NUS National University of Singapore | School of Computing

CS5340
Uncertainty Modeling in AI

Lecture 7:
Parameter Learning with Complete Data

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AY 2018/19

Semester 1

Course Schedule

Week	Date	Topic	Remarks
1	15 Aug	Introduction to probabilities and probability distributions	
2	22 Aug	Fitting probability models	Hari Raya Haji*
3	29 Aug	Bayesian networks (Directed graphical models)	
4	05 Sep	Markov random Fields (Undirected graphical models)	
5	12 Sep	I will be traveling	No Lecture
6	19 Sep	Variable elimination and belief propagation	
-	26 Sep	Recess week	No lecture
7	03 Oct	Factor graph and the junction tree algorithm	
8	10 Oct	Parameter learning with complete data	
9	17 Oct	Mixture models and the EM algorithm	
10	24 Oct	Hidden Markov Models (HMM)	
11	31 Oct	Monte Carlo inference (Sampling)	
12	07 Nov	Variational inference	
13	14 Nov	Graph-cut and alpha expansion	

* **Make-up lecture**: 25 Aug (Sat), 9.30am-12.30pm, LT 15

Acknowledgements

- A lot of slides and content of this lecture are adopted from:

1. Michael I. Jordan “An introduction to probabilistic graphical models”, 2002, Chapter 9
2. Kevin Murphy, “Machine learning: a probabilistic approach”, Chapters 10.4, 19.5, and 19.6.3
3. Daphne Koller and Nir Friedman, “Probabilistic graphical models”, Chapter 17
4. David Barber, “Bayesian reasoning and machine learning”, Chapters 9.1, 9.2, 9.3, 9.4, 9.6

Learning Outcomes

- Students should be able to:

1. Compute the unknown parameters of discrete/continuous **DGMs** using MLE and MAP.
2. Compute the unknown parameters of **MRFs** using stochastic maximum likelihood, and iterative proportional fitting.
3. Compute the unknown parameters of **CRFs** using stochastic gradient descent.

Motivation

- From lecture 2, we know how to get the unknown parameter θ of a single random variable probability distributions $p(x|\theta)$ from observed data.

- In lectures 5 and 6, we learned how to do exact inference given a DGM/UGM $p(x_1, \dots, x_M|\theta)$ with multiple random variables.

Motivation

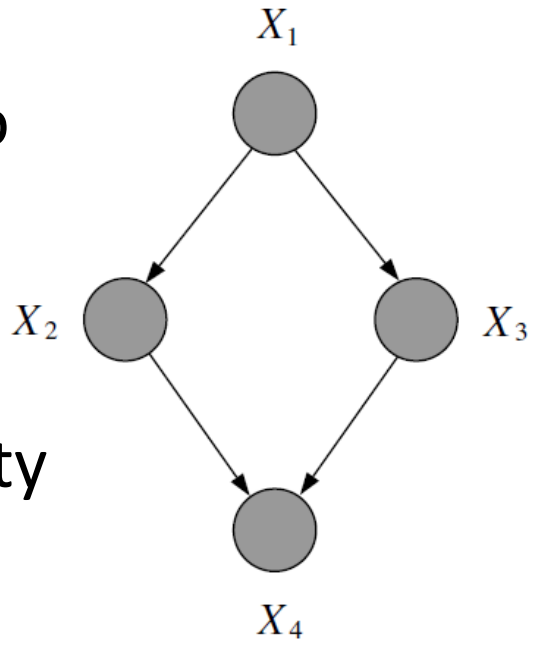
- We will now look into the details of the unanswered question on:

How to get the unknown parameter θ of a DGM/UGM $p(x_1, \ldots, x_M|\theta)$ from fully observed data?

The Basic Idea

- Let's first consider a simple example to illustrate the basic idea.

- The graphical model shown in the figure has the following joint probability distribution:



$$p(x \mid \theta) = p(x_1 \mid \theta_1)p(x_2 \mid x_1, \theta_2)p(x_3 \mid x_1, \theta_3)p(x_4 \mid x_2, x_3, \theta_4).$$

Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

The Basic Idea

- Finding the maximum log-likelihood of each parameter θ_i can be carried out independently!

$$p(x \mid \theta) = p(x_1 \mid \theta_1)p(x_2 \mid x_1, \theta_2)p(x_3 \mid x_1, \theta_3)p(x_4 \mid x_2, x_3, \theta_4).$$

Taking the log of $p(x|\theta)$ converts the product into sums

$$\log p(x|\theta) = \log p(x_1|\theta_1) + \log p(x_2|x_1, \theta_2) + \log p(x_3|x_1, \theta_3) + \log(x_4|x_2, x_3, \theta_4)$$

Maximum log-likelihood of θ_1:

$$\underset{\theta_1}{\operatorname{argmax}} \log p(x|\theta) = \underset{\theta_1}{\operatorname{argmax}} \{\log p(x_1|\theta_1) + \log p(x_2|x_1, \theta_2) + \log p(x_3|x_1, \theta_3) + \log(x_4|x_2, x_3, \theta_4)\}$$

$$= \underset{\theta_1}{\operatorname{argmax}} \log p(x_1|\theta_1)$$

independent of θ_1, hence can be removed

The Basic Idea

- In general, the maximum log-likelihood of each parameter θ_i is given by:

$$\underset{\theta_i}{\operatorname{argmax}} \log p(x|\theta) = \underset{\theta_i}{\operatorname{argmax}} \log p\left(x_i \middle| x_{\pi_i}, \theta_i\right)$$

- Equivalent to solving separate maximum likelihood problems for each node conditioned on its parents.

