MCMC Sampling (wrap-up)

CS772A: Probabilistic Machine Learning

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Example Recap: Gibbs Sampling

- Bayesian linear regression: $p(y_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) = \mathcal{N}(y_n|\boldsymbol{w}^\top \boldsymbol{x}_n, \beta^{-1})$, $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|0, \lambda^{-1}I)$, $p(\lambda) = \text{Gamma}(\lambda|a, b)$, $p(\beta) = \text{Gamma}(\beta|c, d)$. Gibbs sampler for $p(w, \lambda, \beta|\boldsymbol{X}, \boldsymbol{y})$ will be
- Initialize λ, β as $\lambda^{(0)}, \beta^{(0)}$. For iteration $t = 1,2, \dots, T$
  - Generate a random sample of $\boldsymbol{w}$ by sampling from its CP as

$$\boldsymbol{w}^{(t)} \sim \mathcal{N}(\boldsymbol{w}|\boldsymbol{\mu}^{(t-1)}, \boldsymbol{\Sigma}^{(t-1)})$$

where

$$\boldsymbol{\Sigma}^{(t-1)} = \left(\beta^{(t-1)}\boldsymbol{X}^\top\boldsymbol{X} + \lambda^{(t-1)}\right)^{-1}$$

$$\boldsymbol{\mu}^{(t-1)} = \left(\boldsymbol{X}^\top\boldsymbol{X} + \frac{\lambda^{(t-1)}}{\beta^{(t-1)}}\right)^{-1} \boldsymbol{X}^\top\boldsymbol{y}$$

  - Generate a random sample of λ by sampling from its CP as

$$\lambda^{(t)} \sim \text{Gamma}\left(\lambda|a + \frac{D}{2}, b + \frac{\boldsymbol{w}^{(t)^\top}\boldsymbol{w}^{(t)}}{2}\right)$$

  - Generate a random sample of β by sampling from its CP as

$$\beta^{(t)} \sim \text{Gamma}\left(\beta|c + \frac{N}{2}, d + \frac{\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}^{(t)}\|^2}{2}\right)$$

- The posterior's approximation is the set of collected samples

Gibbs Sampling: Some Comments

- One of the most popular MCMC algorithm
- Only needs CPs which can be easily obtained (especially for locally conjugate models).
  - Just look at the joint distribution of data and unknown, write its factorization, and look at only the terms that contain the variable for which you want to compute the CP
- Many variations exist, e.g.,
  - Blocked Gibbs: sample more than one component jointly (sometimes possible)
  - Rao-Blackwellized Gibbs: Can collapse (i.e., integrate out) the unneeded components while sampling. Also called "collapsed" Gibbs sampling
  - MH within Gibbs: If CPs are not easy to sample distributions
- Instead of sampling from CPs, an alternative is to use the mode of the CPs
  - Called the "Iterative Conditional Mode" (ICM) algorithm
  - ICM doesn't give the posterior though – it's more like ALT-OPT to get (approx) MAP estimate

Using MCMC samples to make predictions

- Using the S samples $\boldsymbol{Z}^{(1)}, \boldsymbol{Z}^{(2)}, \dots, \boldsymbol{Z}^{(S)}$, our approx. $p(\boldsymbol{Z}) \approx \frac{1}{S}\sum_{s=1}^{S} \delta_{\boldsymbol{Z}^{(s)}}(\boldsymbol{Z})$
- Any expectation that depends on $p(\boldsymbol{Z})$ can be approximated as

$$\mathbb{E}[f(\boldsymbol{Z})] = \int f(\boldsymbol{Z})p(\boldsymbol{Z})d\boldsymbol{Z} \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{Z}^{(s)})$$

- For Bayesian lin. reg., assuming $\boldsymbol{w}, \beta, \lambda$ to be unknown, the PPD approx. will be

