Generative Classification, Exponential Family Distributions

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Recap: (Bayesian) Logistic Regression

Models the conditional probability of label given features as

$$p(y = 1 | \boldsymbol{x}, \boldsymbol{w}) = \sigma(\boldsymbol{w}^{\top} \boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^{\top} \boldsymbol{x})} = \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x})}{1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x})}$$

where ${m w} \in \mathbb{R}^D$ is the weight vector. Can assume a prior $p({m w}) = \mathcal{N}(0, \lambda^{-1}{m I})$

- MLE, MAP, fully Bayesian inference can be carried out for this model
 - Due to non-conjugacy, fully Bayesian approach requires approximate inference!
- ullet Can extend it to multinomial logistic (aka "softmax") regression for K>2 classes

$$p(y = k | \mathbf{x}, \mathbf{W}) = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x})}{\sum_{k=1}^{K} \exp(\mathbf{w}_k^{\top} \mathbf{x})} \qquad k = 1, \dots, K$$

where $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_K]$. Inference similar to logistic regression.

Generative Classification

• Logistic/Softmax Regression models the conditional probability of labels given features directly

$$\begin{array}{lll} \text{Logistic:} & \rho(y=1|\mathbf{x},\mathbf{w}) & = & \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} \\ \\ \text{Softmax:} & \rho(y=k|\mathbf{x},\mathbf{W}) & = & \frac{\exp(\mathbf{w}_k^{\top}\mathbf{x})}{\sum_{k=1}^K \exp(\mathbf{w}_k^{\top}\mathbf{x})} & k=1,\ldots,K \end{array}$$

- These are examples of Discriminative Classification (directly define a class discriminator function!)
- Another alternative is to use Generative Classification
 - \bullet Doesn't define the distribution of y given x directly but as a two step process
 - Step 1: Using training data, estimate class-marginals p(y) and class-conditional p(x|y)
 - Step 2: Use these to compute conditional probability of label given features as

$$p(y = k|x) = \frac{p(x, y = k)}{p(x)} = \frac{p(x, y = k)}{\sum_{k=1}^{K} p(x, y = k)} = \frac{p(y = k)p(x|y = k)}{\sum_{k=1}^{K} p(y = k)p(x|y = k)}$$

• Note: p(y) and p(x|y) can be learned using point estimation or fully Bayesian inference(we have already seen several examples of learning such distributions from data)

Generative Classification: The "Generative Story"

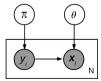
- Assuming binary labels, we can define a "generative story" for each example (x_i, y_i)
 - ullet First draw ("generate") a binary label $y_i \in \{0,1\}$

$$y_i \sim \mathsf{Bernoulli}(\pi)$$

• Now draw ("generate") the feature vector x_i from the distribution of class $y_i \in \{0,1\}$

$$x_i|y_i \sim p(x|\theta_{y_i})$$

• Writing $\theta = (\theta_0, \theta_1)$, the above generative model shown in "plate notation" (shaded = observed)



• Note that the above implicity defines a joint distribution of the form $p(\mathbf{x},y) = p(y)p(\mathbf{x}|y)$

Generative Classification: Learning Procedure

- Recall the rule: $p(y = k|\mathbf{x}) = \frac{p(y=k)p(\mathbf{x}|y=k)}{\sum_{k=1}^{K} p(y=k)p(\mathbf{x}|y=k)}$. How do we learn p(y) and $p(\mathbf{x}|y)$?
- Need to choose the distribution p(y). It has to be a discrete distribution, e.g.,
 - For binary y, $p(y) = p(y|\pi) = \text{Bernoulli}(\pi)$ with $\pi \in (0,1)$
 - For $y \in \{1, \dots, K\}$, $p(y) = p(y|\pi) = \text{multinoulli}(\pi)$ where $\pi = [\pi_1, \dots, \pi_K]$ with $\sum_{k=1}^K \pi_k = 1$
- Need to choose the distribution p(x|y). Its form will depend on the type of x, e.g.,
 - ullet For $x\in\mathbb{R}^D$, we can choose p(x|y) as a multivariate Gaussian (one for each class)

$$p(x|y=k) = p(x|\theta_k) = \mathcal{N}(x|\mu_k, \Sigma_k)$$

- Given training data, we can estimate these distributions. Note: In the fully Bayesian approach
 - Instead of $p(y_*|\hat{\pi})$, we'd infer $p(y_*|\mathbf{y}) = \int p(y_*|\pi)p(\pi|\mathbf{y})d\pi$
 - Instead of $p(x_*|\hat{\theta}_k)$, we'd infer $p(x_*|\mathbf{X}_k) = \int p(x_*|\theta_k)p(\theta_k|\mathbf{X}_k)d\theta_k$ (\mathbf{X}_k : inputs from class k)
- We have already looked at various examples for estimating distributions (via point estimation and Bayesian inference), e.g., for Bernoulli, Gaussian, etc., given data

