

#### **Probabilistic Graphical Models**

#### **Generalized linear models**

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Reading: KF-chap 17

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### Parameterizing graphical models

• Bayesian network:

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#### where $\boldsymbol{\varepsilon}$ is an error term of unmodeled effects or random noise



$$p(y_i \mid x_i; \theta) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

• We can use LMS algorithm, which is a gradient ascent/descent approach, to estimate the parameter

## **Recall Linear Regression**

related by the equation:

 $y_i = \theta^T \mathbf{X}_i + \varepsilon_i$ 

• Let us assume that the target variable and the inputs are



### Recall: Logistic Regression (sigmoid classifier, perceptron, etc.)

• The condition distribution: a Bernoulli

$$p(y | x) = \mu(x)^{y} (\mathbf{1} - \mu(x))^{1-y}$$

where  $\mu$  is a logistic function

$$\mu(x) = \frac{1}{1 + e^{-\theta^T x}}$$



• We can used the brute-force gradient method as in LR

 But we can also apply generic laws by observing the p(y|x) is an exponential family function, more specifically, a generalized linear model!

### Parameterizing graphical models

• Markov random fields

$$p(\mathbf{x}) = \frac{1}{Z} \exp\left\{-\sum_{c \in C} \phi_c(\mathbf{x}_c)\right\} = \frac{1}{Z} \exp\left\{-H(\mathbf{x})\right\}$$



#### **Restricted Boltzmann Machines**



 $p(x,h \mid \theta) = \exp \left\{ \sum_{i=1}^{n} \phi_{i}(x_{i}) + \sum_{i=1}^{n} \phi_{i}(h_{j}) + \sum_{i=1}^{n} \phi_{i,j}(x_{i},h_{j}) - A(\theta) \right\}$ i, j



#### **Conditional Random Fields**



• Discriminative

$$p_{\theta}(y \mid x) = \frac{1}{Z(\theta, x)} \exp\left\{\sum_{c} \theta_{c} f_{c}(x, y_{c})\right\}$$

• *X*<sub>*i*</sub>'s are assumed as features that are inter-dependent

• When labeling *X<sub>i</sub>* future observations are taken into account

### **Conditional Distribution**



$$p_{\theta}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp\left(\sum_{e \in E,k} \lambda_k f_k(e, \mathbf{y} \mid_e, \mathbf{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathbf{y} \mid_v, \mathbf{x})\right)$$

- x is a data sequence
- y is a label sequence
- *v* is a vertex from vertex set V = set of label random variables
- e is an edge from edge set E over V
- $f_k$  and  $g_k$  are given and fixed.  $g_k$  is a Boolean vertex feature;  $f_k$  is a Boolean edge feature
- k is the index number of the features
- $\theta = (\lambda_1, \lambda_2, \dots, \lambda_n; \mu_1, \mu_2, \dots, \mu_n); \lambda_k \text{ and } \mu_k$  are parameters to be estimated
- y|<sub>e</sub> is the set of components of y defined by edge e
- y|<sub>v</sub> is the set of components of y defined by vertex v

**X**<sub>1</sub> ... **X**<sub>n</sub>

#### **2-D Conditional Random Fields**



$$\mathbf{p}_{\theta}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\theta, \mathbf{x})} \exp\left\{\sum_{c} \theta_{c} \mathbf{f}_{c}(\mathbf{x}, \mathbf{y}_{c})\right\}$$

- Allow arbitrary dependencies on input
- Clique dependencies on labels
- Use approximate inference for general graphs

### Exponential family, a basic building block



• For a numeric random variable X

 $p(x \mid \eta) = h(x) \exp\left\{\eta^T T(x) - A(\eta)\right\}$  $= \frac{1}{Z(\eta)} h(x) \exp\left\{\eta^T T(x)\right\}$ 

is an **exponential family distribution** with natural (canonical) parameter  $\eta$ 

- Function T(x) is a sufficient statistic.
- Function  $A(\eta) = \log Z(\eta)$  is the log normalizer.
- Examples: Bernoulli, multinomial, Gaussian, Poisson, gamma,...