Joint posterior over all unknowns

Thus, in this case, the PPD is a sum of S Gaussians

$$\int p(y_*|\boldsymbol{x}_*, \boldsymbol{w}, \beta)p(\boldsymbol{w}, \beta, \lambda|\boldsymbol{X}, \boldsymbol{y})d\boldsymbol{w}d\beta d\lambda \approx \frac{1}{S}\sum_{s=1}^{S} p\left(y_*\middle|\boldsymbol{x}_*, \boldsymbol{w}^{(s)}, \beta^{(s)}\right)$$

Can also think of it as an ensemble consisting of S members

Sampling based approximation of PPD

Mean and variance of y_* can be computed using sum of Gaussian properties

Mean: $\mathbb{E}[\boldsymbol{w}^\top \boldsymbol{x}_*] \approx \frac{1}{S}\sum_{s=1}^{S} \boldsymbol{w}^{(s)\top} \boldsymbol{x}_*$

Variance: Exercise! Use definition of variance and use Monte-Carlo approximation

- Sampling based approx. for PPD of other models can also be obtained likewise

Using Gradients in MCMC: Langevin Dynamics

- MCMC uses a random-walk based proposal to generate the next sample, e.g.,

And then accept/reject (MH)

$$\theta^{(t)} \sim \mathcal{N}(\theta^{(t-1)}, \eta_t)$$

Will use $\boldsymbol{\theta}$ to denote all the unknowns

Can use automatic differentiation methods for this

- Langevin dynamics: Use (unnormalized) posterior's gradient info in the proposal as

Likelihood

Prior

Move towards the mode of the posterior (like finding MAP est)

$$\theta^* = \theta^{(t-1)} + \frac{\eta_t}{2}\nabla_\theta[\log p(\mathcal{D}|\theta) + \log p(\theta)]\big|_{\theta^{(t-1)}}$$

And then accept/reject (MH)

η set s.t. acceptance rate is around 0.6

$$\theta^{(t)} \sim \mathcal{N}(\theta^*, \eta_t)$$

Same as doing a gradient ascent step towards the posterior and injecting noise $\epsilon_t \sim \mathcal{N}(0, \eta_t)$. Noise ensures we aren't stuck at the MAP solution

Using gradient info in the proposal helps us move faster towards high-prob regions

- Note that the above is equivalent to

Helps also incorporate the curvature info of the posterior

If gradient is pre-multiplied by a preconditioner matrix $M(\theta^{(t-1)})$: Simplified Manifold MALA

And then accept/reject (MH)

$$\boxed{\theta^{(t)} = \theta^{(t-1)} + \frac{\eta_t}{2}\nabla_\theta[\log p(\mathcal{D}|\theta) + \log p(\theta)]\big|_{\theta^{(t-1)}} + \epsilon_t}$$

Known as Metropolis-Adjusted Langevin Algorithm (MALA)

One option to use for $M(\theta^{(t-1)})$ is the second derivative of the unnorm. posterior

- After some waiting period T_0, iterates $\{\theta^{(t)}\}_{t=T_0+1}^{T_0+S}$ are MCMC samples from $p(\theta|\mathcal{D})$

"Bayesian Learning via Stochastic Gradient Langevin Dynamics" by Welling and Teh (2011)

Langevin Dynamics: A Closer Look

- Is generating MCMC samples really as easy as computing MAP?
- Recall the form of Langevin Dynamics updates

And then accept/reject (MH)

$$\boxed{\theta^{(t)} = \theta^{(t-1)} + \frac{\eta_t}{2}\nabla_\theta[\log p(\mathcal{D}|\theta) + \log p(\theta)]\Big|_{\theta^{(t-1)}} + \epsilon_t}$$

Same as our target posterior

- Equivalent to discretization of an SDE with equilibrium distribution $\propto \exp(\log p(\mathcal{D}, \theta))$

