The Exponential Family & Generalized Linear Models CSC2541 Tutorial 2, Winter 2022

Jenny Bao

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Overview

The Exponential Family

- ► Formula & basics
- ▶ Examples: Bernoulli, Gaussian, ...

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Useful identities

Generalized Linear Models

The Exponential Family

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\mathbf{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\mathbf{x}))$$

- \blacktriangleright η : natural parameters
- u(x): sufficient statistic
- > $\mathcal{Z}(\eta)$: partition function, ensures the distribution $p(\mathbf{x}|\eta)$ is normalized.

continuous:
$$\mathcal{Z}(\boldsymbol{\eta}) = \int h(\boldsymbol{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\boldsymbol{x})) d\boldsymbol{x}$$

discrete: $\mathcal{Z}(\boldsymbol{\eta}) = \sum_{\boldsymbol{x}} h(\boldsymbol{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\boldsymbol{x}))$

Example 1: Bernoulli



$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\mathbf{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\mathbf{x}))$$

Bernoulli distribution:

$$p(x|\mu) = \text{Bern}(x|\mu) = \mu^{x}(1-\mu)^{1-x}$$

Put in the exponential family form:

$$\operatorname{Bern}(x|\mu) = (1-\mu) \left(\frac{\mu}{1-\mu}\right)^{x}$$
$$= \underbrace{(1-\mu)}_{\frac{1}{Z(\eta)}} \cdot \underbrace{1}_{h(x)} \cdot \exp\left\{\left(\underbrace{\log\frac{\mu}{1-\mu}}_{\eta}\right) \cdot \underbrace{x}_{u(x)}\right\}$$

$$\blacktriangleright \implies \mu = \sigma(\eta), \ \mathcal{Z}(\eta) = \sigma(-\eta)$$

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Exercise: put the multinomial distribution in the standard form for exponential family

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Example 2: Gaussian (μ)



$$p(\boldsymbol{x}|\boldsymbol{\eta}) = rac{1}{\mathcal{Z}(\boldsymbol{\eta})} h(\boldsymbol{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\boldsymbol{x}))$$

Gaussian distribution (treating only μ as parameter, assuming σ is constant):

$$p(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$
$$= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x - \frac{\mu^2}{2\sigma^2}\right)$$
$$= \underbrace{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)}_{h(x)} \cdot \underbrace{\exp\left(-\frac{\mu^2}{2\sigma^2}\right)}_{\frac{1}{2(\eta)}} \exp\left(\underbrace{\frac{\mu}{\sigma^2}}_{\eta^{\top}} \underbrace{x}_{u(x)}\right)$$

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Example 3: Gaussian (μ and σ)



$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})} h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\mathbf{x}))$$

Gaussian distribution (treating both μ and σ as parameters):

$$p(x|\mu,\sigma^{2}) = \frac{1}{\sqrt{2\pi}}\sigma^{-1}\exp(-\frac{1}{2\sigma^{2}}(x-\mu)^{2})$$

= $\frac{1}{\sqrt{2\pi}}\sigma^{-1}\exp(-\frac{1}{2\sigma^{2}}x^{2} + \frac{\mu}{\sigma^{2}}x - \frac{\mu^{2}}{2\sigma^{2}})$
= $\underbrace{\frac{1}{\sqrt{2\pi}}}_{h(x)} \cdot \underbrace{\sigma^{-1}\exp(-\frac{\mu^{2}}{2\sigma^{2}})}_{\frac{1}{\frac{1}{\mathcal{E}(\eta)}}}\exp(\underbrace{\left[-\frac{\mu}{2\sigma^{2}}\right]}_{\eta^{\top}} \cdot \underbrace{\left[x\right]}_{u(x)}$

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The Exponential Family

Other members of the exponential family:

Poisson, gamma, exponential, beta, Dirichlet, …

Why studying the exponential family?

