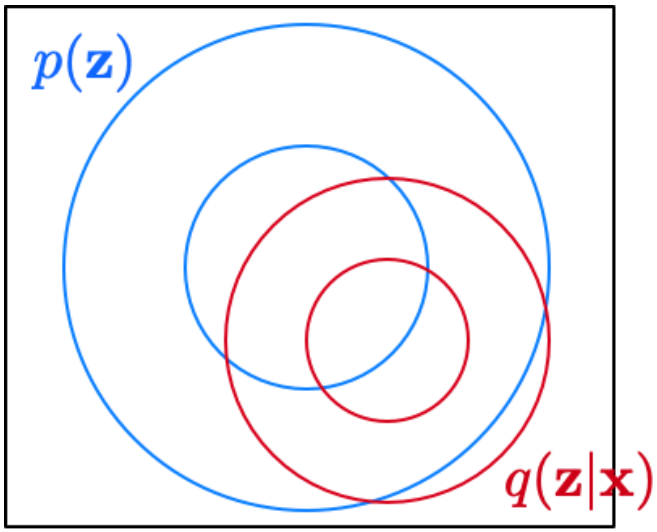


— Hernandez-Lobato et al., Probabilistic Backpropagation

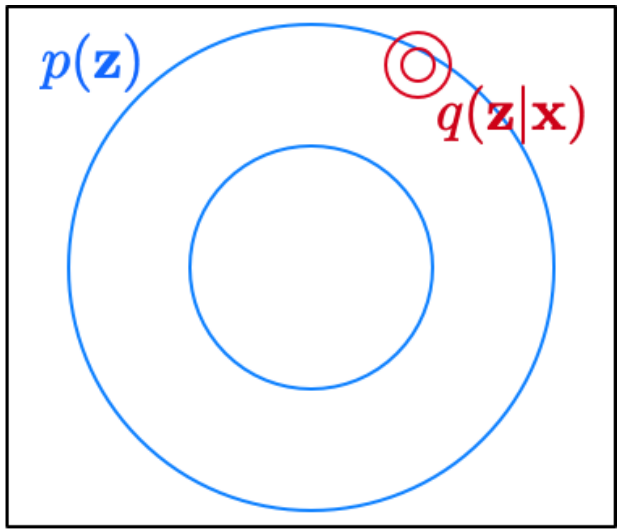
- So what are variational BNNs good for?

Description Length Regularization

- What variational BNNs are really doing is regularizing the description length of the weights.
- Intuition: the more concentrated the posterior is, the more bits it requires to describe the location of the weights to adequate precision.
- A more concentrated q generally implies a higher KL from the prior.



small KL divergence,
small description length



large KL divergence,
large description length

Description Length Regularization

- The KL term $\mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w}))$ can be interpreted as the number of bits required to describe $\mathbf{w}$ to adequate precision.
  - This can be made precise using the bits-back argument. This is beyond the scope of the class, but see here for a great explanation:

    `https://youtu.be/0IoLKnAg6-s`
- A classic result from computational learning theory ("Occam's Razor") bounded the generalization error a learning algorithm that selected from K possible hypotheses.
  - It requires $\log K$ bits to specify the hypothesis.
  - PAC-Bayes gives analogous bounds for the generalization error of variational BNNs, where $\mathrm{D}_{\mathrm{KL}}(q(\mathbf{w}) \,\|\, p(\mathbf{w}))$ behaves analogously to $\log K$.
    - This is one of the few ways we have to prove that neural nets generalize.
    - See Dziugaite et al., "Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data".

Uses of BNNs

- **Guiding exploration**
  - **Bayesian optimization:** Snoek et al., 2015, "Scalable Bayesian optimization using deep neural networks"
  - **Curriculum learning:** Graves et al., 2017, "Automated curriculum learning for neural networks"
  - **Intrinsic motivation in reinforcement learning:** Houthooft et al., 2016, "Variational information maximizing exploration"
- **Network compression:** Louizos et al., 2017, "Bayesian compression for deep learning"
- **Predicting generalization:** Jiang et al., 2019, "Fantastic generalization measures and where to find them": measures based on PAC-Bayesian/MDL ideas were the most predictive of generalization
- Lots more references in CSC2541, "Scalable and Flexible Models of Uncertainty"
  - `https://csc2541-f17.github.io/`

Variational Bayes and Curvature

Variational Bayes and Curvature

- We introduced the Laplace approximation, where uncertainty comes directly from the curvature:

$$p(\mathbf{w} \mid \mathcal{D}) \approx \mathcal{N}(\mathbf{w}; \mathbf{w}_{\text{MAP}}, \mathbf{H}^{-1})$$

$$\mathbf{H} = -\nabla^2 \log p(\mathcal{D} \mid \mathbf{w})$$

- But the Laplace approximation is often a very poor model of uncertainty. Variational Bayes is often better (at least for capturing a single mode).