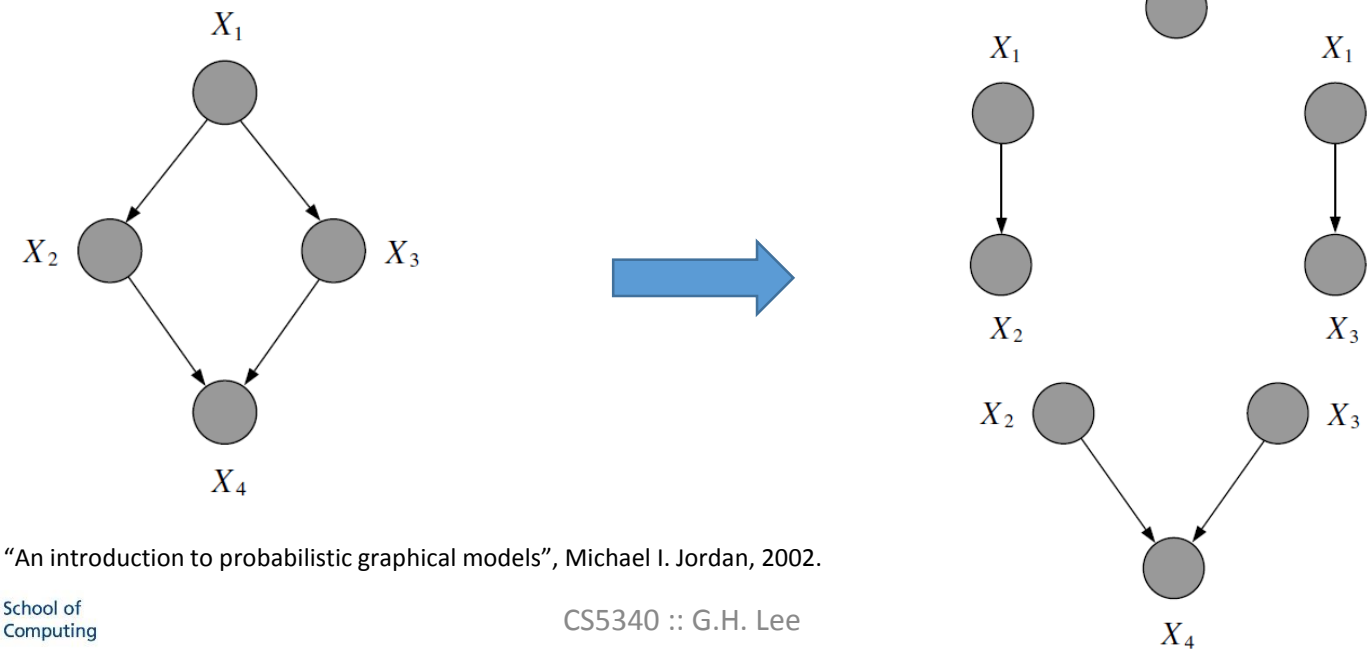


Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

The Basic Idea

- In similar vein, we can solve for the Maximum a Posterior (MAP) of each parameter separately:

$$\underset{\theta_i}{\operatorname{argmax}} \log p(\theta|x) = \underset{\theta_i}{\operatorname{argmax}} \log p(x|\theta)p(\theta)$$

$$= \underset{\theta_i}{\operatorname{argmax}} \{\log p(x_i|x_{\pi_i}, \theta_i) + \log p(\theta_i)\}$$

where $\theta = (\theta_1, \ldots, \theta_M)$

Parameter Learning: DGM

- Let $G = (U, E)$ be a directed graph, where U is the set of nodes and E the set of edges.
- We associate a random vector X with the graph, where vector components are indexed by the nodes.
- X_u denotes the random variable associated with node $u \in U$, and x_u denotes a realization of X_u.

Parameter Learning: DGM

- To each node $u \in U$, we associate a local conditional probability distribution $p(x_u|x_{\pi_u}, \theta_u)$.
- π_u denotes the set of indices of the parents of u and where θ_u is a parameter vector.
- The overall probability associated with the graph G is a product of the local probabilities:

$$p(x_U|\theta) = \prod_{u \in U} p\left(x_u|x_{\pi_u}, \theta_u\right), \qquad \theta = \left(\theta_1, \ldots, \theta_{|U|}\right)$$

Complete Observation

A complete observation is an assignment of values to ALL of the random variables X_U in the model.

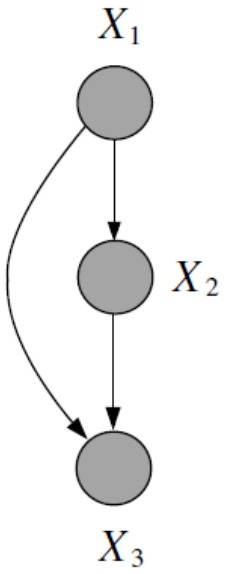


Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

Complete Observation

- In many problems, data are assumed to consists of a set of N independent, identically distributed (i.i.d.) observations.
- Requires no special treatment within the graphical model formalism – we simply replicate the basic graph structure N times.

Complete Observation

- For N i.i.d. observations, the graphical model simply becomes an augmentation of N disconnected replicates of G.

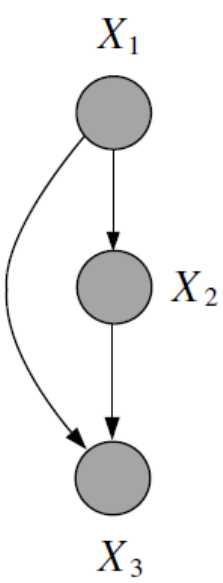
- We denote the augmented graphical model as:

$$G^{(N)} = \left(U^{(N)}, E^{(N)}\right)$$

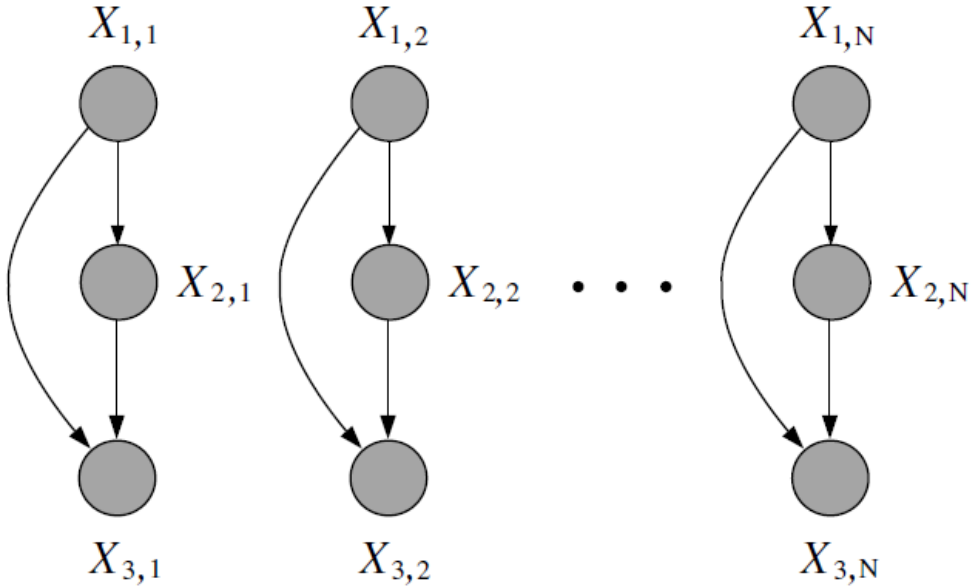
- Nodes $U^{(N)}$ are indexed using a pair of labels (u, n), where $u \in U$ designates a node in G and $n \in \{1, \ldots, N\}$ designates the replication number.