# Example: Multivariate Gaussian Distribution



• For a continuous vector random variable  $X \in \mathbb{R}^k$ :

$$p(x|\mu, \Sigma) = \frac{1}{(2\pi)^{k/2} |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right\}$$
  
Moment parameter  
$$= \frac{1}{(2\pi)^{k/2}} \exp\left\{-\frac{1}{2} \operatorname{tr}(\Sigma^{-1} x x^T) + \mu^T \Sigma^{-1} x - \frac{1}{2} \mu^T \Sigma^{-1} \mu - \log|\Sigma|\right\}$$

- Exponential family representation  $\eta = \left[\Sigma^{-1}\mu; -\frac{1}{2}\operatorname{vec}(\Sigma^{-1})\right] = \left[\eta_1, \operatorname{vec}(\eta_2)\right], \quad \eta_1 = \Sigma^{-1}\mu \text{ and } \eta_2 = -\frac{1}{2}\Sigma^{-1}$   $T(x) = \left[x; \operatorname{vec}(xx^T)\right]$   $A(\eta) = \frac{1}{2}\mu^T \Sigma^{-1}\mu + \log|\Sigma| = -\frac{1}{2}\operatorname{tr}(\eta_2\eta_1\eta_1^T) - \frac{1}{2}\log(-2\eta_2)$   $h(x) = (2\pi)^{-k/2}$ 
  - Note: a *k*-dimensional Gaussian is a  $(d+d^2)$ -parameter distribution with a  $(d+d^2)$ element vector of sufficient statistics (but because of symmetry and positivity,
    parameters are constrained and have lower degree of freedom)

### **Example: Multinomial distribution**

• For a binary vector random variable  $\mathbf{X} \sim \text{multi}(\mathbf{X} \mid \pi)$ ,

$$(x|\pi) = \pi_1^{x_1} \pi_2^{x_1} \cdots \pi_K^{x_K} = \exp\left\{\sum_k x_k \ln \pi_k\right\}$$
$$= \exp\left\{\sum_{k=1}^{K-1} x_k \ln \pi_k + \left(1 - \sum_{k=1}^{K-1} x_K\right) \ln\left(1 - \sum_{k=1}^{K-1} \pi_k\right)\right\}$$
$$= \exp\left\{\sum_{k=1}^{K-1} x_k \ln\left(\frac{\pi_k}{1 - \sum_{k=1}^{K-1} \pi_k}\right) + \ln\left(1 - \sum_{k=1}^{K-1} \pi_k\right)\right\}$$

• Exponential family representation

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$$\eta = \left[ \ln\left(\frac{\pi_k}{\pi_K}\right); \mathbf{0} \right]$$
$$T(x) = [x]$$
$$A(\eta) = -\ln\left(1 - \sum_{k=1}^{K-1} \pi_k\right) = \ln\left(\sum_{k=1}^{K} e^{\eta_k}\right)$$
$$h(x) = 1$$
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### Why exponential family?

• Moment generating property

$$\frac{dA}{d\eta} = \frac{d}{d\eta} \log Z(\eta) = \frac{1}{Z(\eta)} \frac{d}{d\eta} Z(\eta)$$
$$= \frac{1}{Z(\eta)} \frac{d}{d\eta} \int h(x) \exp\{\eta^T T(x)\} dx$$
$$= \int T(x) \frac{h(x) \exp\{\eta^T T(x)\}}{Z(\eta)} dx$$
$$= E[T(x)]$$

$$\frac{d^2 A}{d\eta^2} = \int T^2(x) \frac{h(x) \exp\{\eta^T T(x)\}}{Z(\eta)} dx - \int T(x) \frac{h(x) \exp\{\eta^T T(x)\}}{Z(\eta)} dx \frac{1}{Z(\eta)} \frac{d}{d\eta} Z(\eta)$$
$$= E[T^2(x)] - E^2[T(x)]$$
$$= Var[T(x)]$$

#### **Moment estimation**



- We can easily compute moments of any exponential family distribution by taking the derivatives of the log normalizer  $A(\eta)$ .
- The  $q^{\text{th}}$  derivative gives the  $q^{\text{th}}$  centered moment.

$$\frac{dA(\eta)}{d\eta} = \text{mean}$$
$$\frac{d^2A(\eta)}{d\eta^2} = \text{variance}$$

. . .