Many convenient properties

- Sufficient statistics for maximum likelihood
- Many convenient identities for $\mathcal{Z}(\eta)$ (the partition function)
 - Relates concepts such as the Fisher information matrix

Can be used to derive the Generalized Linear Models (GLM)

Maximum likelihood & sufficient statistics

Consider i.i.d. data $X = \{x_1, ..., x_N\}$. Find η to maximize $p(X|\eta)$ (maximum likelihood).

$$p(\boldsymbol{X}|\boldsymbol{\eta}) = \prod_{i=1}^{N} \frac{1}{\mathcal{Z}(\boldsymbol{\eta})} \left(h(\boldsymbol{x}_{i}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\boldsymbol{x}_{i})) \right)$$
$$= \left(\frac{1}{\mathcal{Z}(\boldsymbol{\eta})}\right)^{N} \left(\prod_{i=1}^{N} h(\boldsymbol{x}_{i})\right) \exp(\boldsymbol{\eta}^{\top} \sum_{i=1}^{N} \boldsymbol{u}(\boldsymbol{x}_{i}))$$

Take derivative of the log-likelihood and set it to 0.

$$abla_{\eta} \log p(\boldsymbol{X}|\boldsymbol{\eta}) = -N
abla_{\eta} \log \mathcal{Z}(\boldsymbol{\eta}) + \sum_{i=1}^{N} \boldsymbol{u}(\boldsymbol{x}_{i}) = 0$$

$$\implies
abla_{\eta} \log \mathcal{Z}(\boldsymbol{\eta}) = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{u}(\boldsymbol{x}_{i})$$

Maximum likelihood & sufficient statistics

$$abla_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta}) = rac{1}{N} \sum_{i=1}^{N} \boldsymbol{u}(\boldsymbol{x}_i)$$

The maximum-likelihood solution η only depends on $\sum_{i=1}^{N} u(x_i)$.

• Hence u(x) is called the sufficient statistic

Examples:

- **Bernoulli:** u(x) = x. Only need to store $\sum_i x_i$.
- Gaussian (μ and σ): $u(x) = \begin{bmatrix} x & x^2 \end{bmatrix}^{\top}$. Need to store both $\sum_i x_i$ and $\sum_i x_i^2$.

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\mathbf{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\mathbf{x}))$$

1. $\nabla_{\eta} \log \mathcal{Z}(\eta) = \mathbb{E}_{x \sim \rho(x|\eta)}[\boldsymbol{u}(x)] =: \boldsymbol{\xi}$ (moments)

Derivation:

$$\nabla_{\eta} \log \mathcal{Z}(\eta) = \frac{1}{\mathcal{Z}(\eta)} \nabla_{\eta} \int h(x) \exp(\eta^{\top} u(x)) dx$$
$$= \frac{1}{\mathcal{Z}(\eta)} \int h(x) \exp(\eta^{\top} u(x)) u(x) dx$$
$$= \int \frac{1}{\mathcal{Z}(\eta)} h(x) \exp(\eta^{\top} u(x)) u(x) dx$$
$$= \mathbb{E}_{x \sim \rho(x|\eta)} [u(x)]$$

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})} h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\mathbf{x}))$$

1. $\nabla_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta}) = \mathbb{E}_{\boldsymbol{x} \sim \boldsymbol{\rho}(\boldsymbol{x}|\boldsymbol{\eta})}[\boldsymbol{u}(\boldsymbol{x})] =: \boldsymbol{\xi}$ (moments)

- \blacktriangleright There's a 1-to-1 mapping between $\eta\leftrightarrowoldsymbol{\xi}$
- \triangleright ξ is an alternative parameterization for the exponential family

$$p(\pmb{x}|\pmb{\eta}) \leftrightarrow p(\pmb{x}|\pmb{\xi})$$

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$$p(\boldsymbol{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\boldsymbol{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\boldsymbol{x}))$$
1.
$$\nabla_{\boldsymbol{\eta}}\log\mathcal{Z}(\boldsymbol{\eta}) = \mathbb{E}_{\boldsymbol{x}\sim p(\boldsymbol{x}|\boldsymbol{\eta})}[\boldsymbol{u}(\boldsymbol{x})] =: \boldsymbol{\xi} \quad (\text{moments})$$