Complete Observation

Example:



A graphical model G, where $U = \{1,2,3\}$



$G^{(N)}$ obtained by making N replicates of G

n^{th} complete observation is denoted $X_{U,n} = (x_{1,n}, x_{2,n}, x_{3,n})$

Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

Complete Observation

- We can write the entire set of observed data in the completely observed setting as:

$$\mathcal{D} = (x_{U,1}, x_{U,2}, \ldots, x_{U,N})$$

- The probability model for $G^{(N)}$ is thus given by:

$$p(\mathcal{D} \mid \theta) = \prod_n p(x_{U,n} \mid \theta) \quad \text{(Naïve Bayes)}$$

$$= \prod_n \prod_u p(x_{u,n} \mid x_{\pi_u,n}, \theta_u)$$

$$\Rightarrow \log p(\mathcal{D}|\theta) = \sum_n \sum_u \log p(x_{u,n}|x_{\pi_u,n}, \theta_u) \quad \text{Log-likelihood}$$

Maximum Log-Likelihood

- Taking the maximum log-likelihood over parameter θ_u gives:

$$\underset{\theta_u}{\operatorname{argmax}} \log p(\mathcal{D}|\theta) = \underset{\theta_u}{\operatorname{argmax}} \sum_n \log p(x_{u,n}|x_{\pi_u,n}, \theta_u)$$

- We can ignore all terms that do not involve θ_u.

- Implies that it is sufficient to estimate θ_u with the local subset of observations:

$$\{x_{u,n}, x_{\pi_u,n}\}_{n=1}^{N}$$

Maximum A Posteriori (MAP)

- Taking the maximum a posteriori (MAP) over parameter θ_u gives:

$$\underset{\theta_u}{\operatorname{argmax}} \log p(\theta \,|\mathcal{D}) =$$

$$\underset{\theta_u}{\operatorname{argmax}} \left\{ \sum_n \log p(x_{u,n}|x_{\pi_u,n}, \theta_u) + \log p(\theta_u) \right\}$$

- $p(\theta_u)$ is the conjugate prior of the likelihood distribution.

Maximum Log-Likelihood: Discrete Case

- Likelihood is given by Categorical distribution:

$$p\left(x_u \middle| x_{\pi_u}, \lambda_u\right) = \mathrm{Cat}_{x_u|x_{\pi_u}}[\lambda_u]$$

$$= \prod_{c=1}^{C} \prod_{k=1}^{K} \lambda_{uck}^{x_{uck}} = \lambda_{uck}, \quad s.t. \quad \sum_k \lambda_{uck} = 1$$

- The parameter $\lambda_u = \{\lambda_{u11}, \dots, \lambda_{uck}, \dots, \lambda_{uCK}\}$.
- C is total number of states that X_{π_u} takes, and K is the total number of states that X_u takes.
- $X_{uck} = 1$ when $X_u = k$ and $X_{\pi_u} = c$, $X_{uck} = 0$ otherwise.

Maximum Log-Likelihood: Discrete Case

- Putting the likelihood into the maximum log-likelihood, we get:

$$\underset{\lambda_{uc1}, \ldots, \lambda_{ucK}}{\operatorname{argmax}} \sum_{n=1}^{N} \sum_{c=1}^{C} \sum_{k=1}^{K} \log \lambda_{uck}^{x_{uck,n}}, \quad s.t. \quad \sum_k \lambda_{uck} = 1$$

- Sum over c is dropped since we optimize over the parameters of each configuration of X_{π_u}:

$$\Longrightarrow \underset{\lambda_{uc1}, \ldots, \lambda_{ucK}}{\operatorname{argmax}} \sum_{n=1}^{N} \sum_{k=1}^{K} \log \lambda_{uck}^{x_{uck,n}}, \quad s.t. \quad \sum_k \lambda_{uck} = 1$$

times we observe ($x_u = k, x_{\pi_u} = c$)

$$\Longrightarrow \underset{\lambda_{uc1}, \ldots, \lambda_{ucK}}{\operatorname{argmax}} \sum_{k=1}^{K} \log \lambda_{uck}^{N_{uck}}, \quad s.t. \quad \sum_k \lambda_{uck} = 1$$

Maximum Log-Likelihood: Discrete Case

- Applying Lagrange multiplier ν on the constraint, we get the auxiliary function :

$$\mathcal{L} = \sum_{k=1}^{K} N_{uck} \log \lambda_{uck} + \upsilon \left(\sum_{k} \lambda_{uck} - 1 \right)$$

- Take derivative of $\mathcal{L}$ w.r.t λ_{uck} and υ, set to zero and solve for λ_{uck}:

$$\hat{\lambda}_{uck} = \frac{N_{uck}}{\sum_{m=1}^{K} N_m}$$

Normalized counts of # times we observed $x_u = k, x_{\pi_u} = c$

Maximum A Posteriori: Discrete Case

- We use the Dirichlet distribution as conjugate prior:

$$p(\lambda_{uc1}, \dots, \lambda_{ucK}) = \mathrm{Dir}_{\lambda_{uc1,\dots,ucK}}[\alpha_{uc1}, \dots \alpha_{ucK}]$$

$$= \frac{\Gamma[\sum_{k=1}^{K} \alpha_{uck}]}{\prod_{k=1}^{K} \Gamma[\alpha_{uck}]} \prod_{k=1}^{K} \lambda_{uck}^{\alpha_{uck}-1},$$

$$\text{s.t. } \lambda_{uck} \in [0,1],\ \sum_k \lambda_{uck} = 1$$

- K hyperparameters $\alpha_{uck} > 1$ for each random variable X_u and a state of its parents $X_{\pi_u} = c$.