Above update is its discretiization

Note that this is continuous time

$$d\theta_t = -\nabla L(\theta_t)dt + \sqrt{2}dB_t$$

where $L(\theta_t) = -\log p(\mathcal{D}, \theta_t)$ and $(B_t)_{t\geq 0}$ is Brownian motion s.t. ΔB_t are i.i.d. Gaussian r.v.s

- Discretization introduces some error which is corrected by MH accept/reject step
- Note: As learning rate η_t decreases, discretization error also decreases and rejection rate tends to zero
- Note: Gradient computations require all the data (thus slow)
  - Solution: Use stochastic gradients - Stochastic Gradient Langevin Dynamics (SGLD)

Stochastic Gradient Langevin Dynamics (SGLD)

- An "online" MCMC method: Langevin Dynamics with minibatches to compute gradients
- Given minibatch $\mathcal{D}_t = \{x_{t1}, x_{t2}, \dots, x_{tN_t}\}$, the (stochastic) Langevin dynamics update:

$$\theta^* = \theta^{(t-1)} + \frac{\eta_t}{2}\nabla_\theta\left[\frac{N}{|\mathcal{D}_t|}\sum_{n=1}^{N_t}\log p(\boldsymbol{x}_{tn}|\theta) + \log p(\theta)\right]$$

Almost as fast as doing SGD updates ☺

And then accept/reject (MH)

$$\theta^{(t)} \sim \mathcal{N}(\theta^*, \eta_t)$$

- Choice of the learning rate is important. For convergence, $\eta_t = a(b+t)^{-\kappa}$
  - Switching to constant learning rates (after a few iterations) often helps convergence
- As η_t becomes very very small, acceptance prob. becomes close to 1

No need for accept/reject (MH)

- Recent flurry of work on this topic (see "Bayesian Learning via Stochastic Gradient Langevin Dynamics" by Welling and Teh (2011) and follow-up works)

