Exponential Family Distributions

CS772A: Probabilistic Machine Learning Piyush Rai

Plan today

- PPD for Logistic regression
- Model Selection and Model Averaging
- More on Laplace's Approximation
 - How to make LA scalable when θ is very high dimensional Exponential family distributions
- Exponential Family Distributions



LR: Posterior Predictive Distribution

The posterior predictive distribution can be computed as

$$p(y_* = 1 | x_*, X, y) = \int p(y_* = 1 | w, x_*) p(w | X, y) dw$$
Integral not tractable and must be approximated sigmoid Gaussian (if using Laplace approx.)

- Monte-Carlo approximation is one possible way to approximate such integrals
 - Draw M samples w_1, w_2, \dots, w_M , from the posterior p(w|X, y)
 - Now approximate the PPD as follows

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{X}, \mathbf{y}) \approx \frac{1}{M} \sum_{m=1}^{M} p(y_* = 1 | \mathbf{w}_m, \mathbf{x}_*) = \frac{1}{M} \sum_{m=1}^{M} \sigma(\mathbf{w}_m^{\mathsf{T}} \mathbf{x}_n)$$

In contrast, when using MLE/MAP solution \widehat{w}_{opt} , the plug-in pred. distribution

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}) = \int p(y_* = 1 | \boldsymbol{w}, \boldsymbol{x}_*) p(\boldsymbol{w} | \boldsymbol{X}, \boldsymbol{y}) d\boldsymbol{w}$$

$$\approx p(y_* = 1 | \widehat{\boldsymbol{w}}_{opt}, \boldsymbol{x}_*) = \sigma(\widehat{\boldsymbol{w}}_{opt}^{\mathsf{T}} \boldsymbol{x}_n)$$



LR: Plug-in Prediction vs Bayesian Averaging

- Plug-in prediction uses a single w (point est) to make prediction
- \blacksquare PPD does an averaging using all possible $oldsymbol{w}$'s from the posterior



More on Marginalization

PPD is a weighted average over all possible parameter values of one model

$$p(y_*|\mathbf{x}_*, \mathcal{D}, m) = \int p(y_*|\mathbf{x}_*, \theta, m) p(\theta|\mathcal{D}, m) d\theta$$
Note: *m* is just a model identifier; can ignore when writing

$$\approx \frac{1}{S} \sum_{i=1}^{S} p(y_*|\mathbf{x}_*, \theta^{(i)}, m)$$
Each $\theta^{(i)}$ is drawn i.i.d. from the distribution $p(\theta|\mathcal{D}, m)$.
Above integral replaced by a "Monte-Carlo Averaging" (an approximation when PPD integral is intractable).

PPD marginalization can be done even over several choices of models

Marginalization over all
weights of a single model
$$m$$
 $p(y_*|x_*, D, m) = \int p(y_*|x_*, \theta, m)p(\theta|D, m)d\theta$
Marginalization over all finite
choices $m = 1, 2, ..., M$ of
the model $p(y_*|x_*, D) = \sum_{m=1}^{M} p(y_*|x_*, D, m)p(m|D)$
For example, deep nets with
different architectures
Like a double averaging
(over all model choices, and
over all weights of each
model choice)
Naven't yet told you how
to compute this quantity
but will see shortly
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Model Selection and Model Averaging

• Can use Bayes rule to find the best model from a set of models m = 1, 2, ..., M



Recap: Laplace's Approximation

Consider a posterior distribution that is intractable to compute

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}, \theta)}{p(\mathcal{D})} = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

Laplace approximation approximates the above using a Gaussian distribution



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Laplace's approx. is based on a second-order Taylor approx. of the posterior