Maximum A Posteriori: Discrete Case

- Putting the conjugate prior into

$$\underset{\lambda_u}{\text{argmax}}\left\{\sum_n \log p(x_{u,n}|x_{\pi_u,n},\lambda_u) + \log p(\lambda_u)\right\},$$

- We get:

$$\underset{\lambda_{uc1},\ldots,\lambda_{ucK}}{\text{argmax}} \left\{\sum_n \log \text{Cat}_{x_{u,n}|x_{\pi_u,n}}[\lambda_u] + \log \text{Dir}_{\lambda_{uc1\ldots ucK}}[\alpha_{uc1},\ldots \alpha_{ucK}]\right\}, \text{ s.t. } \sum_k \lambda_{uck} = 1$$

Independent of λ_{uck}

$$= \underset{\lambda_{uc1},\ldots,\lambda_{ucK}}{\text{argmax}} \left\{\sum_k \left(\sum_n \log \lambda_{uck}^{x_{uck,n}} + \log \lambda_{uck}^{\alpha_{uck}-1}\right) + \log \frac{\Gamma[\sum_{k=1}^K \alpha_{uck}]}{\prod_{k=1}^K \Gamma[\alpha_{uck}]}\right\}, \text{ s.t. } \sum_k \lambda_{uck} = 1$$

times we observe ($x_u = k, x_{\pi_u} = c$)

$$= \underset{\lambda_{uc1},\ldots,\lambda_{ucK}}{\text{argmax}} \left\{\sum_k \left(\log \lambda_{uck}^{N_{uck} + \alpha_{uck} - 1}\right)\right\}, \qquad \text{s.t. } \sum_k \lambda_{uck} = 1$$

Maximum A Posteriori: Discrete Case

- Applying Lagrange multiplier ν on the constraint, we get the auxiliary function :

$$\mathcal{L} = \sum_{k=1}^{K} (N_{uck} + \lambda_{uck} - 1) \log \lambda_{uck} + \upsilon \left(\sum_{k} \lambda_{uck} - 1 \right)$$

- Take derivative of $\mathcal{L}$ w.r.t λ_{uck} and υ, set to zero and solve for λ_{uck}:

$$\hat{\lambda}_{uck} = \frac{N_{uck} + \alpha_{uck} - 1}{\sum_{m=1}^{K} (N_{ucm} + \alpha_{ucm} - 1)}$$

Maximum Log-Likelihood: Continuous Case

- Likelihood is given by linear-Gaussian model:

$$p\left(x_u \middle| x_{\pi_u}, \theta_{x_u|x_{\pi_u}}\right) = \text{Norm}_{x_u|x_{\pi_u}}[w_{u0}, \ldots, w_{uC}, \sigma_u^2]$$

$$= \frac{1}{\sqrt{2\pi\sigma_u^2}} \exp\left\{-0.5 \frac{\left(x_u - \left(\sum_{c \in x_{\pi_u}} w_{uc} x_{uc} + w_{u0}\right)\right)^2}{\sigma_u^2}\right\}$$

- The parameter $\theta_{x_u|x_{\pi_u}} = \{w_{u0}, \ldots, w_{uC}, \sigma_u^2\}$.
- Mean $\mu_u = \sum_{c \in x_{\pi_u}} w_{uc} x_{uc} + w_{u0}$ is a weighted sum of the parent nodes x_{π_u}.
- C is the total number of parent nodes.

Maximum Log-Likelihood: Continuous Case

- Putting the likelihood into the maximum log-likelihood, we get:

$$\underset{\theta_{x_u|x_{\pi_u}}}{\text{argmax}} \sum_{n=1}^{N} \log p(x_{u,n}|x_{\pi_u,n}, \theta_{x_u|x_{\pi_u}})$$

$$= \underset{\theta_{x_u|x_{\pi_u}}}{\text{argmax}} \sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma_u^2}} \exp\left\{-\frac{\left(x_{u,n}-\left(\sum_{c\in x_{\pi_u}} w_{uc}x_{uc,n}+w_{u0}\right)\right)^2}{2\sigma_u^2}\right\}$$

$$= \underset{\theta_{x_u|x_{\pi_u}}}{\text{argmax}} \sum_{n=1}^{N} \underbrace{\left\{-\frac{1}{2}\log(2\pi\sigma_u^2) - \frac{1}{2\sigma_u^2}\left(x_{u,n} - \left(\sum_{c\in x_{\pi_u}} w_{uc}x_{uc,n} + w_{u0}\right)\right)^2\right\}}_{L}$$

Maximum Log-Likelihood: Continuous Case

- Take the derivative of L w.r.t to $w_{u0,}\, w_{uc}$ and equating to zero, we get $C + 1$ equations:

$$\frac{\partial L}{\partial w_{u0}} = \sum_{n=1}^{N} \left(x_{u,n} - \left(w_{u1} x_{u1,n} + \ \ldots + \ w_{uC} x_{uC,n} + w_{u0} \right) \right) = 0$$

$$\frac{\partial L}{\partial w_{u1}} = \sum_{n=1}^{N} \left(x_{u,n} - \left(w_{u1} x_{u1,n} + \ \ldots + \ w_{uC} x_{uC,n} + w_{u0} \right) \right) x_{u1,n} = 0$$

$$\vdots$$

$$\frac{\partial L}{\partial w_{uC}} = \sum_{n=1}^{N} \left(x_{u,n} - \left(w_{u1} x_{u1,n} + \ \ldots + \ w_{uC} x_{uC,n} + w_{u0} \right) \right) x_{uC,n} = 0$$

- Which can be used to solve for the $C + 1$ unknowns $w_{u0,}\, w_{u1}, \ldots w_{uC}$.

- Finally, take the derivative of L w.r.t to σ_u^2 and equate to zero, to solve for σ_u^2.

Maximum A Posteriori: Continuous Case

- We define the prior of the linear Gaussian parameters $\theta_{x_u|x_{\pi_u}} = \{w_{u0}, \ldots, w_{uC}, \sigma_u^2\}$ as:

$$p(w_{u0}, \ldots w_{uC}, \sigma_u^2) = p(\sigma_u^2)p(w_{u0}, \ldots w_{uC}|\sigma_u^2)$$

$$= p(\sigma_u^2) \prod_{c \in x_{\pi_u}} p(w_{uc}|\sigma_u^2) \qquad \text{(Naïve Bayes)}$$

- $p(w_{uc}|\sigma_u^2)$ follows the univariate normal distribution:

$$p(w_{uc}|\mu_u, \sigma_u^2) = \frac{1}{\sqrt{2\pi\sigma_u^2}} \exp - \frac{(w_{uc} - \mu_u)^2}{2\sigma_u^2} = \text{Norm}_{w_{uc}}[\mu_u, \sigma_u^2]$$

- where μ_u is a hyperparameter.