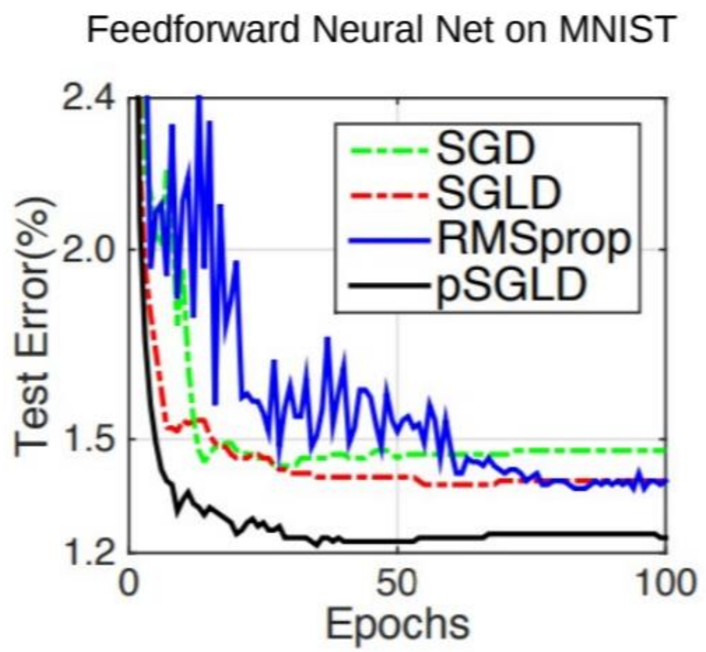
Improvements to SGLD

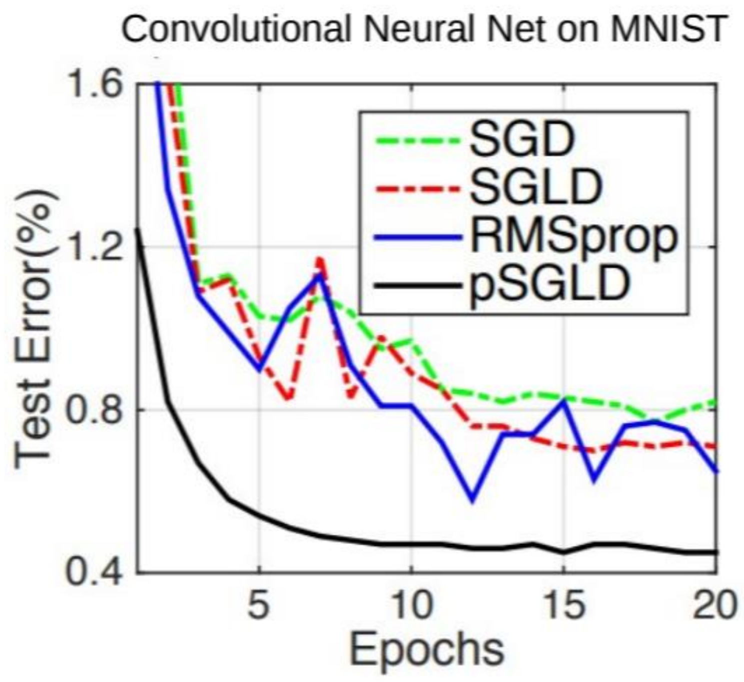
- The basic SGLD, although fairly simple, has many limitations, e.g.
  - Exhibits slow convergence and mixing. Uses same learning rate η_t in all dimensions of θ
  - Doesn't apply to models where θ is constrained (e.g., non-neg or prob. vector)
  - Needs to the model to be differentiable (since it needs $\nabla_\theta \log p(\mathcal{D}, \theta)$)
- A lot of recent work on improving the basic SGLD to handle such limitations
- Introducing the curvature information in the gradients, e.g.,
  - Bayesian Posterior Sampling via Stochastic Gradient Fisher Scoring (Ahn et al, 2012), and Preconditioned Stochastic Gradient Langevin Dynamics for Deep Neural Networks (Li et al, 2016)
  - These methods use a preconditioner matrix in the learning rate to improve convergence
  - This also allows different amounts of updates in different dimensions
- SLGD in Riemannian space to handle constrained variables
  - Stoch. Grad. Riemannian Langevin Dynamics on the Probability Simplex (Patterson and Teh, 2013)

Based on reparametrizing the constrained variables to make them unconstrainted

Applications of SGLD

- Popular for Bayesian neural networks and other complex Bayesian models
- Reason: SGLD = backprop based updates + Gaussian noise





(Figure: Preconditioned Stochastic Gradient Langevin Dynamics for Deep Neural Networks (Li et al, 2016))

Other Recent "SGD-inspired" Sampling Algorithms

- Run SGD and use SGD iterates $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_T$ to construct a Gaussian approximation
- Recently Maddox et al (2019) proposed an idea using stochastic weight avging (SWA)

$$\theta_{SWA} = \frac{1}{T}\sum_{t=1}^{T}\theta_t$$

$$\overline{\theta^2} = \frac{1}{T}\sum_{t=1}^{T}\theta_t^2, \quad \Sigma_{\text{diag}} = \text{diag}(\overline{\theta^2} - \theta_{SWA}^2)$$

$$p(\theta|\mathcal{D}) \approx \mathcal{N}(\theta_{SWA}, \Sigma_{\text{diag}})$$

Approach known as SWA-Gaussian (SWAG)

- If we want full cov., we can use a low-rank approx. of $\boldsymbol{\Sigma}$ (see Maddox et al for details)
- Reason it works: SGD is asymptotically Normal under certain conditions
- For a more detailed theory of SGD and MCMC, may also refer to this very nice paper: Stochastic Gradient Descent as Approximate Bayesian Inference (Mandt et al, 2017)
- Such algos can give not too accurate but very fast posterior approx for complex models

A Simple Baseline for Bayesian Uncertainty in Deep Learning, Maddox et al (2019)

