Readings: K&F 11.4, 11.5, 20.1, 20.2, 20.3, 20.4

Approximate Inference & Learning undirected Models

Lecture 17 – May 23, 2011
CSE 515, Statistical Methods, Spring 2011

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Outline

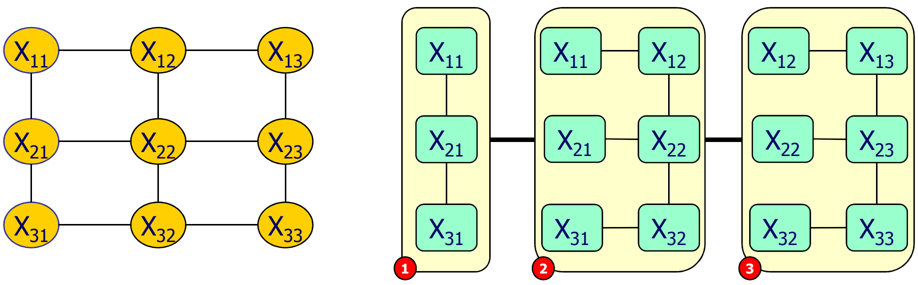
- Approximate Inference
  - Inference as optimization
  - Generalized Belief Propagation
  - Propagation with approximate messages ←
    - Factorized messages
    - Approximate message propagation
  - Structured variational approximations
- Learning Undirected Models

Propagation w. Approximate Msgs

- General idea
  - Perform BP (or GBP) as before, but propagate messages that are only approximate
  - Modular approach
    - General inference scheme remains the same
    - Can plug in many different approximate message computations

Factorized Messages

- Keep internal structure of the cliques in the tree
- Calibration involves sending messages that are joint over three variables
- Idea: simplify messages using factored representation
  - Example: $\tilde{\delta}_{1\to 2}[X_{11}, X_{21}, X_{31}] = \tilde{\delta}_{1\to 2}[X_{11}]\tilde{\delta}_{1\to 2}[X_{21}]\tilde{\delta}_{1\to 2}[X_{31}]$

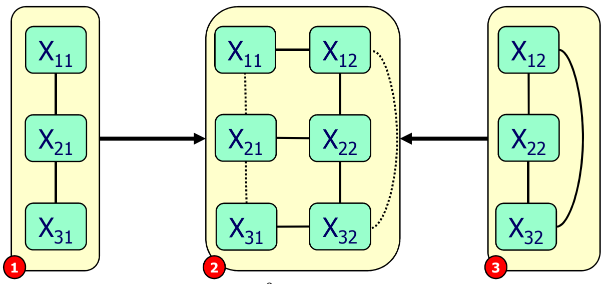


Markov network

Clique tree

Computational Savings 1/2

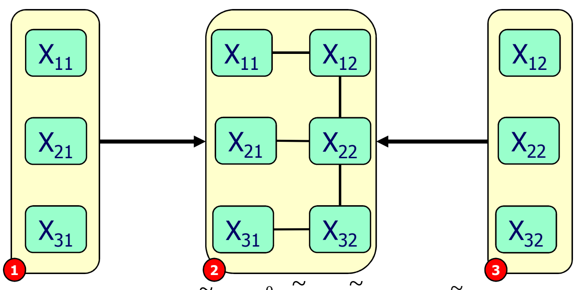
- Answering queries in Cluster 2
  - Exact inference: $\pi_2 = \pi_2^0 \cdot \delta_{1\to 2} \cdot \delta_{3\to 2}$
    - Exponential in joint space of cluster 2 (6 variables)



$\delta_{1\to 2}[X_{11}, X_{21}, X_{31}]$ $\pi_2 = \pi_2^0 \cdot \delta_{1\to 2} \cdot \delta_{3\to 2}$ $\delta_{3\to 2}[X_{12}, X_{22}, X_{32}]$

Computational Savings 2/2

- Answering queries in Cluster 2
  - Exact inference: $\pi_2 = \pi_2^0 \cdot \delta_{1\to 2} \cdot \delta_{3\to 2}$
    - Exponential in joint space of cluster 2 (6 variables)
  - Approximate inference with factored messages
    - Notice that subnetwork with factored messages is a tree
    - Perform efficient exact inference on subtree to answer queries