Maximum A Posteriori: Continuous Case

- $p(\sigma_u^2)$ follows the inverse gamma distribution:

$$p(\sigma_u^2|\alpha_u,\beta_u) = \frac{\beta_u^{\alpha_u}}{\Gamma(\alpha_u)}(\sigma_u^2)^{-\alpha_u-1}\exp\left(-\frac{\beta_u}{\sigma_u^2}\right) = \text{InvGam}_{\sigma_u^2}[\alpha_u,\beta_u]$$

- (α_u,β_u) are the hyperparameters that describe the shape and scale of the distribution.
- $\alpha_u > 0$ and $\beta_u > 0$.
- $\Gamma(\alpha_u)$ denotes the gamma function.

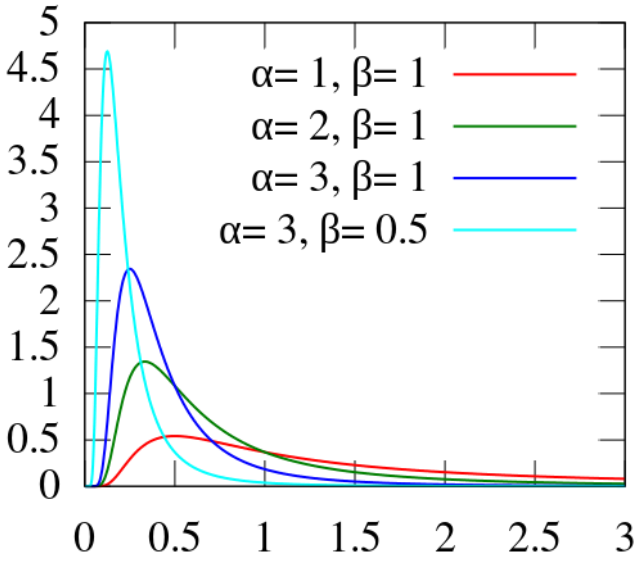


Image source: https://en.wikipedia.org/wiki/Inverse-gamma_distribution

Maximum A Posteriori: Continuous Case

- Putting the likelihood and conjugate prior into

$$\underset{\theta_{x_u|x_{\pi_u}}}{\text{argmax}} \left\{ \sum_n \log p(x_{u,n}|x_{\pi_u,n}, \theta_{x_u|x_{\pi_u}}) + \log \underbrace{p(\theta_{x_u|x_{\pi_u}})}_{p(\sigma_u^2)p(w_{u0},\ldots w_{uC}|\sigma_u^2)} \right\},$$

- We get:

$$\underset{\theta_{x_u|x_{\pi_u}}}{\text{argmax}} \{ \sum_n \log \text{Norm}_{x_{u,n}|x_{\pi_u,n}}[w_{u0}, \ldots, w_{uC}, \sigma_u^2] + \underbrace{\log \text{InvGam}_{\sigma_u^2}[\alpha_u, \beta_u] + \sum_c \log p(w_{uc}|\sigma_u^2)}_{L} \}$$

Maximum A Posteriori: Continuous Case

- Take the derivative of L w.r.t to $w_{u0,}\, w_{uc}$ and equating to zero:

$$\frac{\partial L}{\partial w_{u0}} = 0$$
$$\frac{\partial L}{\partial w_{u1}} = 0$$
$$\vdots$$
$$\frac{\partial L}{\partial w_{uC}} = 0$$

$C + 1$ equations to solve for the $C + 1$ unknowns $\{w_{u0}, \ldots, w_{uC}\}$.

- Finally, take the derivative of L w.r.t to σ_u^2 and equate to zero, to solve for σ_u^2.

Parameter Learning: UGM (MRF)

- Consider a Markov Random Field (MRF) in log-linear form, where c indexes the cliques:

$$p(\mathbf{y}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\sum_c \boldsymbol{\theta}_c^T \boldsymbol{\phi}_c(\mathbf{y})\right)$$

- The scaled log-likelihood is given by:

$$\ell(\boldsymbol{\theta}) \triangleq \frac{1}{N} \sum_{i}^{N} \log p(\mathbf{y}_i|\boldsymbol{\theta}) = \frac{1}{N} \sum_{i}^{N} \left[\sum_c \boldsymbol{\theta}_c^T \boldsymbol{\phi}_c(\mathbf{y}_i) - \log Z(\boldsymbol{\theta})\right]$$

Parameter Learning: UGM (MRF)

- Since MRFs are in the exponential family, we know that this function is convex in θ.
- So it has a unique global maximum, which we can find using gradient-based optimizers.
- In particular, the derivative for the weights of a particular clique c is given by:

$$\frac{\partial \ell}{\partial \boldsymbol{\theta}_c} = \frac{1}{N} \sum_i^N \left[\boldsymbol{\phi}_c(\mathbf{y}_i) - \frac{\partial}{\partial \boldsymbol{\theta}_c} \log Z(\boldsymbol{\theta}) \right]$$

Parameter Learning: UGM (MRF)

- The derivative of the log partition function w.r.t. θ_c is the expectation of the c^{th} feature under the model:

$$\frac{\partial \log Z(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_c} = \mathbb{E}\left[\phi_c(\mathbf{y})|\boldsymbol{\theta}\right] = \sum_{\mathbf{y}} \phi_c(\mathbf{y}) p(\mathbf{y}|\boldsymbol{\theta})$$

Proof:

$$\frac{\partial \log Z(\theta)}{\partial \theta_c} = \frac{1}{Z(\theta)} \frac{\partial Z(\theta)}{\partial \theta_c}, \quad \text{where} \quad Z(\theta) = \sum_y \exp\left(\sum_c \theta_c^T \phi_c(y)\right)$$

$$\Rightarrow \frac{\partial Z(\theta)}{\partial \theta_c} = \sum_y \exp\left(\sum_c \theta_c^T \phi_c(y)\right) \phi_c(y)$$

$$\Rightarrow \frac{\partial \log Z(\theta)}{\partial \theta_c} = \frac{1}{Z(\theta)} \sum_y \phi_c(y) \exp\left(\sum_c \theta_c^T \phi_c(y)\right)$$

$$= \sum_y \phi_c(y) \underbrace{\frac{1}{Z(\theta)} \exp\left(\sum_c \theta_c^T \phi_c(y)\right)}_{p(y|\theta)} = \sum_y \phi_c(y)\ p(y|\theta)$$

Parameter Learning: UGM (MRF)

- Hence the gradient of the log-likelihood is:

$$\frac{\partial \ell}{\partial \boldsymbol{\theta}_c} = \underbrace{\left[\frac{1}{N}\sum_{i}^{N} \boldsymbol{\phi}_c(\mathbf{y}_i)\right]}_{\text{Clamped term}} - \underbrace{\mathbb{E}\left[\boldsymbol{\phi}_c(\mathbf{y})\right]}_{\text{Unclamped/contrastive term}}$$

- Clamped term: y is fixed to its observed values.
- Unclamped/contrastive term: y is a free variable.
- Unclamped term requires inference in the model, once per gradient step, and this makes UGM learning much slower than DGM.