Hamiltonian/Hybrid Monte Carlo (HMC)

- HMC (Neal, 1996) is an "auxiliary variable sampler" and incorporates gradient info
- Uses the idea of simulating a Hamiltonian Dynamics of a physical system
- Consider the target posterior $p(\theta|\mathcal{D}) \propto \exp(-U(\theta))$
- Think of $\boldsymbol{\theta}$ as "position" then $U(\theta) = -\log p(\mathcal{D}|\theta)p(\theta)$ is like "potential energy"
- Let's introduce an auxiliary variable - the momentum $\boldsymbol{r}$ of the system
- Can now define a joint distribution over the position and momentum as

$$p(\theta, \boldsymbol{r}|\mathcal{D}) \propto \exp\left(-U(\theta) - \frac{1}{2}\boldsymbol{r}^\top M^{-1}\boldsymbol{r}\right) \propto p(\theta|\mathcal{D})p(\boldsymbol{r})$$

- The total energy (potential + kinetic) or the Hamiltonian of the system

Constant w.r.t. time

$$H(\theta, \boldsymbol{r}) = U(\theta) - \frac{1}{2}\boldsymbol{r}^\top M^{-1}\boldsymbol{r} = U(\theta) + K(\boldsymbol{r})$$

- Given a sample $(\theta, \boldsymbol{r})$ from $p(\theta, \boldsymbol{r})$, ignoring $\boldsymbol{r}$, $\boldsymbol{\theta}$ will be a sample from $p(\theta|\mathcal{D})$

Generating Samples in HMC

- Given an initial $(\boldsymbol{\theta}, \boldsymbol{r})$, Hamiltonian Dynamics defines how $(\boldsymbol{\theta}, \boldsymbol{r})$ changes w.r.t. time t

$$\frac{\partial \theta}{\partial t} = \frac{\partial H}{\partial \boldsymbol{r}} = \frac{\partial K}{\partial \boldsymbol{r}}$$
$$\frac{\partial \boldsymbol{r}}{\partial t} = -\frac{\partial H}{\partial \theta} = -\frac{\partial U}{\partial \theta}$$

$$\left(H(\theta, \boldsymbol{r}) = U(\theta) + \tfrac{1}{2}\boldsymbol{r}^\top M^{-1}\boldsymbol{r} = U(\theta) + K(\boldsymbol{r}) \right)$$

- We can use these equations to update $(\boldsymbol{\theta}, \boldsymbol{r}) \rightarrow (\boldsymbol{\theta}^*, \boldsymbol{r}^*)$ by discretizing time

Reason: Getting analytical solutions for the above requires integrals which is in general intractable

- For $s = 1{:}S$, sample as follows
  - Initialize $\theta_0 = \theta^{(s-1)}$, $\boldsymbol{r}_* \sim \mathcal{N}(0, \mathbf{I})$ and $\boldsymbol{r}_0 = \boldsymbol{r}_* - \frac{\rho}{2}\frac{\partial U}{\partial \theta}|_{\theta_0}$
  - Do L "leapfrog" steps with learning rates $\rho_\ell = \rho$ for $\ell < L$ and $\rho_L = \rho/2$
    - For $\ell = 1{:}L$

$$\theta_\ell = \theta_{\ell-1} + \rho \frac{\partial K}{\partial \boldsymbol{r}}|_{\boldsymbol{r}_{\ell-1}}$$
$$\boldsymbol{r}_\ell = \boldsymbol{r}_{\ell-1} - \rho_\ell \frac{\partial U}{\partial \theta}|_{\theta_\ell}$$