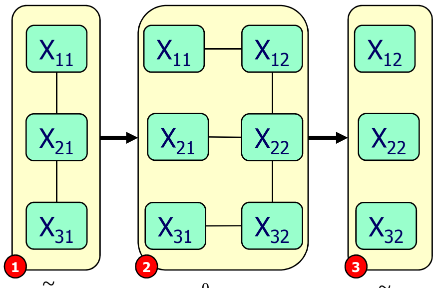
$\tilde{\delta}_{1\to 2}[X_{11}, X_{21}, X_{31}]$ $\tilde{\pi}_2 = \pi_2^0 \cdot \tilde{\delta}_{1\to 2} \cdot \tilde{\delta}_{3\to 2}$ $\tilde{\delta}_{3\to 2}[X_{12}, X_{22}, X_{32}]$

Factor Sets

- A factor set $\phi=\{\phi_1,\ldots,\phi_k\}$ provides a compact representation for high-dimensional factor $\phi_1\times,\ldots,\times\phi_k$
- Belief propagation
  - Multiplication of factor sets
    - Easy: simply the union of the factors in each factor set multiplied
  - Marginalization of factor set: inference in simplified network
    - Example: compute $\delta_{2\to3}$

$$\tilde{\delta}_{2\to3} = \rho\left(\sum_{X_{11},X_{21},X_{31}} \pi_2^0 \cdot \tilde{\delta}_{1\to2}\right)$$

$$= \tilde{\delta}_{2\to3}[X_{12}]\tilde{\delta}_{2\to3}[X_{22}]\tilde{\delta}_{2\to3}[X_{32}]$$



$\tilde{\delta}_{1\to2}$ π_2^0 $\tilde{\delta}_{2\to3}$

M-projection

$$P(X_1, X_2, X_3) \approx P(X_1)P(X_2)P(X_3)$$

Global Approximate Inference

- Inference as optimization
- Generalized Belief Propagation
  - Define algorithm
  - Constructing cluster graphs
  - Analyze approximation guarantees
- Propagation with approximate messages
  - Factorized messages
  - Approximate message propagation
- Structured variational approximations

Approximate Message Propagation

- Input
  - Clique tree (or cluster graph)
  - Assignments of original factors π^0 to clusters/cliques
  - The factorized form of each sepset
    - Can be represented by a network for each edge C_i—C_j that specifies the factorization (in previous examples we assumed empty network)
- Two strategies for approximate message propagation
  - Sum-product message passing scheme
  - Belief update messages

Sum-Product Propagation

- Same propagation scheme as in exact inference
  - Select a root
  - Propagate messages towards the root
    - Each cluster collects messages from its neighbors and sends outgoing messages when possible
  - Propagate messages from the root
- Each message passing performs inference on cluster
- Terminates in a fixed number of iterations
- Note: final marginals at each variable are not exact

Message Passing: Belief Propagation

- Same as BP but with approximate messages
- Initialize the clique tree
  - For each clique C_i set $\tilde{\pi}_i \leftarrow \prod_{\phi:\alpha(\phi)=i} \phi$
  - For each edge C_i—C_j set $\tilde{\mu}_{i,j} \leftarrow 1$
- While unset cliques exist
  - Select C_i—C_j
  - Send message from C_i to C_j
    - Marginalize the clique over the sepset $\tilde{\sigma}_{i\to j} \leftarrow \rho\left(\sum_{C_i - S_{i,j}} \tilde{\pi}_i\right)$

Approximation

    - Update the belief at C_j $\tilde{\pi}_j \leftarrow \tilde{\pi}_j \dfrac{\tilde{\sigma}_{i\to j}}{\tilde{\mu}_{i,j}}$
    - Update the sepset at C_i–C_j $\tilde{\mu}_{i,j} \leftarrow \tilde{\sigma}_{i\to j}$

Two message passing schemes differ in approximate inference

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Structured Variational Approx.