• When the sufficient statistic is a stacked vector, partial derivatives need to be considered.

#### **Moment vs canonical parameters**

- The moment parameter µ can be derived from the natural (canonical) parameter
  - $\frac{dA(\eta)}{d\eta} = E[T(x)]^{\text{def}} = \mu$
- $A(\eta)$  is convex since

 $\frac{d^2 A(\eta)}{d\eta^2} = Var[T(x)] > \mathbf{0}$ 

• Hence we can invert the relationship and infer the canonical parameter from the moment parameter (1-to-1):

$$\eta = \psi(\mu)$$

• A distribution in the exponential family can be parameterized not only by  $\eta$  – the canonical parameterization, but also by  $\mu$  – the moment parameterization.

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## **MLE for Exponential Family**

• For *iid* data, the log-likelihood is

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$$(\eta; D) = \log \prod_{n} h(x_{n}) \exp\left\{\eta^{T} T(x_{n}) - A(\eta)\right\}$$
$$= \sum_{n} \log h(x_{n}) + \left(\eta^{T} \sum_{n} T(x_{n})\right) - NA(\eta)$$

• Take derivatives and set to zero:

$$\frac{\partial \ell}{\partial \eta} = \sum_{n} T(x_{n}) - N \frac{\partial A(\eta)}{\partial \eta} = \mathbf{0}$$
$$\Rightarrow \frac{\partial A(\eta)}{\partial \eta} = \frac{1}{N} \sum_{n} T(x_{n})$$
$$\Rightarrow \hat{\mu}_{MLE} = \frac{1}{N} \sum_{n} T(x_{n})$$

- This amounts to **moment matching**.
- We can infer the canonical parameters using  $\hat{\eta}_{MLE} = \psi(\hat{\mu}_{MLE})$



#### Sufficiency

- For  $p(x|\theta)$ , T(x) is sufficient for  $\theta$  if there is no information in X regarding  $\theta$  beyond that in T(x).
  - We can throw away X for the purpose of inference w.r.t.  $\theta$ .



#### **Examples**

• Gaussian:

$$\eta = \left[\Sigma^{-1}\mu; -\frac{1}{2}\operatorname{vec}(\Sigma^{-1})\right]$$
$$T(x) = \left[x; \operatorname{vec}(xx^{T})\right]$$
$$A(\eta) = \frac{1}{2}\mu^{T}\Sigma^{-1}\mu + \frac{1}{2}\log|\Sigma|$$
$$h(x) = (2\pi)^{-k/2}$$

$$\Rightarrow \mu_{MLE} = \frac{1}{N} \sum_{n} T_1(x_n) = \frac{1}{N} \sum_{n} x_n$$

Multinomial:

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$$\eta = \left[ \ln\left(\frac{\pi_k}{\pi_K}\right); \mathbf{0} \right]$$

$$T(x) = [x]$$

$$A(\eta) = -\ln\left(1 - \sum_{k=1}^{K-1} \pi_k\right) = \ln\left(\sum_{k=1}^{K} e^{\eta_k}\right)$$

$$h(x) = \mathbf{1}$$

$$\Rightarrow \mu_{MLE} = \frac{1}{N} \sum_{n} x_n$$

• Poisson:

$$\eta = \log \lambda$$
$$T(x) = x$$
$$A(\eta) = \lambda = e^{\eta}$$
$$h(x) = \frac{1}{x!}$$

$$\Rightarrow \mu_{MLE} = \frac{1}{N} \sum_{n} x_{n}$$

#### **Bayesian est.**



### Generalized Linear Models (GLIMs)

- The graphical model
  - Linear regression
  - Discriminative linear classification
  - Commonality:
    - model  $E_p(Y) = \mu = f(\theta^T X)$
    - What is p()? the cond. dist. of Y.
    - What is f()? the response function.
- GLIM
  - The observed input x is assumed to enter into the model via a linear combination of its elements  $\xi = \theta^T x$
  - The conditional mean μ is represented as a function f(ξ) of ξ, where f is known as the response function
  - The observed output y is assumed to be characterized by an exponential family distribution with conditional mean  $\mu$ .





