Introduction to Variational Inference and its Applications

Valentina Staneva

Senior Data Scientist, eScience Institute



Estimating Posteriors: Sampling Techniques

MCMC Methods

- iterative dependent sampling
- sampling in high dimensions is hard
- slow convergence, hard diagnostics

Importance Sampling

- independent samples from approximate distribution
- weight degenaracy
- requires even larger samples

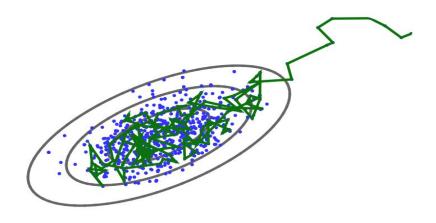


Image Source

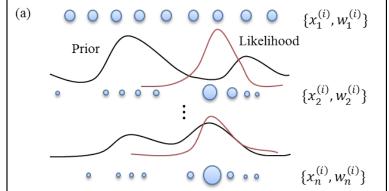


Image Source



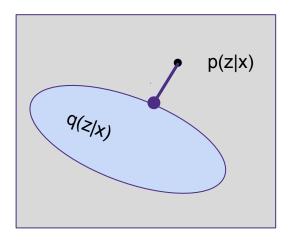
Estimating Posteriors: Optimization Techniques

Expectation-Maximization (EM) Variational Inference

finds only the mode, not the complete distribution

9 Prior Posterior Likelihood MAP Density MLE 95% CI 2 0.2 0.0 0.4 0.6 0.8 1.0

- select a distribution family q(z|x)
- minimize D(q(z|x), p(z|x))





Minimization Loss

Minimize KL divergence

$$D_{KL}(Q(Z|X)||P(Z|X)) = \int_Z Q(Z|X) \log rac{Q(Z|X)}{P(Z|X)} dZ$$

Maximize Evidence Lower Bound (ELBO)

$$\mathcal{L}(Q) = -D_{KL}(Q(Z|X)||P(Z)) + \mathbb{E}_{Q(Z|X)}\log(P(X|Z))$$

Notes

- Sometimes the first term can be computed analytically.
- The second term is obtained by sampling from Q(Z|X)



Stochastic Variational Inference

Stochastic Gradient Descent:

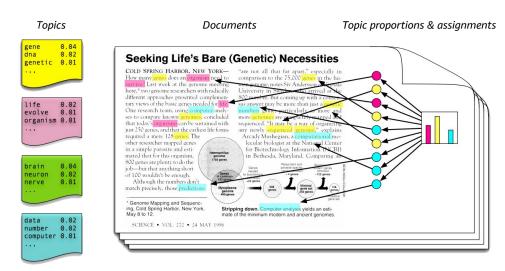
- evaluate gradient at individual (or batch of observations)
- reduce time step to optimize function

Stochastic Variational Inference:

- evaluate gradients at individual (or batch of observations)
- keep time step fixed to achieve stationary distribution



Example: Topic Models



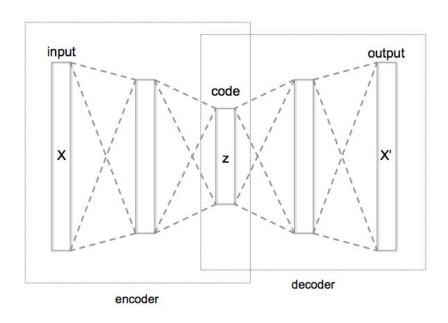
Generate j'th word in document i:

- Choose topic z_i,j ~ Multinomial(θ_i)
- Choose word w_i,j ~ Multinomial($\varphi(z_i)$)
- $\theta \sim \text{Dirichlet}(\alpha)$ (topic distribution per document)
- φ ~ Dirichlet(β) (word distribution of topic)

Sample from a distribution for which the latent variables are decoupled. [Blei'03]



Autoencoders



https://en.wikipedia.org/wiki/Autoencoder#/media/File:Autoencoder_structure.png

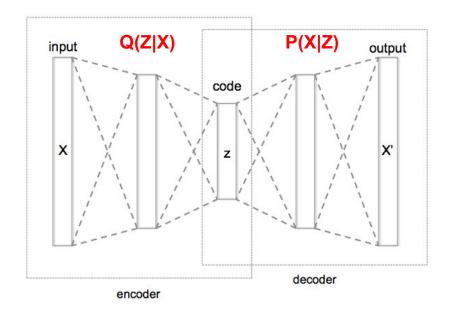
- Minimize reconstruction cost
- Mappings represented by a neural network



Note, when only one hidden layer: X = WZ (matrix decomposition)

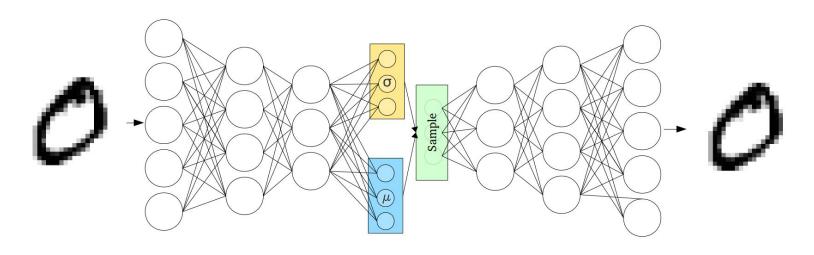
Variational Autoencoders

```
decoder = generative network p(z), p(x|z)
encoder = inference network q(z|x)
reconstruction cost = -E_Q(Z|X)[log(P(Z|X))]
regularization = D_{KL}(Q(Z|X)||P(Z))
```





Example: MNIST Digits



Find low dimensional latent variables z from which we can generate the digits.

$$Q:z|x\sim \mathcal{N}(\mu,\sigma I)$$
 where (μ,σ) = inference_network(x)

$$P:z\sim \mathcal{N}(0,I)$$

$$P: x_i | z \sim Bernoulli(logit)$$
 where logit = generative_network(z)



Computations

Why Tensorflow & Keras?

- GPU support
- automatic differentiation
- stochastic gradient descent methods
- built-in tools for batch processing and evaluation
- can add deep models

Tensorflow Probability
Edward Library



References

- Auto-Encoding Variational Bayes
- Stochastic Variational Inference
- Stochastic Gradient Descent for Variational Inference
- Keras MNIST Example (dense layers)
- Colab MNIST Example (conv layers)
- https://github.com/valentina-s/Variational_Inference
- Tensorflow Probability Examples