- Select a simple family of distributions **Q**
- Find $Q \in \mathbf{Q}$ that maximizes $F[P_F, Q]$

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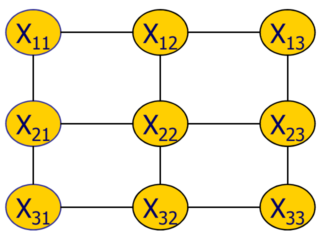
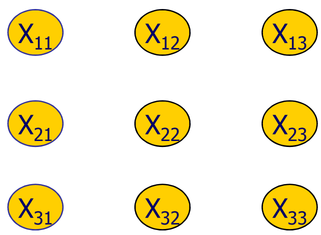
Mean Field Approximation

- $Q(x) = \Pi Q(X_i)$
- Q loses much of the information of P_F
- Approximation is computationally attractive
  - Every query in Q is simple to compute
  - Q is easy to represent



P_F – Markov grid network



Q – Mean field network

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Mean Field Approximation

- The energy functional is easy to compute, even for networks where inference is complex
  - The energy functional for a fully factored distribution Q can be rewritten simply as a sum of expectations, each one over a small set of variables.

$$F[P_F, Q] = \sum_{\phi \in F} E_Q[\ln \phi] + H_Q(\mathbf{U})$$

$$E_Q[\ln \phi] = \sum_{\mathbf{u}_\phi} Q(\mathbf{u}_\phi) \ln \phi(\mathbf{u}_\phi) = \sum_{\mathbf{u}_\phi} \left(\prod_{X_i \in \mathbf{u}_\phi} Q(x_i) \right) \ln \phi(\mathbf{u}_\phi)$$

$$H_Q(\mathbf{U}) = \sum_i H_Q(X_i)$$

  - The complexity of this expression depends on the size of the factors in P_F, and not on the topology of the network.

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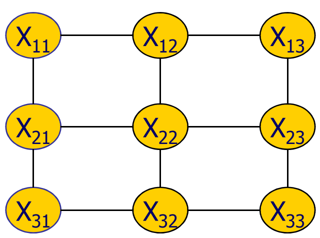
Mean Field Maximization

- Maximizing the Energy Functional of Mean-Field
  - Find $Q(x) = \Pi Q(X_i)$ that maximizes $F[P_F,Q]$
  - Subject to for all i: $\Sigma_{x_i} Q(x_i)=1$



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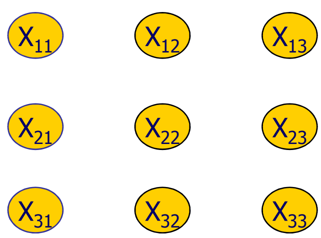

Q – Mean field network

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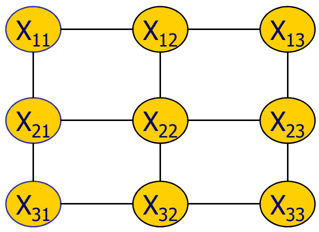
Mean Field Maximization

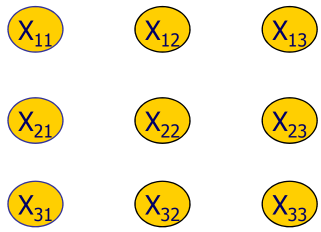
- Theorem: $Q(X_i)$ is a local maximum of the mean field given $Q(X_1),\ldots Q(X_{i-1}),Q(X_{i+1}),\ldots Q(X_n)$ if and only if

$$Q(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in F} E_Q[\ln \phi \mid x_i] \right\}$$

  - Proof in K&F on pages 451-452



P_F – Markov grid network



Q – Mean field network

Mean Field Maximization: Intuition

- We can rewrite $Q(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in F} E_Q[\ln \phi \mid x_i] \right\}$ as:

$$Q(x_i) = \frac{1}{Z_i} \exp\left\{ E_Q[\ln P_F(x_i \mid \mathbf{X}_{-i})] \right\} \boxed{\exp\left\{ E_Q[\ln ZP_F(\mathbf{X}_{-i})] \right\}}$$

Doesn't depend on x_i.
This constant can be "absorbed" into the normalizing function.

$$Q(x_i) = \frac{1}{\tilde{Z}_i} \exp\left\{ E_Q[\ln P_F(x_i \mid \mathbf{X}_{-i})] \right\}$$