Generative Classification: Some Benefits



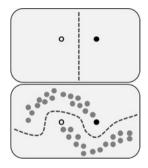
- Can incorporate class prior information (relative frequencies of classes) via p(y)
- Can be used in semi-supervised learning (SSL) settings (when only part of the data is labeled)
 - Usually learned in an alterating fashion
 - "Guess" the missing labels using the current estimates of p(y) and p(x|y)

$$p(y = k|x) = \frac{p(y = k)p(x|y = k)}{\sum_{k=1}^{K} p(y = k)p(x|y = k)}$$

- ② Update p(y) and p(x|y) using the examples with guessed labels + the other labeled examples
- Not limited to learning linear boundaries (unlike logistic/softmax while is a linear models)
 - ullet Form of the class-conditional p(x|y) controls the shape of the learned decision boundary
- Can leverage recent advances in generative models to learn very flexible forms for p(x|y)

An Aside: Why Unlabeled Examples Might Help in Classification?

• The unlabeled example give us a (rough) sense of what each class looks like



• SSL algorithms can leverage this information via the class-conditional p(x|y)

Exponential Family (Pitman, Darmois, Koopman, Late 1930s)

• Defines a class of distributions. An Exponential Family distribution is of the form

$$p(\mathbf{x}|\theta) = \frac{1}{Z(\theta)}h(\mathbf{x})\exp[\theta^{\top}\phi(\mathbf{x})] = h(\mathbf{x})\exp[\theta^{\top}\phi(\mathbf{x}) - A(\theta)]$$

- $m{\circ}$ $m{x} \in \mathcal{X}^m$ is the random variable being modeled (where \mathcal{X} denotes some space, e.g., \mathbb{R} or $\{0,1\}$)
- $oldsymbol{\theta} \in \mathbb{R}^d$: Natural parameters or canonical parameters defining the distribution
- $\phi(\mathbf{x}) \in \mathbb{R}^d$: Sufficient statistics (another random variable)
 - Why "sufficient": $p(x|\theta)$ as a function of θ depends on x only via $\phi(x)$
- $Z(\theta) = \int h(\mathbf{x}) \exp[\theta^{\top} \phi(\mathbf{x})] d\mathbf{x}$: Partition function
- $A(\theta) = \log Z(\theta)$: Log-partition function (also called the <u>cumulant function</u>)
- h(x): A constant (doesn't depend on θ)

Expressing a Distribution in Exponential Family Form

A general trick to represent any distribution (assuming it is exp-family dist.) in exp-family form

• Write the given distribution as $\exp(\log p())$ and simplify, e.g., for the Binomial

$$\exp\left(\log \operatorname{Binomial}(x|N,p)\right) = \exp\left(\log \binom{N}{x} p^{x} (1-p)^{N-x}\right)$$

$$= \exp\left(\log \binom{N}{x} + x \log p + (N-x) \log(1-p)\right)$$

$$= \binom{N}{x} \exp\left(x \log \frac{p}{1-p} - N \log(1-p)\right)$$

• Now compare the resulting expression with the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp(\theta^{\top} \phi(\mathbf{x}) - A(\theta))$$

.. to identify the natural parameters, sufficient statistics, log-partition function, etc.

(Univariate) Gaussian as Exponential Family

• Let's try to write a univariate Gaussian in the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp[\theta^{\top} \phi(\mathbf{x}) - A(\theta)]$$

Recall the standard definition of a univariate Gaussian

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] = \frac{1}{\sqrt{2\pi}} \exp\left[\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}x^2 - \frac{\mu^2}{2\sigma^2} - \log\sigma\right]$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left[\left[-\frac{\mu}{\sigma^2}\right]^{\top} \begin{bmatrix} x \\ x^2 \end{bmatrix} - \left(\frac{\mu^2}{2\sigma^2} - \log\sigma\right)\right]$$

$$\bullet h(x) = \frac{1}{\sqrt{2\pi}}$$

$$\bullet \ \theta = \begin{bmatrix} \frac{\mu}{\sigma_1^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}, \ \text{and} \ \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} -\frac{\theta_1}{2\theta_2} \\ -\frac{1}{2\theta_2} \end{bmatrix}$$