L usually set to 5 and learning rate tuned to make acceptance rate around 90%

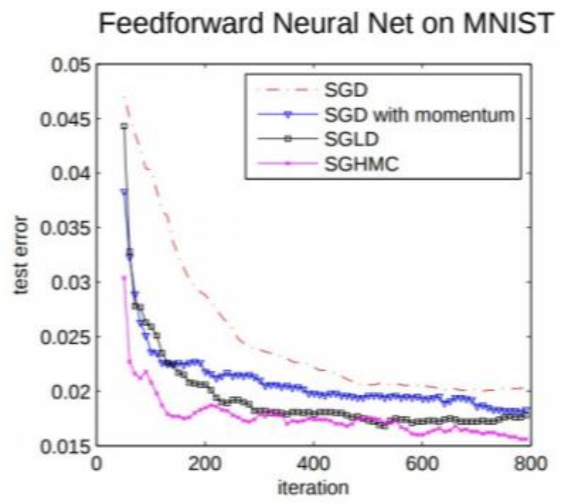
  - Perform MH accept/reject test on $(\boldsymbol{\theta}_L, \boldsymbol{r}_L)$. If accepted $\boldsymbol{\theta}^{(s)} = \boldsymbol{\theta}_L$

A single sample generated by taking L steps

- The momentum forces exploring different regions instead of getting driven to regions where the MAP solution is

HMC in Practice

- HMC typically has very low rejection rate (that too, primarily due to discretization error)
- Performance can be sensitive to L (no. of leapfrog steps) and step-sizes, tuning hard
- A lot of renewed interest in HMC (you may check out NUTS - No U-turn Sampler – doesn't require setting L)
  - Prob. Prog. packages e.g., Tensorflow Prob., Stan, etc, contain implementations of HMC
- Can also do HMC on minibatches (Stochastic Gradient HMC - Chen et al, 2014)
- An illustration: SGHMC vs other methods on MNIST classification (Bayesian neural net)



(Figure: Stochastic Gradient Hamiltonian Monte Carlo (Chen et al, 2014))

Parallel/Distributed MCMC

- Suppose our goal is to compute the posterior of $\theta \in \mathbb{R}^D$ (assuming N is very large)

$$p(\theta|\mathbf{X}) \propto p(\theta)p(\mathbf{X}|\theta) = p(\theta)\prod_{n=1}^{N} p(\mathbf{x}_n|\theta)$$

- Suppose we have J machines with data partitioned as $\mathbf{X} = \{\mathbf{X}^{(j)}\}_{j=1}^{J}$
- Let's assume that the posterior $p(\theta|\mathbf{X})$ factorizes as

$$p(\theta|\mathbf{X}) = \prod_{i=1}^{J} p^{(j)}(\theta|\mathbf{X}^{(j)})$$

- Here $p^{(j)}(\theta|\mathbf{X}^{(j)}) \propto p(\theta)^{1/J} \prod_{\mathbf{x}_n \in \mathbf{X}^{(j)}} p(\mathbf{x}_n|\theta)$ is known as the "subset posterior"
- Assume the j^{th} machine generates T MCMC samples $\{\theta_{j,t}\}_{t=1}^{T}$
- We need a way to combine these subset posteriors using a "consensus"

$$\hat{\theta}_1, \ldots, \hat{\theta}_T = \texttt{CONSENSUSSAMPLES}(\{\theta_{j,1}, \ldots, \theta_{j,T}\}_{j=1}^{J})$$

Parallel/Distributed MCMC

- Many ways to compute the consensus samples. Let's look at two of them
- Approach 1: Weighted Average: $\hat{\theta}_t = \sum_{j=1}^{J} W_j \theta_{j,t}$ where W_j can be learned as follows
  - Assuming Gaussian likelihood and Gaussian prior on θ

$$
\begin{aligned}
\bar{\Sigma}_j &= \text{sample covariance of } \{\theta_{j,1}, \ldots, \theta_{j,T}\} \\
\Sigma &= (\Sigma_0^{-1} + \sum_{j=1}^{J} \bar{\Sigma}_j^{-1})^{-1} \quad (\Sigma_0 \text{ is the prior's covariance}) \\
W_j &= \Sigma(\Sigma_0^{-1}/J + \bar{\Sigma}_j^{-1})
\end{aligned}
$$