- $Q(x_i)$ is the geometric average of $P_F(x_i|\mathbf{X}_{-i})$
  - Relative to the probability distribution Q
  - In this sense, marginal is "consistent" with other marginals
- In P_F we can also represent marginals

$$P_F(x_i) = \sum_{\mathbf{x}_{-i}} P_F(\mathbf{x}_{-i}) P_F(x_i \mid \mathbf{x}_{-i}) = E_{P_F}[P_F(x_i \mid \mathbf{x}_{-i})]$$

  - Arithmetic average with respect to P_F

Mean Field: Algorithm

- Since terms that do not involve x_i can be "absorbed" into the normalization constant,
- Simplify: $Q(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in F} E_Q[\ln \phi \mid x_i] \right\}$
- To: $Q(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi : X_i \in Scope(\phi)} E_Q[\ln \phi(U_\phi, x_i)] \right\}$
  - Note: $Q(x_i)$ does not appear on right hand side
    - Can solve and reach optimal $Q(x_i)$ in one step
    - Note: step is only optimal given all other $Q(X_j)$ $(j \neq i)$
    - Suggests an iterative algorithm: in each step, find the optimal $Q(x_i)$, given all the other $Q(X_j)$ $(j \neq i)$
    - Convergence guaranteed to local maxima since each step improves $F[P_F, Q]$

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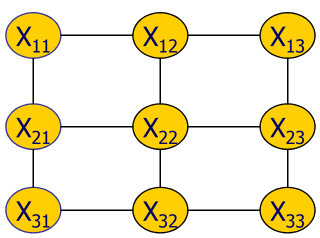
Structured Approximations

- Can use Q that are increasingly complex
- As long as Q is easy (=inference feasible) efficient update equations can be derived

Maximize $F[P_F, Q]$



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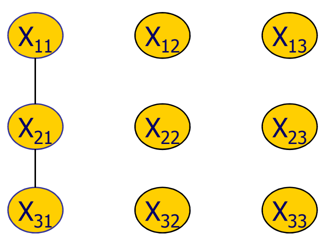

Q – Mean field network

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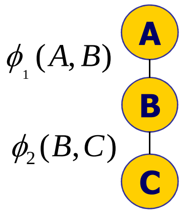
LEARNING UNDIRECTED GRAPHICAL MODELS

Learning Undirected Graphs

- The likelihood function
  - Log-linear representation
  - Properties of the likelihood function
- Learning parameters (weights)
  - Maximum likelihood estimation
  - Generatively vs Discriminatively
- Learning with alternative goals
- Learning with incomplete data
- Learning structure (features)

The Likelihood Function 1/2



- Consider the very simple network, parameterized by two potentials ϕ_1(A,B) and ϕ_2(B,C)
- The log-likelihood of an instance <a,b,c> :

$$\ln P(a,b,c) = \ln \phi_1(a,b) + \ln \phi_2(b,c) - \ln Z$$

  - where Z is the partition function that ensures the distribution sums up to 1.
- Now, consider the log-likelihood function for a data set D containing M instances:

$$l(\boldsymbol{\theta}:D) = \sum_m \left[\ln \phi_1(a[m],b[m]) + \ln \phi_2(b[m],c[m]) - \ln Z(\boldsymbol{\theta})\right]$$

$$= \sum_{a,b} M[a,b] \ln \phi_1(a,b) \sum_{b,c} M[b,c] \ln \phi_2(b,c) - M \ln Z(\boldsymbol{\theta})$$

The Likelihood Function 2/2

$$l(\boldsymbol{\theta}:D) = \sum_{a,b} M[a,b] \ln \phi_1(a,b) + \sum_{b,c} M[b,c] \ln \phi_2(b,c) - M \ln Z(\boldsymbol{\theta})$$

- Sufficient statistics that summarize the data: the joint counts M[a,b], M[b,c] in D
- The first and second term involves ϕ_1 and ϕ_2 alone, respectively.
- The third term is the log-partition function ln Z, where

$$Z(\boldsymbol{\theta}) = \sum_{a,b,c} \phi_1(a,b)\phi_2(b,c)$$

  - ln Z is a function of both ϕ_1 and ϕ_2; it couples the two potentials in the likelihood function.
  - Consider MLE: In BNs, we could estimate each parameter independently of the other ones. Here, when changing ϕ_1, Z changes, possibly changing the value of ϕ_2 that maximizes ln Z($\boldsymbol{\Theta}$). → In MNs, we cannot estimate each parameter independently.

