Probabilistic Graphical Models

Lecture 5: Conditional Random Fields

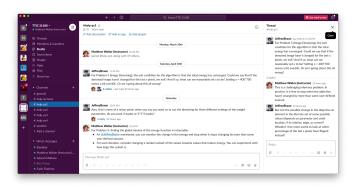
Matthew Walter

TTI-Chicago

April 21, 2020

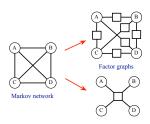
Problem Set 1 and Slack

- See Canvas for updates on Problem Set 1
- Don't forget to join the Slack channel #help-ps1
- See Slack channel for discussion and hints



Factor Graphs (Revisited)

- ullet The Markov network H does not make explicit the structure of the distribution, i.e., maximum cliques vs. complete graph subsets
- A factor graph is a bipartite undirected graph with variable nodes (oval) and factor nodes (square). Edges exist only between variable nodes and factor nodes
- Each factor node is associated with a single potential, the scope of which is the variables that are the factor's neighbors



Distribution is the same as an MRF, just a different data structure

Boltzmann Distribution (Revisited)

ullet We can rewrite a factor $\phi(oldsymbol{D}): \mathsf{Val}(oldsymbol{D}) o \mathbb{R}^+$ as

$$\phi(\mathbf{D}) = \exp(-\psi(\mathbf{D}))$$

where $\psi(D) = -\log \phi(D)$ is the **energy function** (not surprisingly, derived from statistical physics)

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- ullet $\sum_{k=1}^K \psi_k(oldsymbol{D}_k)$ is referred to as the "free energy"
- Gives rise to interpretation as energy minimization

$$\arg \max P(X_1, \dots, X_n) = \arg \min \sum_{k=1}^K \psi_k(\boldsymbol{D}_k)$$

Log-Linear Markov Networks with Features (Revisited)

- A **feature** is a function $f: \mathsf{Val}(\boldsymbol{D}_i) \to \mathbb{R}$
- ullet A distribution P is a **log-linear model** over a Markov network H if it is associated with
 - A set of features ${m F}=\{f_1({m D}_1),\ldots,f_K({m D}_M)\}$ where ${m D}_i$ is a complete subgraph in H
 - A set of weights $\{w_1, \ldots, w_M\}$

such that

$$P(X_1,\ldots,X_n) \propto \exp\left(-\sum_{i=1}^M w_i f_i(\boldsymbol{D}_i)\right)$$

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- Multiple features can be defined over the same variables
- Log-linear model can represent tabular potentials, but is more general
- Features and weights can be reused for different factors
- Historically, features designed by hand and weights learned from data



Left Image

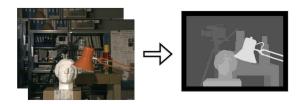


Right Image

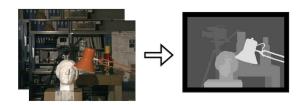


Disparity Image

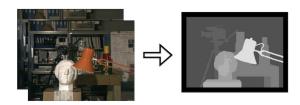
• Dense stereo reconstruction: For every pixel (i_l,j_l) in left image, we are interested in the image-space distance (**disparity**) y_{i_l,j_l} to the corresponding pixel (i_r,j_r) in the right image



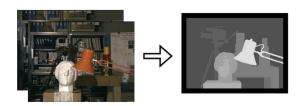
• We could model this as a Markov random field



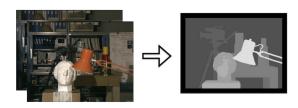
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- ullet Joint distribution $P(oldsymbol{Y},oldsymbol{X})$ over disparity $oldsymbol{Y}$ and pixel intensities $oldsymbol{X}$:



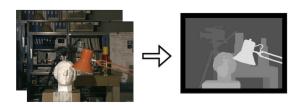
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 - Both involve a (conditional) distribution over natural images!!!