Detour: Hessian and Fisher Information Matrix

- Hessian is related to the Fisher Information Matrix (FIM)
- Gradient of the log likelihood is also called score function: $s(\theta) = \nabla_{\theta} \log p(y|\theta)$
 - Note: At some places (some generative models) $\nabla_{\mathbf{y}} \log p(\mathbf{y}|\boldsymbol{\theta})$ also called score function
- Expectation of score function is zero: $\mathbb{E}_{p(y|\theta)}[s(\theta)] = 0$ (exercise)
- Fisher Information Matrix (FIM) is covariance matrix of score function
- $\mathbf{F} = \mathbb{E}_{p(y|\theta)} [(s(\theta) 0)(s(\theta) 0)^{\mathsf{T}}] = \mathbb{E}_{p(y|\theta)} [\nabla_{\theta} \log p(y|\theta) \nabla_{\theta} \log p(y|\theta)^{\mathsf{T}}]$ Note: If we have a prior $p(\theta)$ too, then also add the second derivative of $\log p(\theta)$ $\mathbf{F} = -\mathbb{E}_{p(y|\theta)} [\nabla_{\theta}^{2} \log p(y|\theta)], \text{ i.e., negative of expected Hessian (exercise)}$
- Each entry F_{ii} tells us how "sensitive" the model is w.r.t. the pair (θ_i, θ_i)
 - Each <u>diagonal</u> entry $F_{ii} = (\nabla_{\theta_i} \log p(y|\theta))^2$ tells "important" θ_i is by itself

• Can compute empirical FIM using data: $\hat{\mathbf{F}} = \frac{1}{N} \sum_{n=1}^{N} [\nabla_{\theta} \log p(y_n | \theta) \nabla_{\theta} \log p(y_n | \theta)^{\mathsf{T}}]$

Laplace Approx. for High-Dimensional Problems

- For high-dim θ , Laplace's approx $p(\theta|\mathcal{D}) \approx \mathcal{N}(\theta|\theta_{MAP}, \Lambda^{-1})$ can be expensive
- Many methods to address this, e.g.,
 - Use a diagonal of (empirical) Fisher as the precision

 $\Lambda \approx \text{diag}(\mathbf{F})$



- Use a block-diagonal approximation* of Λ (better than diagonal approx)
- For deep nets, use LA only for some weights + point estimates for others
 - Option 1: Use LA only for last layer weights "last layer Laplace's approximation" (LLLA)
 - Option 2: Use LA for weights from an identified "subnetwork"





Exp. Family (Pitman, Darmois, Koopman, 1930s)

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

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

• $x \in \mathcal{X}^m$ is the r.v. being modeled (\mathcal{X} denotes some space, e.g., \mathbb{R} or $\{0,1\}$)

- $\theta \in \mathbb{R}^d$: Natural parameters or canonical parameters defining the distribution
- $\phi(x) \in \mathbb{R}^d$: Sufficient statistics (another random variable)
 - Knowing this quantity suffices to estimate parameter heta from 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 <u>cumulant function</u>)
- $h(\mathbf{x})$: A constant (doesn't depend on θ)

Expressing a Distribution in Exp. Family Form

- Recall the form of exp-fam distribution $p(x|\theta) = h(x)\exp[\theta^{\top}\phi(x) A(\theta)]$
- To write any exp-fam dist p() in the above form, write it as $exp(\log p())$

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

• Now compare the resulting expression with the exponential family form $p(x|\theta) = h(x)\exp[\theta^{\top}\phi(x) - A(\theta)]$

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



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(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 PDF of a univar Gaussian (already has exp, so less work needed :))

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

$$\theta = \begin{bmatrix} \frac{\mu}{\sigma_1^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \quad \phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix} \quad \text{, and } \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} -\frac{\theta_1}{2\theta_2} \\ -\frac{1}{2\theta_2} \end{bmatrix}$$
$$h(x) = \frac{1}{\sqrt{2\pi}} \qquad A(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sigma = \frac{-\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi)$$

Other Examples

- Many other distribution belong to the exponential family
 - Bernoulli
 - Beta
 - Gamma
 - Multinoulli/Multinomial
 - Dirichlet
 - Multivariate Gaussian
 - .. and many more (<u>https://en.wikipedia.org/wiki/Exponential_family</u>)
- Note: Not all distributions belong to the exponential family, e.g.,
 - Uniform distribution (x ~ Unif(a, b))
 - Student-t distribution
 - Mixture distributions (e.g., mixture of Gaussians)



Log-Partition Function

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

$$\frac{dA}{d\theta} = \mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi(\boldsymbol{x})]$$

$$\frac{d^{2}A}{d\theta^{2}} = \mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi^{2}(\boldsymbol{x})] - \left[\mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi(\boldsymbol{x})]\right]^{2} = \operatorname{var}[\phi(\boldsymbol{x})]$$

- 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?