2. $\nabla_{\eta} \log p(\boldsymbol{x}|\boldsymbol{\eta}) = \boldsymbol{u}(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\eta})}[\boldsymbol{u}(\boldsymbol{x})]$

Derivation:

$$egin{aligned}
abla_{\eta} \log p(oldsymbol{x}|oldsymbol{\eta}) &= -
abla_{\eta} \log \mathcal{Z}(oldsymbol{\eta}) +
abla_{\eta}(oldsymbol{\eta}^{ op}oldsymbol{u}(oldsymbol{x})) \ &= -\mathbb{E}_{oldsymbol{x}\sim p(oldsymbol{x}|oldsymbol{\eta})}[oldsymbol{u}(oldsymbol{x})] + oldsymbol{u}(oldsymbol{x})) \end{aligned}$$

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\mathbf{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\mathbf{x}))$$

1.
$$\nabla_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta}) = \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\eta})}[\boldsymbol{u}(\mathbf{x})] =: \boldsymbol{\xi}$$
 (moments)
2. $\nabla_{\boldsymbol{\eta}} \log p(\mathbf{x}|\boldsymbol{\eta}) = \boldsymbol{u}(\mathbf{x}) - \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\eta})}[\boldsymbol{u}(\mathbf{x})]$

Recall, in maximum likelihood, we have

$$\nabla_{\boldsymbol{\eta}} \sum_{i=1}^{N} \log p(\boldsymbol{x}_{i} | \boldsymbol{\eta}) = N\left(\underbrace{\frac{1}{N} \sum_{i=1}^{N} \boldsymbol{u}(\boldsymbol{x}_{i})}_{\text{empirical moments } \hat{\boldsymbol{\xi}}} - \underbrace{\nabla_{\boldsymbol{\eta}} \log \boldsymbol{\mathcal{Z}}(\boldsymbol{\eta})}_{\text{moments } \boldsymbol{\xi}}\right)$$
$$= N \cdot (\hat{\boldsymbol{\xi}} - \boldsymbol{\xi}) = 0$$

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Maximum likelihood \rightarrow moment matching

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})}h(\mathbf{x})\exp(\boldsymbol{\eta}^{\top}\boldsymbol{u}(\mathbf{x}))$$

1.
$$\nabla_{\eta} \log \mathcal{Z}(\eta) = \mathbb{E}_{x \sim p(x|\eta)}[\boldsymbol{u}(x)] =: \boldsymbol{\xi}$$
 (moments)
2. $\nabla_{\eta} \log p(x|\eta) = \boldsymbol{u}(x) - \mathbb{E}_{x \sim p(x|\eta)}[\boldsymbol{u}(x)]$
3.1. $\nabla_{\eta}^{2} \log \mathcal{Z}(\eta) = \operatorname{Cov}(\boldsymbol{u}(x)) = -\nabla_{\eta}^{2} \log p(x|\eta)$

Derivation:
$$\nabla^2_{\boldsymbol{\eta}} \log p(\boldsymbol{x}|\boldsymbol{\eta}) = \nabla_{\boldsymbol{\eta}} \boldsymbol{u}(\boldsymbol{x}) - \nabla^2_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta}) = -\nabla^2_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta})$$

$$\nabla_{\eta}^{2} \log \mathcal{Z}(\eta) = \nabla_{\eta} \mathbb{E}_{x \sim p(x|\eta)} [\boldsymbol{u}(x)]$$

the grad-log trick $\rightarrow = \mathbb{E}_{x \sim p(x|\eta)} [\nabla_{\eta} \log p(x|\eta) \boldsymbol{u}(x)^{\top}]$
 $= \mathbb{E}_{x \sim p(x|\eta)} [(\boldsymbol{u}(x) - \mathbb{E}_{x \sim p(x|\eta)} [\boldsymbol{u}(x)]) \boldsymbol{u}(x)^{\top}]$
 $\mathbb{E}[(\boldsymbol{u} - \mathbb{E}[\boldsymbol{u}])\mathbb{E}[\boldsymbol{u}]] = 0 \rightarrow = \mathbb{E}[(\boldsymbol{u}(x) - \mathbb{E}[\boldsymbol{u}(x)]) (\boldsymbol{u}(x) - \mathbb{E}[\boldsymbol{u}(x)])^{\top}]$
 $= \operatorname{Cov}(\boldsymbol{u}(x))$