•
$$A(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sigma = \frac{-\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi)$$

Other Examples

- Many other distribution belong to the exponential family
 - Bernoulli
 - Beta
 - Gamma
 - Multinoulli/Multinomial
 - Dirichlet
 - Multivariate Gaussian
 - .. and many more (https://en.wikipedia.org/wiki/Exponential_family)
- Note: Not all distributions belong to the exponential family, e.g.,
 - Uniform distribution $(x \sim \text{Unif}(a, b))$
 - Student-t distribution
 - Mixture distributions (e.g., mixture of Gaussians)
- If the support of the distribution depends on its parameters, then it is not an exp. family dist.

Log-Partition Function

- $A(\theta) = \log Z(\theta) = \log \int h(x) \exp[\theta^{\top} \phi(x)] dx$ is the log-partition function
- $A(\theta)$ is also called the cumulant function
- Derivatives of $A(\theta)$ can be used to generate the cumulants of the sufficient statistics $\phi(x)$
- Exercise: Assume θ to be a scalar (thus $\phi(\mathbf{x})$ is also scalar). Show that the first and the second derivatives of $A(\theta)$ are

$$\begin{array}{lcl} \frac{dA}{d\theta} & = & \mathbb{E}_{p(\mathbf{x}|\theta)}[\phi(\mathbf{x})] = \mathsf{mean}[\phi(\mathbf{x})] \\ \\ \frac{d^2A}{d\theta^2} & = & \mathbb{E}_{p(\mathbf{x}|\theta)}[\phi^2(\mathbf{x})] - \left[\mathbb{E}_{p(\mathbf{x}|\theta)}[\phi(\mathbf{x})]\right]^2 = \mathsf{var}[\phi(\mathbf{x})] \end{array}$$

- Note: The above result also holds when θ and $\phi(x)$ are vector-valued (the "var" will be "covar")
- Important: $A(\theta)$ is a **convex function** of θ . Why?
- Exercise: For Binomial, using its expression of $A(\theta)$, derive the first and second cumulants of $\phi(x)$

MLE for Exponential Family Distributions

• Suppose we have data $\mathcal{D} = \{x_1, \dots, x_N\}$ drawn i.i.d. from an exponential family distribution

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp \left[\theta^{\top} \phi(\mathbf{x}) - A(\theta)\right]$$

• To do MLE, we need the overall likelihood. This is simply a product of the individual likelihoods

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{N} p(\mathbf{x}_i|\theta) = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \sum_{i=1}^{N} \phi(\mathbf{x}_i) - NA(\theta)\right] = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \phi(\mathcal{D}) - NA(\theta)\right]$$

- ullet To estimate heta via MLE (and even MAP), we only need $\phi(\mathcal{D}) = \sum_{i=1}^N \phi(\mathbf{x}_i)$ and N
- Size of $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$ does not grow with N (same as the size of each $\phi(\mathbf{x}_i)$)
- Only exponential family distributions have finite-sized sufficient statistics
 - No need to store all the data; can simply store and recursively update the sufficient statistics with more and more data
 - Very useful when doing probabilistic/Bayesian inference with large-scale data sets. Also useful in online parameter estimation problems.

Bayesian Inference for Exponential Family Distributions

• We saw that the total likelihood given N i.i.d. observations $\mathcal{D}\{x_1,\ldots,x_N\}$

$$p(\mathcal{D}|\theta) \propto \exp\left[\theta^{ op}\phi(\mathcal{D}) - \textit{NA}(\theta)
ight] \qquad ext{where} \quad \phi(\mathcal{D}) = \sum_{i=1}^N \phi(m{x}_i)$$

ullet Let's choose the following prior (note: it looks similar in terms of heta within the exponent)

$$oxed{p(heta|
u_0,oldsymbol{ au}_0) = h(heta) \exp\left[heta^ op_{oldsymbol{ au}} - oldsymbol{
u}_0 A(heta) - A_c(
u_0,oldsymbol{ au}_0)
ight]}$$

