CS281: Advanced ML **September 20, 2017**

Lecture 6: Exponential Families

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6.1 Introduction

(Wainwright and Jordan presents a more detailed coverage of the material in this lecture, beginning in section 3.2.)

This lecture, we will unify all of the fundamentals presented so far:

$p(\theta)$	$p(x)$	$p(y \mid x) / p(x, y)$
Beta, Dir	Discrete	Classification
MVN, IW	MVN	Linear Regression
	Exponential Families	**Generalized Linear Models**
	Undirected Graphic Models	Conditional UGM
	Variational Inference	

We will focus on coming up with a general form for Discrete and MVN through exponential families. We will also come up with a general form for classification and linear regression through generalized linear models.

6.2 Definition of Exponential Family

A pdf is said to belong to the exponential family if it has the form:

$$\begin{aligned} p(x \mid \theta(\mu)) &= \frac{1}{Z(\theta)} h(x) \exp\{\theta^T \phi(x)\} \\ &= h(x) \exp\{\theta^T \phi(x) - A(\theta)\} \end{aligned}$$

where

μ	mean parameters
$\theta(\mu)$	natural / canonical / exponential parameters
$Z(\theta), A(\theta)$	also written as $Z(\theta(\mu))$ or $Z(\mu)$, the partition function and log partition function
$\phi(x)$	sufficient statistics of x, potential functions, "features"
$h(x)$	scaling term; in most cases, we have $h(x) = 1$

Note that representations in the exponential family form can be "minimal" or "overcomplete". A representation is **minimal** if there is a unique θ associated with the distribution. A representation is **overcomplete** if there is a linear dependence between the features. For example, in the case of the Bernoulli distribution, if we let $\phi(x) = [\mathbb{1}\{x = 0\}, \mathbb{1}\{x = 1\}]$, we know $1 = \mathbb{1}\{x = 0\} + \mathbb{1}\{x = 1\}$ and θ would not be uniquely identifiable.

6.3 Examples of Exponential Families

6.3.1 Bernoulli/Categorical

First, we consider the Bernoulli as an exponential family. Like last lecture, we rewrite the distribution as an exp of log.

$$
\begin{aligned}
\text{Ber}(x|\mu) &= \mu^x(1-\mu)^{(1-x)} \\
&= \exp\{x\log\mu + (1-x)\log(1-\mu)\} \\
&= \underbrace{1}_{h(x)}\exp\{\underbrace{\log\left(\frac{\mu}{1-\mu}\right)}_{\theta}\underbrace{x}_{\phi(x)} + \underbrace{\log(1-\mu)}_{-A(\mu)}\}
\end{aligned}
$$

For the **minimal form**, we have

$$
\begin{aligned}
h(x) &= 1 \\
\phi_1(x) &= x \\
\theta_1(\mu) &= \log\frac{\mu}{1-\mu}(\text{“log odds”}) \\
\mu &= \sigma(\theta) \\
A(\mu) &= -\log(1-\mu) \\
A(\theta) &= -\log(1-\sigma(\theta)) = \theta + \log(1+e^{-\theta})
\end{aligned}
$$

For the **overcomplete form**, we have

$$
\begin{aligned}
\phi(x) &= \begin{bmatrix} x \\ 1-x \end{bmatrix} \\
\theta &= \begin{bmatrix} \log\mu \\ \log(1-\mu) \end{bmatrix}
\end{aligned}
$$

For the Categorical/Multinoulli distribution, we have

$$
\theta = \begin{bmatrix} \log\mu_1 \\ \vdots \\ \log\mu_n \end{bmatrix}
$$

where $\sum_c \mu_c = 1$.
Side note: writing the distribution in an overcomplete form means that the features are linearly dependent.

6.3.2 Univariate Gaussians

$$
\begin{aligned}
\mathcal{N}(x \mid \mu, \sigma^2) &= (2\pi\sigma^2)^{1/2}\exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\} \\
&= \underbrace{(2\pi\sigma^2)^{-\frac{1}{2}}}_{A(\mu,\sigma^2)}\exp\{\underbrace{-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x}_{\theta^T\phi(x)} - \underbrace{\frac{1}{2\sigma^2}\mu^2}_{A(\mu,\theta^2)}\}
\end{aligned}
$$

$$
\begin{aligned}
\phi(x) &= \begin{bmatrix} x \\ x^2 \end{bmatrix} \\
\theta &= \begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} \\
A(\mu, \sigma^2) &= \frac{1}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\mu^2 \\
\mu &= -\frac{\theta_1}{2\theta_2} \\
\sigma^2 &= -\frac{1}{2\theta_2} \\
A(\theta) &= -\frac{1}{2}\log(-2\theta_2) - \frac{\theta_1^2}{4\theta_2}
\end{aligned}
$$

6.3.3 Bad distributions

Two simple distributions that do not fit this form are the uniform distribution Uniform(a, b), and the Student-T distribution. The reason that the uniform distribution does not belong in the exponential family is because the support of the uniform distribution depends on the parameters, which is not allowed.