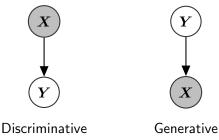


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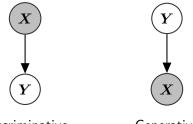


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 - Both involve a (conditional) distribution over natural images!!!
- Requires that we choose a parametric form over the pixel values
- Non-local features (e.g., image gradients) are useful, but difficult to capture with a joint distribution

- ullet Let X denote the input/observation (e.g., an image) and Y be the output (e.g., disparity, label, etc.)
- Flexibility in the structure and parametrization of the model



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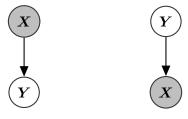


Discriminative

Generative

• Discriminative models are concerned with modeling P(Y | X = x), where X = x is treated as a parameter

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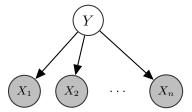
Discriminative

Generative

- Discriminative models are concerned with modeling P(Y | X = x), where X = x is treated as a parameter
- Generative models are interested in the joint distribution $P(\boldsymbol{X},\boldsymbol{Y}) = P(\boldsymbol{X}\,|\,\boldsymbol{Y})P(\boldsymbol{Y})$
 - P(X | Y): Given the target label, generate the input

Generative vs. Discriminative Classifiers: Naive Bayes

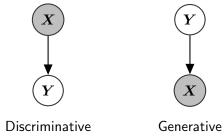
- Classify e-mails as being spam (Y = 1) or not spam (Y = 0)
 - Let $i \in \{1, \dots, n\}$ index English words
 - $X_i = 1$ if word i appears in the e-mail
 - ullet E-mails are drawn from the joint distribution $P(Y,X_1,\ldots,X_n)$
- ullet Words are conditionally independent (d-separated) given Y



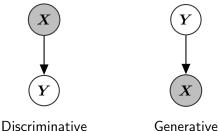
• Prediction follows via Bayes' Rule as

$$P(Y=1 \mid x_1, \dots, x_n) = \frac{P(Y=1) \prod_{i=1}^n P(x_i \mid Y=1)}{\sum_{y=\{0,1\}} P(Y=y) \prod_{i=1}^n P(x_i \mid Y=1)}$$

ullet These are **equivalent** models of P(Y, X)

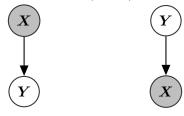


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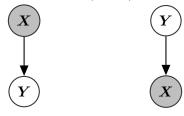


Discriminative

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- ullet But, suppose that we are only interested in $P(oldsymbol{Y}\,|\,oldsymbol{X})$ for prediction
- \bullet A generative model requires representing both $P(\boldsymbol{Y})$ and $P(\boldsymbol{X}\,|\,\boldsymbol{Y})$
 - ullet Generative, since we can $\mathit{generate}\ X$ given Y
 - ullet $P(oldsymbol{Y}\,|\,oldsymbol{X})$ is determined via Bayes' Rule

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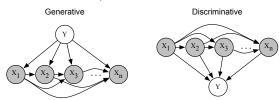
Discriminative

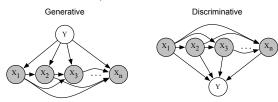
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- ullet But, suppose that we are only interested in $P(oldsymbol{Y}\,|\,oldsymbol{X})$ for prediction
- \bullet A generative model requires representing both $P(\boldsymbol{Y})$ and $P(\boldsymbol{X}\,|\,\boldsymbol{Y})$
 - ullet Generative, since we can $\mathit{generate}\ X$ given Y
 - ullet $P(Y \mid X)$ is determined via Bayes' Rule
- A discriminative model only requires a representation of the conditional distribution $P(\boldsymbol{Y} \mid \boldsymbol{X})$
 - ullet Discriminative, since we can $\emph{discriminate}$ between different Y
 - ullet We never need to estimate $P(oldsymbol{X})$ (which can be hard)

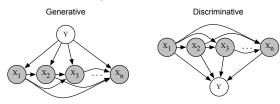


"one should solve the (classification) problem directly and never solve a more general problem as an intermediate step" (Vapnik, 1998)

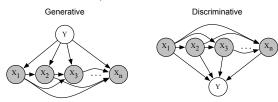




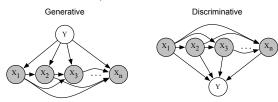
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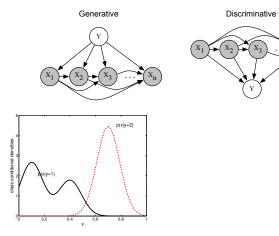