#### GLIM, cont.



- The choice of exp family is constrained by the nature of the data Y
  - Example: y is a continuous vector → multivariate Gaussian
     y is a class label → Bernoulli or multinomial
- The choice of the response function
  - Following some mild constrains, e.g., [0,1]. Positivity ...
  - Canonical response function:  $f = \psi^{-1}(\cdot)$ 
    - In this case  $\theta^T x$  directly corresponds to canonical parameter  $\eta$ .

# Example canonical response functions



| Model                        | Canonical response function          |
|------------------------------|--------------------------------------|
| Gaussian                     | $\mu=\eta$                           |
| Bernoulli                    | $\mu = 1/(1 + e^{-\eta})$            |
| $\operatorname{multinomial}$ | $\mu_i = \eta_i / \sum_j e^{\eta_j}$ |
| Poisson                      | $\mu=e^{\eta}$                       |
| gamma                        | $\mu = -\eta^{-1}$                   |

# MLE for GLIMs with natural response



• Log-likelihood

$$\boldsymbol{\ell} = \sum_{n} \log h(\boldsymbol{y}_{n}) + \sum_{n} \left( \boldsymbol{\theta}^{T} \boldsymbol{x}_{n} \boldsymbol{y}_{n} - A(\boldsymbol{\eta}_{n}) \right)$$

• Derivative of Log-likelihood

$$\frac{d\ell}{d\theta} = \sum_{n} \left( x_{n} y_{n} - \frac{dA(\eta_{n})}{d\eta_{n}} \frac{d\eta_{n}}{d\theta} \right)$$
$$= \sum_{n} \left( y_{n} - \mu_{n} \right) x_{n}$$
$$= X^{T} \left( y - \mu \right)$$

This is a fixed point function because  $\mu$  is a function of  $\theta$ 

- Online learning for canonical GLIMs
  - Stochastic gradient ascent = least mean squares (LMS) algorithm:

$$\theta^{t+1} = \theta^t + \rho (y_n - \mu_n^t) x_n$$
  
where  $\mu_n^t = (\theta^t)^T x_n$  and  $\rho$  is a step size

# Batch learning for canonical GLIMs

• The Hessian matrix

$$H = \frac{d^2 \ell}{d\theta d\theta^T} = \frac{d}{d\theta^T} \sum_n (y_n - \mu_n) x_n = \sum_n x_n \frac{d\mu_n}{d\theta^T}$$
$$= -\sum_n x_n \frac{d\mu_n}{d\eta_n} \frac{d\eta_n}{d\theta^T}$$

$$= -\sum_{n} x_{n} \frac{d\mu_{n}}{d\eta_{n}} x_{n}^{T} \text{ since } \eta_{n} = \theta^{T} x_{n}$$
$$= -X^{T} W X$$



where  $X = [x_n^T]$  is the design matrix and  $W = \text{diag}\left(\frac{d\mu_1}{dn_1}, \dots, \frac{d\mu_N}{dn_N}\right)$ 

which can be computed by calculating the 2<sup>nd</sup> derivative of  $A(\eta_n)$ 

#### **Recall LMS**

• Cost function in matrix form:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{n} (\mathbf{x}_{i}^{T} \theta - y_{i})^{2}$$
$$= \frac{1}{2} (\mathbf{X} \theta - \bar{y})^{T} (\mathbf{X} \theta - \bar{y})^{2}$$



• To minimize  $J(\theta)$ , take derivative and set to zero:

## Iteratively Reweighted Least Squares (IRLS)



$$\theta^{t+1} = \theta^t - H^{-1} \nabla_{\theta} J$$

• We now have

Now:  

$$\theta^{t+1} = \theta^{t} + H^{-1} \nabla_{\theta} \ell$$

$$= \left( X^{T} W^{t} X \right)^{-1} \left[ X^{T} W^{t} X \theta^{t} + X^{T} (y - \mu^{t}) \right]$$

$$= \left( X^{T} W^{t} X \right)^{-1} X^{T} W^{t} z^{t}$$
where the adjusted response is
$$z^{t} = X \theta^{t} + \left( W^{t} \right)^{-1} (y - \mu^{t})$$

• This can be understood as solving the following " Iteratively reweighted least squares " problem

$$\theta^{t+1} = \arg\min_{\theta} (z - X\theta)^T W (z - X\theta)$$

# Example 1: logistic regression (sigmoid classifier)

• The condition distribution: a Bernoulli

$$p(y | x) = \mu(x)^{y} (\mathbf{1} - \mu(x))^{1-y}$$

where  $\mu$  is a logistic function

$$\mu(x) = \frac{1}{1 + e^{-\eta(x)}}$$



- p(y|x) is an exponential family function, with
  - mean:  $E[y | x] = \mu = \frac{1}{1 + e^{-\eta(x)}}$
  - and canonical response function

$$\eta = \xi = \theta^T x$$

IRLS 
$$\frac{d\mu}{d\eta} = \mu(1-\mu)$$
$$W = \begin{pmatrix} \mu_1(1-\mu_1) & & \\ & \ddots & \\ & & \mu_N(1-\mu_N) \\ & & & \vdots \\ & & & \vdots \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ &$$

# Logistic regression: practical issues



• It is very common to use *regularized* maximum likelihood.

$$p(y = \pm \mathbf{1} | x, \theta) = \frac{1}{\mathbf{1} + e^{-y\theta^T x}} = \sigma(y\theta^T x)$$
$$p(\theta) \sim \text{Normal}(\mathbf{0}, \lambda^{-1}I)$$
$$l(\theta) = \sum_n \log(\sigma(y_n\theta^T x_n)) - \frac{\lambda}{2}\theta^T \theta$$

- IRLS takes  $O(Nd^3)$  per iteration, where N = number of training cases and d = dimension of input x.
- Quasi-Newton methods, that approximate the Hessian, work faster.
- Conjugate gradient takes O(Nd) per iteration, and usually works best in practice.
- Stochastic gradient descent can also be used if *N* is large c.f. perceptron rule:

 $\nabla_{\theta} \boldsymbol{\ell} = (\mathbf{1} - \boldsymbol{\sigma}(\boldsymbol{y}_{n} \boldsymbol{\theta}^{T} \boldsymbol{x}_{n})) \boldsymbol{y}_{n} \boldsymbol{x}_{n} - \lambda \boldsymbol{\theta}$ 

#### **Example 2: linear regression**

• The condition distribution: a Gaussian  $p(y|x,\theta,\Sigma) = \frac{1}{(2\pi)^{k/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(y-\mu(x))^T \Sigma^{-1}(y-\mu(x))\right\}$ Rescale  $\Rightarrow h(x) \exp\left\{-\frac{1}{2}\Sigma^{-1}(\eta^T(x)y - A(\eta))\right\}$ where  $\mu$  is a linear function

$$\mu(x) = \theta^T x = \eta(x)$$



• mean:

 $E[y \mid x] = \mu = \theta^T x$ 

and canonical response function

$$\eta_1 = \xi = \theta^T x$$

• IRLS  $\frac{d\mu}{d\eta} = 1$  $= \begin{pmatrix} X^T W^t X \end{pmatrix}^{-1} X^T W^t z^t$  $= \begin{pmatrix} X^T X \end{pmatrix}^{-1} X^T (X \theta^t + (y - \mu^t))$ W = I $= \theta^t + \begin{pmatrix} X^T X \end{pmatrix}^{-1} X^T (y - \mu^t)$ 