$$p(\boldsymbol{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})} h(\boldsymbol{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\boldsymbol{x}))$$
1.
$$\nabla_{\boldsymbol{\eta}} \log \mathcal{Z}(\boldsymbol{\eta}) = \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\eta})} [\boldsymbol{u}(\boldsymbol{x})] =: \boldsymbol{\xi} \quad (\text{moments})$$
2.
$$\nabla_{\boldsymbol{\eta}} \log p(\boldsymbol{x}|\boldsymbol{\eta}) = \boldsymbol{u}(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\eta})} [\boldsymbol{u}(\boldsymbol{x})]$$
3.1.
$$\nabla_{\boldsymbol{\eta}}^{2} \log \mathcal{Z}(\boldsymbol{\eta}) = \operatorname{Cov}(\boldsymbol{u}(\boldsymbol{x})) = -\nabla_{\boldsymbol{\eta}}^{2} \log p(\boldsymbol{x}|\boldsymbol{\eta})$$
3.2.
$$\nabla_{\boldsymbol{\eta}}^{2} \log \mathcal{Z}(\boldsymbol{\eta}) = F_{\boldsymbol{\eta}} \quad (\text{Fisher information matrix})$$
3.3.
$$F_{\boldsymbol{\eta}} = \nabla_{\boldsymbol{\eta}} \boldsymbol{\xi} = J_{\boldsymbol{\xi},\boldsymbol{\eta}} \quad (\text{Jacobian of mapping } \boldsymbol{\eta} \rightarrow \boldsymbol{\xi})$$

We will skip the details for now, as the Fisher information matrix will be covered in lecture 3. Also, discussion on these identities are in Chapter 3 of the course notes.

Consider two familiar models





Linear regression: $\mathcal{L} = \frac{1}{2N} \sum_{i=1}^{N} (t_i - y_i)^2$, where $y_i = \boldsymbol{w}^\top \boldsymbol{x}_i$

$$\implies \nabla_{\mathbf{w}} \mathcal{L} = -\frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) x_i$$

Logistic regression: $\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} -t_i \log y_i - (1 - t_i) \log(1 - y_i)$, where $y_i = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

$$\implies \nabla_{\mathbf{w}} \mathcal{L} = -\frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) x_i$$

Their gradients have the same form (!!!) Why?

(Images taken from CSC311 lecture slides).

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Linear regression, logistic regression, softmax regression all belong to a broader class of models called generalized linear models (GLM).

GLM is derived from the exponential family.

Consider the linear model with features:

$$z = \mathbf{w}^{\top} \phi(\mathbf{x})$$

 $y = a(z)$ (activation)

Assume the labels are distributed according to the exponential family (implied in the loss function)

$$p(t|\eta) = \frac{1}{\mathcal{Z}(\eta)}h(t)\exp(\eta^{\top}u(t))$$

We focus on a special case of the exponential family where u(t) = t.

$$p(t|\eta) = rac{1}{\mathcal{Z}(\eta)}h(t)\exp(\eta^{ op}t)$$

$$z = \mathbf{w}^{\top} \phi(\mathbf{x}), \quad y = a(z)$$
$$\rho(t|\eta) = \frac{1}{\mathcal{Z}(\eta)} h(t) \exp(\eta^{\top} t)$$

Recall, the moments can be computed by differentiating the partition function:

 $\nabla_{\eta} \log \mathcal{Z}(\eta) = \mathbb{E}_{t \sim p(t|\eta)}[u(t)] = \mathbb{E}_{t \sim p(t|\eta)}[t] = y \quad (\text{Prediction probability})$