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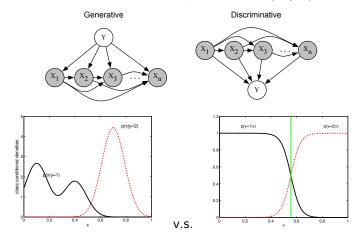


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 - Discriminative model: How do we parametrize P(Y | X)? Allows us to ignore encoding distribution over X

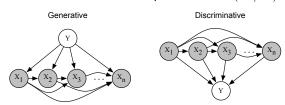
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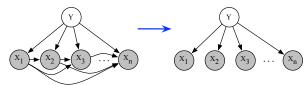
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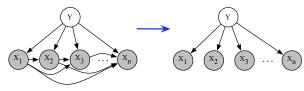
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• For the generative model, ignore the dependencies: assume that $X_i \perp X_{-i} \mid Y$ (naive Bayes)



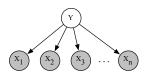
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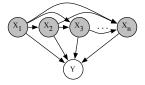
• For the discriminative model, assume that

$$\begin{split} P(Y=1\,|\,\pmb{x};w) &= \frac{e^{w_0 + \sum_{i=1}^n w_i x_i}}{1 + e^{w_0 + \sum_{i=1}^n w_i x_i}} = \frac{1}{1 + e^{-w_0 - \sum_{i=1}^n w_i x_i}} \\ &= \frac{1}{1 + e^{-z}} \quad \text{logistic function} \end{split}$$

Generative (naive Bayes)



Discriminative (logistic regression)



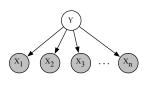
- lacktriangle For the generative model, ignore the dependencies: assume that $X_i \perp m{X}_{-i} \mid m{Y}$ (naive Bayes)
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$$P(Y = 1 \mid \boldsymbol{x}; w) = \frac{e^{w_0 + \sum_{i=1}^{n} w_i x_i}}{1 + e^{w_0 + \sum_{i=1}^{n} w_i x_i}} = \frac{1}{1 + e^{-w_0 - \sum_{i=1}^{n} w_i x_i}}$$

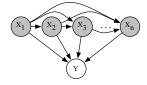
- We can show (problem set) that the first assumption implies the latter
- Every conditional distribution that can be represented via naive Bayes can also be represented using the logistic model

Generative vs. Discriminative Models

Generative (naive Bayes)



Discriminative (logistic regression)



- ullet Unlike naive Bayes, logistic models don't assume $X_i \perp oldsymbol{X}_{-i} \mid oldsymbol{Y}$
- Ignoring dependencies results in double-counting evidence, e.g.,
 - Suppose that $X_i=1$ ("transaction" in e-mail) and $X_j=1$ ("account" in e-mail)
 - \bullet Irrespective of being spam, these always occur together, i.e., $X_i = X_j$
 - Learning with naive Bayes $(P(X_i \mid \boldsymbol{Y}) = P(X_j \mid \boldsymbol{Y}))$ double-counts evidence
 - Learning with logistic regression sets $w_i=0$ for one of the words, thereby ignoring it

Generative vs. Discriminative Models

- ullet Discriminative model requires that $oldsymbol{X}$ be fully observed
 - ullet Generative models allow you to marginalize over unseen variables to compute $P(\boldsymbol{Y}\,|\,\boldsymbol{X}_o)$
- Maximum likelihood estimation of generative models is more efficient than training discriminative models [Ng and Jordan, 2002]¹
 - Consider number of samples necessary to get close to infinite data case
 - ullet Logistic regression requires $\mathcal{O}(n)$ samples
 - Naive Bayes requires $\mathcal{O}(\log n)$ samples
 - Naive Bayes converges with fewer samples, but not necessarily to better estimates

¹Ng and Jordan, "On Discriminative vs. Generative Classifiers: A Comparison of Logistic Regression and Naive Bayes," NeurIPS 2002

Generative vs. Discriminative Models

 Ng and Jordan (2002) show that discriminative logistic regression has lower asymptotic error than a generative naive Bayes classifier, but that naive Bayes converges faster