Log-Linear Model 1/2

- Given a set of features $F=\{f_i(\mathbf{D}_i)\}_{i=1,\ldots,k}$, where $f_i(\mathbf{D}_i)$ is a feature function defined over the variables in $\mathbf{D}_i$, we have:

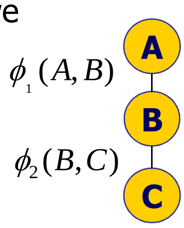
$$P(X_1,\ldots,X_n:\boldsymbol{\theta})=\frac{1}{Z(\boldsymbol{\theta})}\exp\left\{\sum_{i=1}^{k}\theta_i f_i(\mathbf{D}_i)\right\}$$

  - For example, in the previous example, we can define a set of features as:

$$f_1(A,B)=\begin{cases}1 & \text{, when A = a}^1\text{ and B = b}^1\\ 0 & \text{, otherwise}\end{cases}$$

$$f_2(A,B)=\begin{cases}1 & \text{, when A = a}^1\text{ and B = b}^0\\ 0 & \text{, otherwise}\end{cases}$$

:



- Let D be a data set of M instances D={ξ[1],…, ξ[M]}, and let $F=\{f_1,\ldots,f_K\}$ be a set of features that define a model:

$$l(\boldsymbol{\theta}:D)=\sum_i\theta_i\left(\sum_m f_i(\xi[m])\right)-M\ln Z(\boldsymbol{\theta})$$

Log-Linear Model 2/2

$$l(\boldsymbol{\theta}:D)=\sum_i\theta_i\left(\sum_m f_i(d[m])\right)-M\ln Z(\boldsymbol{\theta})$$

- Sufficient statistics: sums of the feature values in the instances in D
- Dividing it by the number of instances M,

$$\frac{1}{M}l(\boldsymbol{\theta}:D)=\sum_i\theta_i\mathbf{E}_D[f_i[\mathbf{d}_i]]-\ln Z(\boldsymbol{\theta})$$

  - where $\mathbf{E}_D[f_i(\mathbf{d}_i)]$ is the empirical expectation of f_i, that is, its average frequency in the data set.

Properties of the Likelihood Function

- The likelihood function is a sum of two functions.

$$l(\boldsymbol{\theta}:D) = \sum_i \theta_i \left(\sum_m f_i(\xi[m]) \right) - M \ln Z(\boldsymbol{\theta})$$

  - The first function is linear in the parameters (increasing the parameters directly increases this term)
  - Let's examine the second term in more detail.

$$\ln Z(\boldsymbol{\theta}) = \ln \sum_\xi \exp\left\{ \sum_i \theta_i f_i(\xi) \right\}$$

  - One important property of the partition function is that it is convex in the parameters **Θ**.
  - Proof? The Hessian – the matrix of the function's second derivatives – is positive semidefinite.
- The likelihood function is convex in **Θ**

Learning Undirected Graphs

- The likelihood function
  - Log-linear representation
  - Properties of the likelihood function
- Learning parameters
  - Maximum likelihood estimation
  - Generatively vs Discriminatively
- Collective classification with HMM, MEMM, CRF
- Learning with incomplete data
- Learning structure (features)
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Maximum Likelihood Estimation 1/2

- The average likelihood is

$$\frac{1}{M} l(\boldsymbol{\theta}:D) = \sum_i \theta_i \mathbf{E}_D[f_i[\mathbf{d}_i]] - \ln Z(\boldsymbol{\theta})$$