These approaches can also be used to make VI parallel/distributed

- Approach 2: Fit J Gaussians, one for each $\{\theta_{j,t}\}_{t=1}^{T}$ and take their product

$$
\begin{aligned}
\bar{\mu}_j &= \text{sample mean of } \{\theta_{j,1}, \ldots, \theta_{j,T}\}, \quad \bar{\Sigma}_j = \text{sample covariance of } \{\theta_{j,1}, \ldots, \theta_{j,T}\} \\
\hat{\Sigma}_J &= (\sum_{j=1}^{J} \bar{\Sigma}_j^{-1})^{-1}, \quad \hat{\mu}_J = \hat{\Sigma}_J(\sum_{j=1}^{J} \bar{\Sigma}_j^{-1}\bar{\mu}_j) \quad (\text{cov and mean of prod. of Gaussians}) \\
\hat{\theta}_t &\sim \mathcal{N}(\hat{\mu}_J, \hat{\Sigma}_J), t = 1, \ldots, T \quad (\text{the final consensus samples})
\end{aligned}
$$

- For detailed proofs and other approaches, may refer to the reference below

Patterns of Scalable Bayesian Inference (Angelino et al, 2016)

Approximate Inference: VI vs Sampling

- VI approximates a posterior distribution $\boldsymbol{p(Z|X)}$ by another distribution $\boldsymbol{q(Z|\phi)}$
- Sampling uses $\boldsymbol{S}$ samples $\boldsymbol{Z^{(1)}, Z^{(2)}, \ldots, Z^{(S)}}$ to approximate $\boldsymbol{p(Z|X)}$
- Sampling can be used within VI (ELBO approx using Monte-Carlo)
- In terms of "comparison" between VI and sampling, a few things to be noted
  - Convergence: VI only has local convergence, sampling (in theory) can give exact posterior
  - Storage: Sampling based approx needs to storage all samples, VI only needs var. params $\boldsymbol{\phi}$
  - Prediction Cost: Sampling always requires Monte-Carlo avging for posterior predictive; with VI, sometimes we can get closed form posterior predictive

PPD if using sampling:

$$p(x_*|X) = \int p(x_*|Z)p(Z|X)dZ \approx \frac{1}{S}\sum_{s=1}^{S} p\left(x_*|Z^{(s)}\right)$$

Closed form if integral is tractable (otherwise Monte Carlo avg still needed for PPD)

PPD if using VI:

$$p(x_*|X) = \int p(x_*|Z)p(Z|X)dZ \approx \int p(x_*|Z)q(Z|\phi)dZ$$

Compressing the S samples into something more compact

- There is some work on "compressing" sampling-based approximations*

*"Compact approximations to Bayesian predictive distributions" by Snelson and Ghaharamani, 2005; and "Bayesian Dark Knowledge" by Korattikara et al, 2015

Inference Methods: Summary

- MLE/MAP: Straightforward for differentiable models (can even use automatic diff.)
- Conjugate models with one "main" parameter: Straightforward posterior updates
- MLE-II/MAP-II: Often useful for estimating the hyperparameters
- EM: If we want to do MLE/MAP for models with latent variables
  - Very general algorithm, can also be made online
  - Used when we want point estimates for some unknowns and posterior over others
  - Can use it for hyperparameter estimation as well
  - Often better than using direct gradient methods
- VI and sampling methods can be used to get full posterior for complex models
  - Quite easy if we have local conjugacy (VI has closed form updates, Gibbs sampler is easy to derive)
  - In other cases, we have general VI with Monte-Carlo gradients, MH sampling
  - MCMC can also make use of gradient info (LD/SGLD)
- For large-scale problems, online/distributed VI/MCMC, or SGD based posterior approx