MLE for Exponential Family Distributions

• Assume data $\mathcal{D} = \{x_1, \dots, x_N\}$ drawn i.i.d. from an exp. family distribution

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

To do MLE, we need the overall likelihood -- a product of the individual likelihoods

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

- To estimate θ (as we'll see shortly), we only need $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$ and N
- Size of $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(x_i)$ does not grow with N (same as the size of each $\phi(x_i)$)
- Only exponential family distributions have finite-sized sufficient statistics
 - No need to store all the data; can simply update the sufficient statistics as data comes
 - Useful in probabilistic inference with large-scale data sets and "online" parameter estimation

Bayesian Inference for Expon. Family Distributions¹⁶

- Already saw that the total likelihood given N i.i.d. observations $\mathcal{D} = \{x_1, \dots, x_N\}$ $p(\mathcal{D}|\theta) \propto \exp\left[\theta^\top \phi(\mathcal{D}) - NA(\theta)\right]$ where $\phi(\mathcal{D}) = \sum_{i=1}^N \phi(x_i)$
- Let's choose the following prior (note: looks similar in terms of θ within exp)

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) = h(\theta) \exp \left[\theta^\top \boldsymbol{\tau}_0 - \boldsymbol{\nu}_0 A(\theta) - A_c(\nu_0, \boldsymbol{\tau}_0)\right]$$

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

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

- Comparing the prior's form with the likelihood, note that
 - ν_0 is like the <u>number of "pseudo-observations"</u> coming from the prior
 - τ_0 is the total sufficient statistics of the pseudo-observations (τ_0 / ν_0 per pseudo-obs)



The Posterior

The likelihood and prior were



- Every exp family likelihood has a conjugate prior having the form above
- Posterior's hyperparams au_0' , u_0' obtained by adding "stuff" to prior's hyperparams



Posterior Predictive Distribution

- Assume some training data $\mathcal{D} = \{x_1, \ldots, x_N\}$ from some exp-fam distribution
- Assume some test data $\mathcal{D}' = \{\tilde{x}_1, \dots, \tilde{x}_{N'}\}$ from the same distribution
- The posterior pred. distr. of \mathcal{D}' Posterior (same form as the Exp. Fam. likelihood prior due to conjugacy) w.r.t. test data $p(\mathcal{D}'|\mathcal{D}) = \int p(\mathcal{D}'|\theta)p(\theta|\mathcal{D})d\theta$ $= \int \left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i)\right] \exp\left[\theta^{\top} \phi(\mathcal{D}') - N'A(\theta)\right] h(\theta) \exp\left[\theta^{\top} (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta) - \underbrace{A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))}_{\text{constant w.r.t. } \theta}\right] d\theta$ This gets further simplified into $p(\mathcal{D}'|\mathcal{D}) = \left| \prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i) \right| = \frac{\int h(\theta) \exp\left[\theta^\top (\tau_0 + \phi(\mathcal{D}) + \phi(\mathcal{D}')) - (\nu_0 + N + N')A(\theta)\right] d\theta}{\exp\left[A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))\right]}$

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



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Posterior Predictive Distribution

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



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

- Therefore the posterior predictive is proportional to
 - Ratio of two partition functions of two "posterior distributions" (one with N + N' examples and the other with N examples)
 - 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 this case $p(\mathcal{D}') = \int p(\mathcal{D}'|\theta) p(\theta) d\theta$ is simply the marginal likelihood of test data \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
- Used in designing Generalized Linear Models: Model p(y|x) using exp. fam distribution
 - Linear regression (with Gaussian likelihood) and logistic regression are GLMs
- Will see several use cases when we discuss approx inference algorithms (e.g., Gibbs sampling, and especially variational inference)