Parameter Learning: UGM (MRF)

- Gradient of the log-likelihood can be rewritten as:

$$\frac{\partial l}{\partial \theta_c} = E_{p_{emp}}[\phi_c(y)] - E_{p(y|\theta)}[\phi_c(y)]$$

- $E_{p_{emp}}[\phi_c(y)] = \frac{1}{N}\sum_{n=1}^{N}\phi_c(y_i)$: Expected feature vector according to the empirical distribution.

- $E_{p(y|\theta)}[\phi_c(y)]$: Expected feature vector according to the model's distribution.

Parameter Learning: UGM (MRF)

- At the optimum, the gradient will be zero:

$$E_{p_{emp}}[\phi_c(y)] - E_{p(y|\theta)}[\phi_c(y)] = 0$$

- **Problem**: $E_{p(y|\theta)}[\phi_c(y)] = \sum_y \phi_c(y)\ p(y|\theta)$ cannot be evaluated in closed-form in terms of the unknown parameters θ!

We **CANNOT** solve for the parameters θ in closed-from!!!

Parameter Learning: UGM (MRF)

Solution:

Use gradient-based optimizers!

- However, the gradient requires inference:

Requires sum over all states of y, which is intractable

$$\frac{\partial l}{\partial \theta_c} = E_{p_{emp}}[\phi_c(y)] - E_{p(y|\theta)}[\phi_c(y)]$$

- Gradient is intractable, hence learning also becomes intractable.
- We can combine approximate inference with gradient-based learning.

Method 1: Stochastic Maximum Likelihood

- This is a stochastic gradient descent method.
- We iteratively updates the parameter θ_{k+1} at the k step using the parameter and gradient from the previous step:

$$\theta_{k+1} \leftarrow \theta_k - \eta g_k$$

- η is the step size, or learning rate.
- $g_k \approx \frac{\partial l}{\partial \theta_c}$ is the gradient that can be approximated with Markov Chain Monte Carlo (MCMC), i.e. sampling.

Method 1: Stochastic Maximum Likelihood

Algorithm : Stochastic maximum likelihood for fitting an MRF

Initialize weights $\boldsymbol{\theta}$ randomly;
$k = 0$, $\eta = 1$;
for *each epoch* **do**
  for *each minibatch of size* B **do** // split the observed data $\mathrm{y}_i, \forall i = 1 \ldots N$ into sets of size B
    for *each sample* $s = 1 : S$ **do**
      Sample $\mathbf{y}^{s,k} \sim p(\mathbf{y}|\boldsymbol{\theta}_k)$;
    $\hat{E}(\phi(\mathbf{y})) = \frac{1}{S}\sum_{s=1}^{S} \phi(\mathbf{y}^{s,k})$;
    for *each training case* i *in minibatch* **do**
      $\mathbf{g}_{ik} = \phi(\mathbf{y}_i) - \hat{E}(\phi(\mathbf{y}))$;
    $\mathbf{g}_k = \frac{1}{B}\sum_{i \in B} \mathbf{g}_{ik}$;
    $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \mathbf{g}_k$;
    $k = k + 1$;
    Decrease step size η;

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

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6 Sample $\mathbf{y}^{s,k} \sim p(\mathbf{y}|\boldsymbol{\theta}_k)$;
7 $\hat{E}(\phi(\mathbf{y})) = \frac{1}{S}\sum_{s=1}^{S} \phi(\mathbf{y}^{s,k})$;
8 **for** *each training case* i *in minibatch* **do**
9 $\mathbf{g}_{ik} = \phi(\mathbf{y}_i) - \hat{E}(\phi(\mathbf{y}))$;
10 $\mathbf{g}_k = \frac{1}{B}\sum_{i \in B} \mathbf{g}_{ik}$;
11 $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \mathbf{g}_k$;
12 $k = k + 1$;
13 Decrease step size η;

// split the observed data $\mathrm{y}_i, \forall i = 1 \ldots N$ into sets of size B

// draw S samples from the model's distribution $p(y|\theta_k)$

// note that we fixed the parameter at θ_k (current estimate)

* We will discuss more about MCMC sampling in Lecture 10

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

Method 1: Stochastic Maximum Likelihood

Algorithm : Stochastic maximum likelihood for fitting an MRF

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// split the observed data $\mathrm{y}_i, \forall i = 1 \ldots N$ into sets of size B

// draw S samples from the posterior distribution $p(y|\theta_k)$

// note that we fixed the parameter at θ_k (current estimate)

// compute the approximated gradient, $g_k \approx \frac{\partial l}{\partial \theta}$

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

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7 $\hat{E}(\phi(\mathbf{y})) = \frac{1}{S}\sum_{s=1}^{S} \phi(\mathbf{y}^{s,k})$; // note that we fixed the parameter at θ_k (current estimate)
8 **for** *each training case* i *in minibatch* **do**
9 $\mathbf{g}_{ik} = \phi(\mathbf{y}_i) - \hat{E}(\phi(\mathbf{y}))$; // compute the approximated gradient, $g_k \approx \frac{\partial l}{\partial \theta}$
10 $\mathbf{g}_k = \frac{1}{B}\sum_{i \in B} \mathbf{g}_{ik}$;
11 $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \mathbf{g}_k$; // stochastic gradient descent update step
12 $k = k + 1$;
13 Decrease step size η;

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

Method 2: Iterative Proportional Fitting (IFP)

- An alternative derivation of the gradient in term of $\psi_c(y_c|\theta_c)$ is given by:

$$\ell(\theta) = \log \prod_i \frac{1}{Z(\theta)} \prod_c \psi_c(y_{i,c}|\theta_c)$$

$$= \sum_i \sum_c \log \psi_c(y_{i,c}|\theta_c) - N \log Z(\theta)$$

$$= \sum_c \sum_{y_c} \underbrace{N(y_c)} \log \psi_c(y_c|\theta_c) - N \log Z(\theta)$$

$N(y_c) = \sum_i \delta(y_c, y_{i,c})$: # times clique c is in configuration y_c in the data

$$\Rightarrow \frac{\partial \ell(\theta)}{\partial \psi_c(y_c)} = \frac{N(y_c)}{\psi_c(y_c)} - \underbrace{N \frac{\partial}{\partial \psi_c(y_c)} \log Z(\theta)}$$

No closed-form!