6.4 Properties of Exponential Families

Most inference problems involve a mapping between natural parameters and mean parameters, so this is a natural framework. Here are three properties of exponential families:

Property 1 Derivatives of $A(\theta)$ provide us the cumulants of the distribution $\mathbb{E}(\phi(x))$, $\text{var}(\phi(x))$:

Proof. For univariate, first order:

$$
\begin{aligned}
\frac{dA}{d\theta} &= \frac{d}{d\theta}(\log Z(\theta)) \\
&= \frac{d}{d\theta}\log \underbrace{\left(\int \exp\{\theta\phi\}h(x)dx\right)}_{\text{needed to integrate to 1}} \\
&= \frac{\int \phi \exp\{\theta\phi\}h(x)dx}{\int \exp(\theta\phi)h(z)dx} \\
&= \frac{\int \phi \exp\{\theta\phi\}h(x)dx}{\exp(A(\theta))} \\
&= \int \phi(x) \underbrace{\exp(\theta\phi(x) - A(\theta))h(x)}_{p(x)} dx \\
&= \int \phi(x)p(x)dx \\
&= \mathbb{E}(\phi(x))
\end{aligned}
$$

The same property holds for multivariates (refer to Murphy 9.2.3 for proof). □

Bernoulli:

$$A(\theta) = \theta + \log(1 + e^{-\theta})$$
$$\frac{dA}{d\theta} = 1 - \frac{e^{-\theta}}{1 + e^{-\theta}} = \underbrace{\frac{1}{1 + e^{-\theta}}}_{\text{sigmoid}} = \sigma(\theta) = \mu$$

Univariate Normal

Exercise 6.1. The univariate normal distribution (parameterized with μ, σ^2) can be written in exponential family form such that its log partition function is $A(\boldsymbol{\theta}) = -\frac{\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi)$ where $\boldsymbol{\theta} = \begin{pmatrix} \mu/\sigma^2 \\ -\frac{1}{2\sigma^2} \end{pmatrix}$. Verify that Property 1 holds.

Property 2 MLE has a nice form (through "moment matching").

Proof.

$$\begin{aligned}
\operatorname*{argmax}_\theta \log p(\text{data} \mid \theta) &= \operatorname*{argmax}_\theta \left(\sum_d \theta^T \phi(x_d) \right) - NA(\theta) \\
&= \operatorname*{argmax}_\theta \theta^T \underbrace{\left(\sum_d \phi(x_d) \right)}_{\text{sum of sufficient statistics}} - \underbrace{NA(\theta)}_{\text{amount of points}}
\end{aligned}$$

We take a derivative to obtain:

$$\begin{aligned}
\frac{d(.)}{d\theta} &= \sum_d \phi(x_d) - N\frac{dA(\theta)}{d\theta} \\
&= \sum_d \phi(x_d) - N\mathbb{E}(\phi(x)) \\
&= 0
\end{aligned}$$

$$E(\phi(x)) = \underbrace{\frac{\sum \phi(x_d)}{N}}_{\text{set mean parameter to sample means that gives us MLE}}$$

□

Property 3 Exponential families have conjugate priors.

Proof. We first introduce some notations.

$$\begin{aligned}
\eta &\coloneqq \text{parameters} \\
\bar{s} &\coloneqq \sum_d \phi(x_d)/N \\
p(\text{data} \mid \eta) &\propto \exp[(N\bar{s})\eta - NA(\eta)] \\
p(\eta \mid N_0, s_0) &\propto \exp[(N_0, \bar{s}_0)\eta - N_0 \underbrace{A(\eta)}_{\text{not log partition, which has to be a function strictly of parameters}}] \\
p(\eta|\text{data}) &\propto \exp((N\bar{s} + N_0\bar{s}_0)^T\eta - (N_0 + N)A(\eta))
\end{aligned}$$

The above two distributions have the same sufficient statistics – so we have a conjugate prior. It also tells us that it is not a coincidence that we kept obtaining pseudo counts. (More references will be put up to describe this).

□

6.5 Definition of Generalized Linear Models

While exponential families generalize $p(x)$, GLMs generalize $p(y|x)$.

$$p(y|x,w) = h(y)\exp\{\theta(\underbrace{\mu(x)}_{\text{predict mean}})^T\phi(y) - A(\theta)\}$$

where $\mu(x) = g^{-1}(w^Tx + b)$ where g is an appropriate linear transformation.
This can be summarized through the following sequence of transformations:

$$x \overset{g^{-1}(w^Tx+b)}{\longrightarrow} \mu \to \theta \to p(y \mid x).$$

6.6 Examples of Generalized Linear Models

We present three examples:

Example 1 Exponential family - Normal distribution with $\sigma^2 = 1$ and g^{-1} is the identity function. This gives us the linear regression:

$$\mu = w^Tx + b \qquad \mathbb{R} \to \mathbb{R}$$

Example 2 Exponential family - Bernoulli distribution and g^{-1} is the sigmoid function $\sigma : \mathbb{R} \to (0,1)$. Now, $\mu = \sigma(w^Tx + b)$ and $\theta = \log\left(\frac{\mu}{1-\mu}\right)$. This is how we define logistic regression. This gives us

$$p(y \mid x) = \sigma(w^Tx + b)^y(1 - \sigma(w^Tx + b))^{1-y}$$

Example 3 Exponential family - Categorical distribution with g^{-1} as the softmax function.

$$\mu_c = \text{softmax}(w_c^Tx + b_c)_c$$
$$\theta_c = \log\mu_c$$