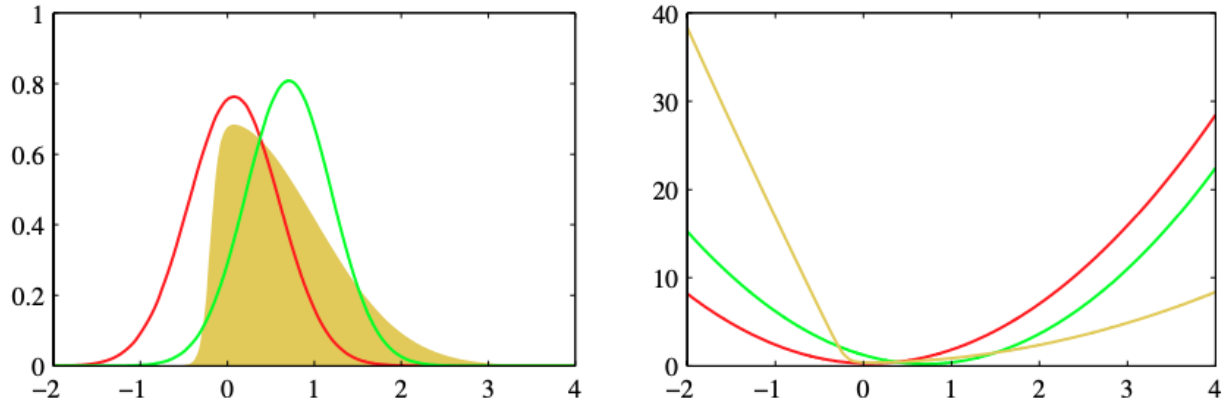


Figure 10.1 Illustration of the variational approximation for the example considered earlier in Figure 4.14. The left-hand plot shows the original distribution (yellow) along with the Laplace (red) and variational (green) approximations, and the right-hand plot shows the negative logarithms of the corresponding curves.

(Bishop, PRML)

Noisy Natural Gradient

Zhang et al., 2018, "Noisy natural gradient as variational inference"

- Consider a proximal objective for variational Bayes, over a family of probability distributions (say, multivariate Gaussians):

$$\min_{\boldsymbol{\phi}} -\mathcal{F}(q_{\boldsymbol{\phi}}) + \mathrm{D}_{\mathrm{KL}}(q_{\boldsymbol{\phi}} \| q_{\boldsymbol{\phi}_0})$$

- As in Lecture 3, taking the infinitesimal limit gives the natural gradient update, called Natural Gradient for Variational Inference (NGVI):

$$\boldsymbol{\phi}^{(k+1)} = \boldsymbol{\phi}^{(k)} + \alpha \mathbf{F}_{\boldsymbol{\phi}}^{-1} \nabla \mathcal{F}(q_{\boldsymbol{\phi}^{(k)}})$$

- **Note:** $\boldsymbol{\phi}$ are the variational parameters, not the network weights. $\mathbf{F}_{\boldsymbol{\phi}}$ is the Fisher information matrix for the multivariate Gaussian distribution, not the pullback metric for the network.

Noisy Natural Gradient

(Zhang et al., 2018)

- Parameterize the multivariate Gaussian by mean $\boldsymbol{\mu}$ and precision matrix $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$
- Stochastic NGVI update rule (derivable using the exponential family identities from NNTD Chapter 3):
  - Sample the network weights $\mathbf{w} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$
  - Update the variational parameters

$$\boldsymbol{\mu} \leftarrow \boldsymbol{\mu} + \alpha \boldsymbol{\Lambda}^{-1} \left[\nabla \log p(y \,|\, \mathbf{x}, \mathbf{w}) - \frac{\lambda}{N\eta} \mathbf{w} \right]$$

$$\boldsymbol{\Lambda} \leftarrow \left(1 - \frac{\lambda\beta}{N}\right) \boldsymbol{\Lambda} + \beta \left[-\nabla^2_{\mathbf{w}} \log p(y \,|\, \mathbf{x}, \mathbf{w}) + \frac{\lambda}{N\eta} \mathbf{I} \right]$$

- Update for $\boldsymbol{\Lambda}$: exponential moving average of the Hessian (justifies the use of moving averages in second-order optimization!)
- Update for $\boldsymbol{\mu}$: stochastic Newton update to the weights

Noisy Natural Gradient

(Zhang et al., 2018)

- All roads lead to $\mathbf{H}$!
- In practice, we approximate $\mathbf{H}$ with $\mathbf{G}$ so that it's PSD
- Imposing structure on $\mathbf{\Lambda}$ corresponds to imposing structure on the variational posterior
  - Diagonal $\mathbf{\Lambda} \Leftrightarrow$ factorial (independent) Gaussian posterior (noisy Adam)
  - K-FAC approximation for $\mathbf{\Lambda} \Leftrightarrow$ matrix variate Gaussian posterior (noisy K-FAC)
    - Unlike the diagonal approximation, this can capture correlations between different weights. So it's not just about optimization!