Method 2: Iterative Proportional Fitting (IFP)

- Derivative of the log partition function:

$$\frac{\partial}{\partial \psi_c(y_c)} \log Z(\theta) = \frac{1}{Z} \frac{\partial Z}{\partial \psi_c(y_c)}$$

$$= \frac{1}{Z} \frac{\partial}{\partial \psi_c(y_c)} \sum_y \prod_D \psi_D(y_D)$$

$$= \frac{1}{Z} \sum_{y \setminus y_c} \frac{\partial}{\partial \psi_c(y_c)} \sum_{y_c} \prod_D \psi_D(y_D)$$

$$= \frac{1}{Z} \sum_{y \setminus y_c} \boxed{\frac{\partial}{\partial \psi_c(y_c)} \sum_{y_c} \psi_c(y_c)} \prod_{D \setminus c} \psi_D(y_D) \qquad = 1$$

$$= \frac{1}{Z} \sum_{y \setminus y_c} \prod_{D \setminus c} \psi_D(y_D)$$

$$= \frac{1}{Z} \frac{\sum_{y \setminus y_c} \psi_c(y_c) \prod_{D \setminus c} \psi_D(y_D)}{\psi_c(y_c)}$$

$$= \frac{\sum_{y \setminus y_c} \frac{\prod_D \psi_D(y_D)}{Z}}{\psi_c(y_c)} = \frac{\sum_{y \setminus y_c} p(y)}{\psi_c(y_c)} = \frac{p(y_c|\psi)}{\psi_c(y_c)}$$

Conditioned on all potentials since $p(y_c|\psi)$ is obtained from marginalization of the full distribution $p(y)$.

Method 2: Iterative Proportional Fitting (IFP)

- Putting the derivative of the log partition function back into the gradient, and equating to zero we get:

$$\frac{N(y_c)}{\psi_c(y_c)} - N\frac{p(y_c|\psi)}{\psi_c(y_c)} = 0$$

- From this we infer:

$$p_{emp}(y_c) \leftarrow \boxed{\frac{N(y_c)}{N}}\frac{1}{\psi_c(y_c)} = \frac{p(y_c|\psi)}{\psi_c(y_c)}$$

- We can solve for $\psi_c(y_c)$ iteratively using the fixed point equation:

$$\psi_c^{t+1}(\mathbf{y}_c) = \psi_c^t(\mathbf{y}_c) \times \frac{p_{\text{emp}}(\mathbf{y}_c)}{p(\mathbf{y}_c|\psi^t)}$$

Element-wise multiplication

Method 2: Iterative Proportional Fitting (IFP)

Algorithm : Iterative Proportional Fitting algorithm for tabular MRFs

```
1 Initialize ψ_c = 1 for c = 1 : C;
2 repeat
3     for c = 1 : C do
4         p_c = p(y_c|ψ);
5         p̂_c = p_emp(y_c);
6         ψ_c = ψ_c * p̂_c / p_c ;
7 until converged;
```

// do marginalization with current ψ: $\sum_{y \setminus y_c} p(y)$

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

Method 2: Iterative Proportional Fitting (IFP)

Algorithm : Iterative Proportional Fitting algorithm for tabular MRFs

```
1 Initialize ψ_c = 1 for c = 1 : C;
2 repeat
3     for c = 1 : C do
4         p_c = p(y_c|ψ);          // do marginalization with current ψ: Σ_{y\y_c} p(y)
5         p̂_c = p_emp(y_c);        // compute empirical probability of current clique c
6         ψ_c = ψ_c * p̂_c / p_c ;
7 until converged;
```