• Ignoring the prior's log-partition function $A_c(\nu_0, \tau_0) = \log \int_{\theta} h(\theta) \exp \left[\theta^{\top} \tau_0 - \nu_0 A(\theta)\right] d\theta$

$$igg| p(heta|
u_0, oldsymbol{ au}_0) \propto h(heta) \exp \left[heta^ op oldsymbol{ au}_0 - oldsymbol{
u}_0 A(heta)
ight]$$

- Comparing the prior's form with the likelihood, we notice that
 - \bullet ν_0 is like the number of "pseudo-observations" coming from the prior
 - τ_0 is the <u>total sufficient statistics</u> of these ν_0 pseudo-observations

The Posterior Distribution

As we saw, the likelihood is

$$p(\mathcal{D}|\theta) \propto \exp\left[\theta^{\top}\phi(\mathcal{D}) - NA(\theta)\right]$$
 where $\phi(\mathcal{D}) = \sum_{i=1}^{N}\phi(\mathbf{x}_i)$

And the prior we chose is

$$p(\theta|\nu_0, oldsymbol{ au}_0) \propto h(\theta) \exp\left[heta^ op oldsymbol{ au}_0 - oldsymbol{
u}_0 A(heta)
ight]$$

• For this form of the prior, the posterior $p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$ will be

$$\boxed{p(\theta|\mathcal{D}) \propto h(\theta) \exp\left[\theta^{\top}(\tau_0 + \phi(\mathcal{D})) - (\textcolor{red}{\nu_0} + N)A(\theta)\right]}$$

- Note that the posterior has the same form as the prior; such a prior is called a **conjugate prior** (note: all exponential family distributions have a conjugate prior having a form shown as above)
- Thus posterior hyperparams $\nu_0{}', \tau_0{}'$ are obtained by simply adding "stuff" to prior's hyperparams $\nu_0{}' \leftarrow \nu_0 + N$ (no. of pseudo-obs + no. of actual obs) $\tau_0{}' \leftarrow \tau_0 + \phi(\mathcal{D})$ (total suff-stats from pseudo-obs + total suff-stats from actual obs)
- Note: Prior's log-partition function $A_c(\nu_0, \tau_0)$ updates to posterior's: $A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))$

The Posterior Distribution

• Assuming the prior $p(\theta|\nu_0, \tau_0) \propto h(\theta) \exp\left[\theta^{\top} \tau_0 - \nu_0 A(\theta)\right]$, the posterior was

$$p(heta|\mathcal{D}) \propto h(heta) \exp\left[heta^ op (au_0 + \phi(\mathcal{D})) - (
u_0 + N)A(heta)
ight]$$

- Assuming $\tau_0 = \nu_0 \bar{\tau}_0$, we can also write the prior as $p(\theta|\nu_0, \bar{\tau}_0) \propto \exp\left[\theta^\top \nu_0 \bar{\tau}_0 \nu_0 A(\theta)\right]$
- ullet Can think of $ar{ au}_0= au_0/
 u_0$ as the average sufficient statistics per pseudo-observation
- The posterior can be written as

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp\left[\theta^{\top} (\nu_0 + N) \frac{\nu_0 \bar{\tau}_0 + \phi(\mathcal{D})}{\nu_0 + N} - (\nu_0 + N) A(\theta)\right]$$

ullet Denoting $ar{\phi}=rac{\phi(D)}{N}$ as the average suff-stats per real observation, the posterior updates are

$$\begin{array}{ccc} \nu_0' & \leftarrow & \nu_0 + N \\ \bar{\tau}_0' & \leftarrow & \frac{\nu_0 \bar{\tau}_0 + N \bar{\phi}}{\nu_0 + N} \end{array}$$

• Note that the posterior hyperparam $\bar{\tau}_0'$ is a convex combination of the average suff-stats $\bar{\tau}_0$ of the ν_0 pseudo-observations and the average suff-stats $\bar{\phi}$ of the N actual observations

- ullet Assume some past (training) data $\mathcal{D} = \{ oldsymbol{x}_1, \dots, oldsymbol{x}_N \}$ generated from an exp. family distribution
- Assme some test data $\mathcal{D}' = \{\tilde{\pmb{x}}_1, \dots, \tilde{\pmb{x}}_{N'}\}$ from the same distribution $(N' \geq 1)$
- ullet The posterior predictive distribution of \mathcal{D}' (probability distribution of new data given old data)

$$p(\mathcal{D}'|\mathcal{D}) = \int p(\mathcal{D}'| heta)p(heta|\mathcal{D})d heta$$