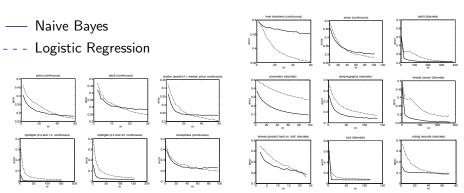
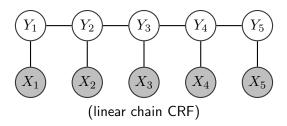
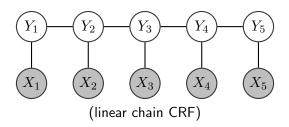


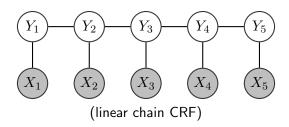
Figure: Error rate vs. number of samples for 15 datasets from the UCI Machine Learning repository. Courtesy: Ng and Jordan, 2002.



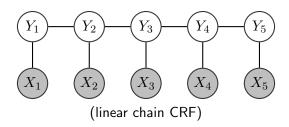
ullet Undirected graph with nodes for Y (target variables) and X (observed variables) (alt., partially directed, with X the parent of Y)



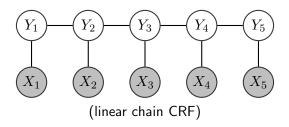
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- Represent conditional distribution $P(\boldsymbol{Y}\,|\,\boldsymbol{X})$ rather than joint distribution $P(\boldsymbol{Y},\boldsymbol{X})$
- ullet Avoid representing dist. over $X\Rightarrow$ no potentials involving only X



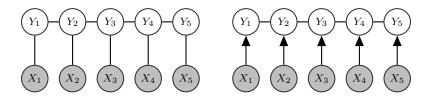
• A conditional random field (CRF) is an undirected graph H over X and Y defined in terms of a set of factors $\phi_1(D_1), \ldots, \phi_m(D_m)$, where $D_i \not\subseteq X$, that encodes the conditional distribution

$$P(Y \mid X) = \frac{1}{Z(X)} \prod_{i=1}^{m} \phi_i(D_i)$$
$$Z(X) = \sum_{Y} \prod_{i=1}^{m} \phi_i(D_i)$$

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- Two variables are connected by an undirected edge if they appear in the scope of the same factor
- ullet Just like a Markov network, except the partition function depends on (i.e., changes with) the observed variables (input) $oldsymbol{X}$
- Trained to maximize conditional (not joint) probability of the output given the input

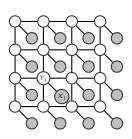
Linear-Chain CRFs



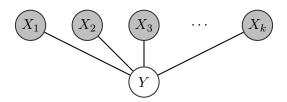
- The linear-chain CRF can be represented as an undirected (left) or partially directed graph (right)
- The conditional distribution factorizes as

$$P(\mathbf{Y} \mid \mathbf{X}) = \frac{1}{Z(\mathbf{X})} \prod_{i=1}^{k-1} \phi(Y_i, Y_{i+1}) \prod_{i=1}^{k} \phi(Y_i, X_i)$$
$$Z(\mathbf{X}) = \sum_{\mathbf{Y}} \prod_{i=1}^{k-1} \phi(Y_i, Y_{i+1}) \prod_{i=1}^{k} \phi(Y_i, X_i)$$





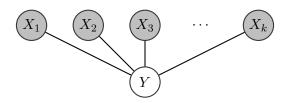
- ullet By not modeling the distribution over $oldsymbol{X}$, we can consider representations of the data with complex, non-parametric interactions
- We can employ a rich set of features without concern over their joint distribution (e.g., image gradients)



- Let $X = \{X_1.X_2, \dots, X_k\}$ and Y be binary random variables
- ullet Assume $oldsymbol{X}$ (observed) and Y are related by the following factors

$$\phi_0(Y) = \exp\{w_0 \mathbb{1}[Y = 1]\}$$

$$\phi_i(X_i, Y) = \exp\{w_i \mathbb{1}[X_i = 1, Y = 1]\}$$



- Let $X = \{X_1.X_2, ..., X_k\}$ and Y be binary random variables
- ullet Assume $oldsymbol{X}$ (observed) and Y are related by the following factors