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

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5         p̂_c = p_emp(y_c);        // compute empirical probability of current clique c
6         ψ_c = ψ_c * p̂_c / p_c ;  // iterative proportional fitting
7 until converged;
```

Source: Kevin Murphy, "Machine Learning: a probabilistic perspective"

Maximum A Posteriori (MAP): MRF (UGM)

- We can also do MAP to learn the unknown parameters in UGM, where we add a prior term:

$$\underset{\theta}{\operatorname{argmax}} \left\{ \sum_i \log p(y_i|\theta) + \underbrace{\log p(\theta)}_{\text{Prior term}} \right\}$$

- A Gaussian prior is often use:

$$p(\theta) = \mathcal{N}(\theta|\mu, \Sigma) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp[-\tfrac{1}{2}(\theta-\mu)^T\Sigma^{-1}(\theta-\mu)]$$

- Where (μ, Σ) are the hyperparameters.

Parameter Learning: UGM (CRF)

- Consider a Conditional Random Field (CRF) in log-linear form, where c indexes the cliques:

$$p(\mathbf{y}|\mathbf{x},\mathbf{w}) = \frac{1}{Z(\mathbf{x},\mathbf{w})}\prod_c \exp(\mathbf{w}_c^T \boldsymbol{\phi}_c(\mathbf{x},\mathbf{y}_c))$$

- $\phi_c(\mathrm{x}, y_c)$ is a feature vector derived from the global inputs x and the local set of labels y_c.

Parameter Learning: UGM (CRF)

- We can modify the gradient based optimization of MRFs to the CRF, the scaled log-likelihood becomes:

$$\ell(\mathbf{w}) \triangleq \frac{1}{N}\sum_{i}^{N}\log p(\mathbf{y}_i|\mathbf{x}_i,\mathbf{w})$$
$$= \frac{1}{N}\sum_{i}^{N}\left[\sum_{c}\mathbf{w}_c^T\boldsymbol{\phi}_c(\mathbf{y}_i,\mathbf{x}_i) - \log Z(\mathbf{w},\mathbf{x}_i)\right]$$

- The gradient now becomes:

$$\frac{\partial \ell}{\partial \mathbf{w}_c} = \frac{1}{N}\sum_{i}^{N}\left[\boldsymbol{\phi}_c(\mathbf{y}_i,\mathbf{x}_i) - \frac{\partial}{\partial \mathbf{w}_c}\log Z(\mathbf{w},\mathbf{x}_i)\right]$$
$$= \frac{1}{N}\sum_{i}^{N}\left[\boldsymbol{\phi}_c(\mathbf{y}_i,\mathbf{x}_i) - \mathbb{E}\left[\boldsymbol{\phi}_c(\mathbf{y},\mathbf{x}_i)\right]\right]$$

We need labeled pairs of data $\{y_i, x_i\}_{i=1}^N$ for learning!

Parameter Learning: UGM (CRF)

$$\frac{\partial \ell}{\partial \mathbf{w}_c} = \frac{1}{N} \sum_i^N [\boldsymbol{\phi}_c(\mathbf{y}_i, \mathbf{x}_i) - \mathbb{E}[\boldsymbol{\phi}_c(\mathbf{y}, \mathbf{x}_i)]]$$

$$\mathbb{E}[\boldsymbol{\phi}_c(\mathrm{y}, \mathrm{x}_i)] = \sum_{\mathrm{y}, \mathrm{x}_i} p(\mathrm{y}|\mathrm{x}_i, \mathrm{w}) \boldsymbol{\phi}_c(\mathrm{y}, \mathrm{x}_i)$$

- The partition function depends on the inputs x_i!
- This means that we cannot bring $\mathbb{E}[\boldsymbol{\phi}_c(\mathrm{y}, \mathrm{x}_i)]$ out of the summation.
- We now have to perform inference for every single training case inside each gradient step, which is $O(N)$ times slower than the MRF case.

Stochastic Gradient Descent

Algorithm: Stochastic Gradient Descent

$w^* = \text{StochasticGradientDescent}(T, \eta)$

Input:

T // number of iterations

$\eta_1, \ldots, \eta_T$ // sequence of learning rates (can be the same)

Output:

$w^* \in \mathbb{R}^D$ // learned weight vector

Algorithm:

$w_{cur} \leftarrow 0$ // initialize parameters to 0

for t=1,...,T **do**

$(x^n, y^n) \in \mathcal{D}'$

$d \leftarrow -\widetilde{\nabla}_w^{(x^n, y^n)} \mathcal{L}(w_{cur})$

$w_{cur} \leftarrow w_{cur} + \eta_t d$

end for

$w^* \leftarrow w_{cur}$

Source: "Structured Learning and Prediction in Computer Vision", Sebastian Nowozin and Christoph H. Lampert, 2013

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$(x^n, y^n) \in \mathcal{D}'$ // pick random subset of data (often 1–3 elements), i.e. $\mathcal{D}' \subset \mathcal{D}$

$d \leftarrow -\widetilde{\nabla}_w^{(x^n, y^n)} \mathcal{L}(w_{cur})$

$w_{cur} \leftarrow w_{cur} + \eta_t d$

end for

$w^* \leftarrow w_{cur}$

This reduces the amount of computation to perform inference for every single training case!

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$d \leftarrow -\widetilde{\nabla}_w^{(x^n, y^n)} \mathcal{L}(w_{cur})$ // gradient approximation

$w_{cur} \leftarrow w_{cur} + \eta_t d$

end for

$w^* \leftarrow w_{cur}$

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Gradient Approximation

- We will approximate the gradient with $\mathcal{D}'$ and MCMC samples from the likelihood $p(\mathrm{y}|\mathrm{x}_i, \mathrm{w})$.

$$\nabla\mathcal{L}(w_c) = \frac{\partial \ell}{\partial \mathbf{w}_c} = \frac{1}{N}\sum_i \left[\phi_c(\mathbf{y}_i, \mathbf{x}_i) - \mathbb{E}\left[\phi_c(\mathbf{y}, \mathbf{x}_i)\right]\right]$$

$$\mathbb{E}[\phi_c(\mathrm{y}, \mathrm{x}_i)] = \sum_{\mathrm{y},\mathrm{x}_i} p(\mathrm{y}|\mathrm{x}_i, \mathrm{w})\phi_c(\mathrm{y}, \mathrm{x}_i)$$

$$\tilde{\nabla}\mathcal{L}(w_c) = \frac{|\mathcal{D}|}{|\mathcal{D}'|}\sum_{(x^n,y^n)\in\mathcal{D}'}\left[\phi_c(x^n, y^n) - \mathbb{E}_{y\sim p(\mathrm{y}|\mathrm{x}_i, \mathrm{w})}\phi_c(x^n, \mathrm{y})\right]$$

Expectation is computed from samples drawn from the likelihood (MCMC sampling)

Stochastic Gradient Descent

Algorithm: Stochastic Gradient Descent

$w^* = \text{StochasticGradientDescent}(T, \eta)$

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T // number of iterations

$\eta_1, \ldots, \eta_T$ // sequence of learning rates (can be the same)

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for t=1,...,T **do**

$(x^n, y^n) \in \mathcal{D}'$ // pick random subset of data (often 1–3 elements), i.e. $\mathcal{D}' \subset \mathcal{D}$

$d \leftarrow -\widetilde{\nabla}_w^{(x^n, y^n)} \mathcal{L}(w_{cur})$ // gradient approximation

$w_{cur} \leftarrow w_{cur} + \eta_t d$ // weight update

end for

$w^* \leftarrow w_{cur}$

Source: "Structured Learning and Prediction in Computer Vision", Sebastian Nowozin and Christoph H. Lampert, 2013

Maximum A Posteriori (MAP): CRF (UGM)

- We can also do a maximum a posteriori estimation of the unknown parameter in CRF:

$$\underset{w}{\operatorname{argmax}} \left\{ \sum_i \log p(y_i | x_i, w) + \log p(w) \right\}$$

- Where a Gaussian prior is often used for $p(w)$.

Summary

- We have looked at how to:

1. Compute the unknown parameters of discrete/continuous **DGMs** using MLE and MAP.
2. Compute the unknown parameters of **MRFs** using stochastic maximum likelihood, and iterative proportional fitting.
3. Compute the unknown parameters of **CRFs** using stochastic gradient descent.