Variational Bayes and Flatness

- Recall: sharp/flat minima claims
  - Gradient noise implicitly regularizes towards flat minima
  - Flat minima generalize better
  - Obvious sharpness measures based on $\mathbf{H}$ aren't invariant to reparameterization
- Variational Bayes
  - Adds noise to the weights
  - KL term encourages flatness (high posterior volume)
  - Strong generalization bounds from PAC-Bayes
  - KL term is invariant to reparameterization
- Is this the right way to think about flatness? I don't know
- Is ordinary SGD training doing anything Bayesian?

SGD and Implicit Variatonal Bayes

SGD and Implicit Variational Bayes

Welling and Teh, 2011, "Bayesian learning via stochastic gradient Langevin dynamics"

- Hamiltonian Monte Carlo (HMC), as pioneered by Neal (1993), is still the gold-standard inference method for BNNs. But it doesn't scale to large datasets because it requires full batch computations.
- Stochastic gradient Langevin dynamics (SGLD) is a scalable alternative which uses stochastic gradients.
- Update rule: compute the mini-batch gradient and add noise

$$\mathbf{w}^{(k)} = \mathbf{w}^{(k-1)} - \alpha \mathbf{g}^{(k)} + \eta^{(k)}$$
$$\eta^{(k)} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{I}),$$

  where $\mathbf{g}$ is a stochastic estimate of the log-likelihood gradient
- As $\alpha \to 0$, $\eta^{(k)}$ dominates the mini-batch noise, and the stationary distribution approaches the true posterior

SGD and Implicit Variational Bayes

- In practice, α has to be very small for the gradient noise to be negligible
- Is ordinary SGD doing something like SGLD?
  - Only if the gradient noise has spherical covariance (unlikely!)

SGD and Implicit Variational Bayes

Mandt, Hoffman, and Blei, 2017, "Stochastic gradient descent as approximate Bayesian inference"

- Analyzes SGD as an Ornstein-Uhlenbeck process, essentially a continuous analogue of the NQM
- Quadratic cost function $\mathcal{J}(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathbf{H}\mathbf{w}$, gradient $g(t) = \mathbf{H}\mathbf{w}(t)$, gradient covariance $\mathbf{C} = \mathbf{A}\mathbf{A}^\top$
- Bayesian posterior: $\mathcal{N}(0, \frac{1}{N}\mathbf{H}^{-1})$
- Stochastic differential equation for the dynamics:

$$\mathrm{d}\mathbf{w}(t) = -\alpha g(t)\,\mathrm{d}t + \frac{\alpha}{\sqrt{B}}\mathbf{A}\,\mathrm{d}W(t)$$

  where W is a white noise process
- Stationary distribution is $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$, where $\mathbf{\Sigma}$ satisfies

$$\mathbf{\Sigma}\mathbf{H} + \mathbf{H}\mathbf{\Sigma} = \frac{\alpha}{B}\mathbf{C}$$

SGD and Implicit Variational Bayes

$$\boldsymbol{\Sigma}\mathbf{H} + \mathbf{H}\boldsymbol{\Sigma} = \frac{\alpha}{B}\mathbf{C}$$

(Mandt et al., 2017)

- If $\mathbf{H}$ and $\mathbf{C}$ are codiagonalizable, then is simplifies to:

$$\boldsymbol{\Sigma} = \frac{\alpha}{2B}\mathbf{H}^{-1}\mathbf{C}$$

- If $\mathbf{H} = \mathbf{C}$ (as in Lecture 7), then we get $\boldsymbol{\Sigma} = \frac{\alpha}{2B}\mathbf{I}$. This is not Bayesian! It ignores posterior uncertainty!
- The optimal preconditioner from a Bayesian standpoint is $\mathbf{C}^{-1}$. Preconditioned SGD converges to $\boldsymbol{\Sigma} = \frac{\alpha}{2B}\mathbf{H}^{-1}$.
  - Justifies the use of adaptive gradient methods, sort of (they precondition by $\mathbf{F}_{\text{emp}}^{-1/2}$, and arguably $\mathbf{F}_{\text{emp}} \approx \mathbf{C}$)
  - If $\mathbf{H} = \mathbf{C} = \mathbf{F}$, then natural gradient descent is doing Bayesian inference. (See also Ahn et al., 2012, "Bayesian posterior sampling via stochastic gradient Fisher scoring")

SGD and Implicit Variational Bayes

(Mandt et al., 2017)
Empirical results (note: axis scale not uniform)