- We've already seen some specific examples of computing the posterior predictive dist., e.g.,
 - Beta-Bernoulli case: Posterior predictive distribution of next coin toss
 - ullet Bayesian linear regression: Posterior predictive distribution of the response y_* of test input x_*
- Nice Property: If the likelihood is an exponential family distribution, prior is conjugate (and thus is the posterior), the posterior predictive always has a closed form expression (shown next)

• Recall the form of the likelihood $p(\mathcal{D}|\theta)$ for exp. family dist.

$$p(\mathcal{D}|\theta) = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \phi(\mathcal{D}) - NA(\theta)\right]$$

The conjugate prior was

$$p(heta|
u_0,oldsymbol{ au}_0) = h(heta) \exp\left[heta^ op au_0 -
u_0 A(heta) - A_c(
u_0,oldsymbol{ au}_0)
ight]$$

• For this choice of the conjugate prior, the posterior was shown to be

$$p(\theta|\mathcal{D}) = h(\theta) \exp \left[\theta^{\top} (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N) A(\theta) - A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D})) \right]$$

• For the test data \mathcal{D}' , the likelihood will be

$$p(\mathcal{D}'|\theta) = \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \exp\left[\theta^\top \phi(\mathcal{D}') - N'A(\theta)\right] \qquad \text{where} \quad \phi(\mathcal{D}') = \sum_{i=1}^{N'} \phi(\tilde{\mathbf{x}}_i)$$

• Therefore the posterior predictive distribution will be

$$\rho(\mathcal{D}'|\mathcal{D}) = \int \rho(\mathcal{D}'|\theta)\rho(\theta|\mathcal{D})d\theta$$

$$= \int \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \exp\left[\theta^{\top}\phi(\mathcal{D}') - N'A(\theta)\right]h(\theta) \exp\left[\theta^{\top}(\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta) - \underbrace{A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))}_{\text{constant w.r.t. }\theta}\right]d\theta$$

• The above gets simplified further into

$$p(\mathcal{D}'|\mathcal{D}) = \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \frac{\int h(\theta) \exp\left[\theta^{\top}(\tau_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}')) - (\nu_0 + N + N')A(\theta)\right] d\theta}{\exp\left[A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))\right]}$$
$$= \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \frac{Z_c(\nu_0 + N + N', \tau_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}'))}{\exp\left[A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))\right]}$$

where
$$Z_c(\nu_0 + N + N', \tau_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}')) = \int h(\theta) \exp\left[\theta^\top (\tau_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}')) - (\nu_0 + N + N')A(\theta)\right] d\theta$$

• Since $A_c = \log Z_c$ or $Z_c = \exp(A_c)$, we can write the posterior predictive distribution as

$$p(\mathcal{D}'|\mathcal{D}) = \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \frac{Z_c(\nu_0 + N + N', \boldsymbol{\tau}_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}'))}{Z_c(\nu_0 + N, \boldsymbol{\tau}_0 + \phi(\mathcal{D}))}$$

$$= \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \exp\left[A_c(\nu_0 + N + N', \boldsymbol{\tau}_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}')) - A_c(\nu_0 + N, \boldsymbol{\tau}_0 + \phi(\mathcal{D}))\right]$$

- Therefore the posterior predictive is proportional to ..
 - .. the ratio of two partition functions of two "posterior distributions" (one with N + N' examples and the other with N examples)
 - .. or exponential of the difference of the corresponding log-partition functions
- Note that the form of Z_c (and A_c) will simply depend on the chosen conjugate prior
- Very useful result. Also holds for N=0
 - In the N=0 case, $p(\mathcal{D}')=\int p(\mathcal{D}'|\theta)p(\theta)d\theta$ is simply the marginal likelihood of \mathcal{D}'

Summary

- Exp. family distributions are very useful for modeling diverse types of data/parameters
- Conjugate priors to exp. family distributions make parameter updates very simple
- Other quantities such as posterior predictive can be computed in closed form
- Useful in designing generative classification models. Choosing class-conditional from exponential family with conjugate priors helps in parameter estimation
- Useful in designing generative models for unsupervised learning
- Uses in designing Generalized Linear Models (GLM): Model p(y|x) using exp. family distribution
 - Linear regression (with Gaussian likelihood) and logistic regression are GLMs
- We will see several use cases when we discuss approximate inference algoritms (e.g., Gibbs sampling, and especially variational inference)