- For a concave function, the maxima are the points at which the gradient is 0

$$\frac{\partial}{\partial \theta_i} \sum_j \theta_j \mathbf{E}_D[f_j[\mathbf{d}_j]] = \mathbf{E}_D[f_i[\mathbf{d}_i]]$$

$$\begin{aligned}\frac{\partial}{\partial \theta_i} \ln Z(\boldsymbol{\theta}) &= \frac{1}{Z(\boldsymbol{\theta})} \sum_\xi \frac{\partial}{\partial \theta_i} \exp\left\{\sum_i \theta_i f_i(\xi)\right\} \\ &= \sum_\xi f_i(\xi) \frac{1}{Z(\boldsymbol{\theta})} \exp\left\{\sum_i \theta_i f_i(\xi)\right\} \\ &= \mathbf{E}_{\boldsymbol{\theta}}[f_i]\end{aligned}$$

- The gradient is $\frac{\partial}{\partial \theta_i} \frac{1}{M} l(\boldsymbol{\theta}:D) = \mathbf{E}_D[f_i[\mathbf{d}_i]] - \mathbf{E}_{\boldsymbol{\theta}}[f_i]$

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Maximum Likelihood Estimation 2/2

- The gradient is

$$\frac{\partial}{\partial \theta_i} l(\boldsymbol{\theta}:D) = M\mathbf{E}_D[f_i[\mathbf{d}_i]] - M\mathbf{E}_{\boldsymbol{\theta}}[f_i]$$

Number of times feature f_i is true in data D

Expected number of times feature f_i is true according to model

- The MLE of parameters $\hat{\boldsymbol{\theta}}$ satisfies, for all i,

$$\mathbf{E}_D[f_i[\mathbf{d}_i]] = \mathbf{E}_{\hat{\boldsymbol{\theta}}}[f_i]$$

- Numerical optimization: gradient ascent method or 2nd order-based (Newton's method)
  - Requires inference at each step (slow!)

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Conditionally Trained Models 1/2

- We often want to use a Markov network to perform a particular inference task, where we have a known set of observed variables **X** and a predetermined set of variables **Y** that we want to query.

- Discriminative training
  - We train the network as a conditional random field (CRF) that encodes a conditional distribution P(**Y**|**X**)
  - Training the model encoding P(**Y**,**X**) – generative training

- Given the training data consisting of pairs D={(**y**[m],**x**[m])}$_{m=1,\ldots,M}$, specifying assignments to **Y** and **X**, an appropriate objective function to use in this situation is the conditional likelihood.

$$l_{\mathbf{Y}|\mathbf{X}}(\boldsymbol{\theta} : D) = \ln P(\mathbf{y}[1,\ldots,M] \mid \mathbf{x}[1,\ldots,M], \boldsymbol{\theta})$$

$$= \sum_{m=1}^{M} \ln P(\mathbf{y}[m] \mid \mathbf{x}[m], \boldsymbol{\theta})$$

Conditionally Trained Models 2/2

- The gradient is

$$\frac{\partial}{\partial \theta_i} l_{\mathbf{Y}|\mathbf{X}}(\boldsymbol{\theta} : D) = \sum_{m=1}^{M} \left(f_i(\mathbf{y}[m], \mathbf{x}[m]) - \mathbf{E}_{\boldsymbol{\theta}}[f_i \mid \mathbf{x}[m]] \right)$$

Number of times feature f_i is true in data D

Expected number of times feature f_i is true according to model

  - Deceptively similar to the generative training case!
  - Key difference: Expected counts (2nd term) are computed as the summation of counts in M models defined by the different values of the conditioning variables **x**[m].

- Inference: In generative training, each gradient step required only a single execution of inference. When training CRFs, we must execute inference for every single training instance m, conditioning on **x**[m]
  - The inference is executed on a simpler model, because conditioning on evidence in a Markov network can only reduce the computational cost.

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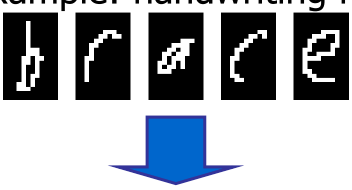
Collective Classification

- Taking a set of interrelated instances and jointly labeling them
- Example: handwriting recognition



x *A sequence of observations*

- Use local information
- Exploit correlations

b r a c e y *Label them with some joint label*

- Let's discuss some of the trade-offs between different models that one can apply to this task.
  - We focus on the context of labeling instances organized in a sequence (HMM, MEMM, CRF)

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Acknowledgement

- These lecture notes were generated based on the slides from Prof Eran Segal.