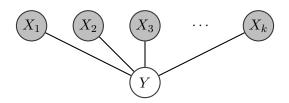
$$\phi_0(Y) = \exp\{w_0 \mathbb{1}[Y = 1]\}$$

$$\phi_i(X_i, Y) = \exp\{w_i \mathbb{1}[X_i = 1, Y = 1]\}$$

The conditional distribution becomes

$$\tilde{P}(Y = 1 \mid x_1, \dots, x_k) = \exp\left\{w_0 + \sum_{i=1}^k w_i x_i\right\}$$

 $\tilde{P}(Y = 0 \mid x_1, \dots, x_k) = 1$



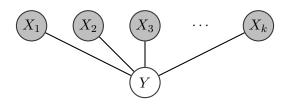
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Recall earlier discriminative (logistic regression) discussion

CRF Parametrization

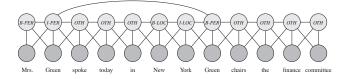
- Factors may depend on a large number of variables
- Typically, parametrize factors using log-linear representation

$$\phi_c(\boldsymbol{X}_c, \boldsymbol{Y}_c) = \exp\left(\boldsymbol{w}_c^{\top} \boldsymbol{f}_c(\boldsymbol{X}_c, \boldsymbol{Y}_c)\right)$$

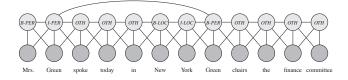
where

- $f_c(X_c, Y_c)$ is a feature vector (e.g., local image gradients)
- $oldsymbol{w}_c$ is a weight vector that is learned from data

- Objective: Given a sentence, segment phrases into different locations, people, organizations, etc.
 - "Mrs. Green spoke today in New York Green chairs the finance committee"
- Entries often span multiple words and label isn't obvious without considering context
- Define a random variable Y_i for each word X_i that expresses its entity type ("BIO notation")
 - B-PER/B-LOC: Beginning of a person/location
 - I-PER/I-LOC: Inside or end of named entity phrase for person/location
 - OTH: Word is not part of an entity

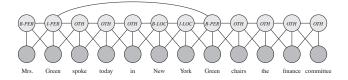


Interested in $P(\boldsymbol{Y} \,|\, \boldsymbol{X}) \Rightarrow \mathsf{Model}$ as a CRF w/ three types of factors



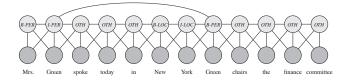
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• $\phi^1(Y_t,Y_{t+1})$: Expresses dependency between neighboring entities (similar to transition distribution in HMMs)



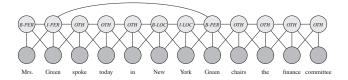
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- $\phi^2(Y_t, X_1, \dots, X_T)$: Expresses dependency between an entity and the entire word sequence (context), encoded via log-linear model
 - \bullet O(1000) features over current word X_t (e.g., capitalized), neighboring words, and entire sequence (e.g., number of sports-related words)



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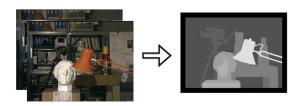
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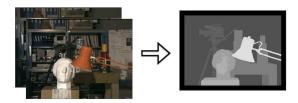
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Graph structure changes depending on sentence

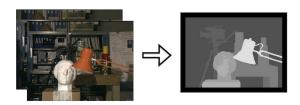


• Given two images X_l and X_r , estimate the disparity $y_{i_l,j_l} \in Y$ between a pixel at (i_l,j_l) in the left image and the corresponding pixel $(i_r,j_r)=(i_l+y_{i_l,j_l},j_l)$ in the right image (assume 1D)



Define local node potential as

$$\phi_{i_l,j_l}(y_{i_l,j_l}, \boldsymbol{X}) \propto \exp\left(-\frac{1}{2\sigma^2} \left(x_l(i_l, j_l) - x_r(i_l + y_{i_l,j_l}, j_l)\right)^2\right)$$



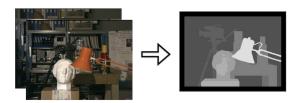
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ullet Define smoothness potential over neighboring pixels s and t

$$\phi_{s,t}(y_s, y_t) \propto \left(-\frac{1}{2\gamma^2}(y_s - y_t)^2\right)$$

Can be defined only for pairs s and t that don't cross boundaries



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There are advantages and disadvantages to MRF and CRF formulations (just as with discriminative and generative classifiers):

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- CRFs require labeled training data and are slower to train