Steepest descent © Eric Xing @ CMU, 2005-2014

$$\stackrel{\rightarrow \infty}{\Rightarrow} \quad \theta = (X^T X)^{-1} X^T Y$$

Normal equation 29



x



## Density estimation

Parametric and nonparametric methods

#### Regression

Linear, conditional mixture, nonparametric

#### Classification

Generative and discriminative approach

# Simple GMs are the building blocks of complex BNs











#### **MLE for general BNs**



• If we assume the parameters for each CPD (a GLIM) are globally independent, and all nodes are fully observed, then the log-likelihood function decomposes into a sum of local terms, one per node:

$$\boldsymbol{\ell}(\boldsymbol{\theta};\boldsymbol{D}) = \log p(\boldsymbol{D} \mid \boldsymbol{\theta}) = \log \prod_{n} \left( \prod_{i} p(\boldsymbol{x}_{n,i} \mid \boldsymbol{x}_{n,\pi_{i}}, \boldsymbol{\theta}_{i}) \right) = \sum_{i} \left( \sum_{n} \log p(\boldsymbol{x}_{n,i} \mid \boldsymbol{x}_{n,\pi_{i}}, \boldsymbol{\theta}_{i}) \right)$$

• Therefore, MLE-based parameter estimation of GM reduces to local est. of each GLIM

#### How to define parameter prior?



Local Distributions

Factorization:  $p(\mathbf{X} = \mathbf{x}) = \prod_{i=1}^{m} p(x_i | \mathbf{x}_{\pi_i})$ 

defined by, e.g., multinomial parameters:

 $p(x_i^k \mid \mathbf{x}_{\pi_i}^j) = \boldsymbol{\theta}_{x_i^k \mid \mathbf{x}_{\pi_i}^j}$ 

Assumptions (Geiger & Heckerman 97,99):

- Complete Model Equivalence
- Global Parameter Independence
- Local Parameter Independence
- Likelihood and Prior Modularity Eric Xing @ CMU, 2005-2014



### Parameter Independence, Graphical View





Provided all variables are observed in all cases, we can perform Bayesian update each parameter independently !!!

### Which PDFs Satisfy Our Assumptions? (Geiger & Heckerman 97,99)

• **Discrete DAG Models:**  $x_i \mid \pi_{x_i}^j \sim \text{Multi}(\theta)$ 

$$P(\theta) = \frac{\Gamma(\sum_{k} \alpha_{k})}{\prod_{k} \Gamma(\alpha_{k})} \prod_{k} \theta_{k}^{\alpha_{k}-1} = C(\alpha) \prod_{k} \theta_{k}^{\alpha_{k}-1}$$

• Gaussian DAG Models:  $x_i \mid \pi_{x_i}^j \sim \text{Normal}(\mu, \Sigma)$ 

Normal prior: 
$$p(\mu | \nu, \Psi) = \frac{1}{(2\pi)^{n/2} |\Psi|^{1/2}} \exp\left\{-\frac{1}{2}(\mu - \nu)'\Psi^{-1}(\mu - \nu)\right\}$$

Normal-Wishart prior:

$$p(\mu | \nu, \alpha_{\mu}, \mathbf{W}) = \operatorname{Normal}(\nu, (\alpha_{\mu}\mathbf{W})^{-1}),$$
  
$$p(\mathbf{W} | \alpha_{w}, \mathbf{T}) = c(n, \alpha_{w}) |\mathbf{T}|^{\alpha_{w}/2} |\mathbf{W}|^{(\alpha_{w}-n-1)/2} \exp\left\{\frac{1}{2}\operatorname{tr}\left\{\mathbf{TW}\right\}\right\},$$

where  $\mathbf{W} = \Sigma^{-1}$ .

### **Summary: Parameterizing GM**

- For exponential family dist., MLE amounts to moment matching
- GLIM:
  - Natural response
  - Iteratively Reweighted Least Squares as a general algorithm
- GLIMs are building blocks of most GMs in practical use
- Parameter independence and appropriate priors