There is a 1-to-1 mapping between $\eta \leftrightarrow y$. Let

$$\eta = \psi(\mathbf{y})$$

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$$z = \mathbf{w}^{\top} \phi(\mathbf{x}), \quad y = a(z)$$

$$\eta = \psi(y)$$

$$p(t|\eta) = \frac{1}{\mathcal{Z}(\eta)} h(t) \exp(\eta^{\top} t)$$

Gradient of log-likelihood w.r.t weights \boldsymbol{w} :

$$\begin{split} \frac{\partial}{\partial \boldsymbol{w}} \sum_{i=1}^{N} \log p(t_i | \eta_i) &= \sum_{i=1}^{N} \frac{\partial}{\partial \eta_i} \log p(t_i | \eta_i) \frac{\partial \eta_i}{\partial y_i} \frac{\partial y_i}{\partial z_i} \frac{\partial z_i}{\partial \boldsymbol{w}} \\ &= \sum_{i=1}^{N} (u(t_i) - \mathbb{E}_{t_i \sim p(t_i | \eta_i)} [u(t_i)]) \psi'(y_i) a'(z_i) \phi(\boldsymbol{x}_i) \\ &= \sum_{i=1}^{N} (t_i - y_i) \psi'(y_i) a'(z_i) \phi(\boldsymbol{x}_i) \end{split}$$

This greatly simplifies if we choose $a = \psi^{-1}$.

$$\eta = \psi(a(z)) = \psi(\psi^{-1}(z)) = z \implies \psi'(y)a'(z) = \frac{\partial\eta}{\partial y}\frac{\partial y}{\partial z} = 1$$

To summarize, when the following conditions are met:

Linear model with activation

$$z = \mathbf{w}^{ op} \phi(\mathbf{x}), \quad y = a(z)$$

The label distribution belongs to the exponential family

$$p(t|\eta) = rac{1}{\mathcal{Z}(\eta)}h(t)\exp(\eta^{\top}t)$$

where $y =
abla_{\eta}\log \mathcal{Z}(\eta)$, and $\eta = \psi(y)$

Activation is chosen as:

$$a(\cdot) = \psi^{-1}(\cdot)$$

Then we have:

$$\frac{\partial}{\partial \boldsymbol{w}} \sum_{i=1}^{N} \log p(t_i | \eta) = \sum_{i=1}^{N} (t_i - y_i) \phi(\boldsymbol{x}_i)$$

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GLM example: logistic regression

Cross-entropy loss (negative log-likelihood):

$$\mathcal{L} = -\log p(t|y) = -t \log y - (1-t) \log(1-y)$$

Corresponding label distribution: Bernoulli

$$p(t|y) = y^{t}(1-y)^{1-t}$$

= (1-y) exp{(log $\frac{y}{1-y}$)t}

We have

$$\eta = \log \frac{y}{1-y} = \psi(y)$$

Then we should choose activation:

$$a(z) = \psi^{-1}(z) = \sigma(z) \quad \checkmark$$

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GLM example: linear regression

Squared loss (negative log-likelihood):

$$\mathcal{L} = -\log p(t|y) = rac{1}{2}(t-y)^2$$

Corresponding label distribution: Gaussian (with fixed σ , WLOG assume $\sigma=1$)

$$p(t|y) = \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2}(t-y)^2\}$$

We have

$$\eta = y = \psi(y)$$

Then we should choose activation:

$$a(z) = \psi^{-1}(z) = z \quad \checkmark$$

Summary

Exponential family

$$p(\mathbf{x}|\boldsymbol{\eta}) = \frac{1}{\mathcal{Z}(\boldsymbol{\eta})} h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\top} \boldsymbol{u}(\mathbf{x}))$$

- Many common distributions belong to this family (Bernoulli, multinomial, Gaussian, Poisson, gamma, ...)
- Sufficient statistics for maximum-likelihood estimation
- Many useful identities stemming from $\mathcal{Z}(\eta)$
 - Moments & empirical moments, MLE as moment matching
 - \blacktriangleright Convenient way to compute the Fisher information matrix F_η

Used to derive the generalized linear models (GLM)