

Probabilistic Graphical Models

Conditional Random Fields

& Case study I: image segmentation

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Reading: See class website

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*Y*₃

X₃

Hidden Markov Model revisit

 Transition probabilities between any two states

$$p(y_t^j = \mathbf{1} | y_{t-1}^i = \mathbf{1}) = a_{i,j},$$

or
$$p(y_t | y_{t-1}^i = 1) \sim \text{Multinomial}(a_{i,1}, a_{i,2}, \dots, a_{i,M}), \forall i \in \mathbb{I}.$$

• Start probabilities

 $p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \dots, \pi_M).$

• Emission probabilities associated with each state

 $p(x_t | y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,2}, \dots, b_{i,K}), \forall i \in \mathbb{I}.$

 y_1

 X_1

 y_2

X₂

or in general: $p(x_t | y_t^i = 1) \sim f(\cdot | \theta_i), \forall i \in \mathbb{I}.$

Xτ

Inference (review)

• Forward algorithm

$$\alpha_{t}^{k} \stackrel{\text{def}}{=} \mu_{t-1 \to t}(k) = P(x_{1}, ..., x_{t-1}, x_{t}, y_{t}^{k} = 1)$$
$$\alpha_{t}^{k} = p(x_{t} \mid y_{t}^{k} = 1) \sum_{i} \alpha_{t-1}^{i} a_{i,k}$$

Backward algorithm

$$\beta_{t}^{k} = \sum_{i} a_{k,i} p(x_{t+1} | y_{t+1}^{i} = 1) \beta_{t+1}^{i}$$

$$\beta_{t}^{k} \stackrel{\text{def}}{=} \mu_{t-1\leftarrow t} (k) = P(x_{t+1}, ..., x_{T} | y_{t}^{k} = 1)$$

$$\gamma_{t}^{i} \stackrel{\text{def}}{=} p(y_{t}^{i} = 1 | x_{1:T}) \propto \alpha_{t}^{i} \beta_{t}^{i} = \sum_{j} \xi_{t}^{i,j}$$

$$\xi_{t}^{i,j} \stackrel{\text{def}}{=} p(y_{t}^{i} = 1, y_{t+1}^{j} = 1, x_{1:T})$$

$$\propto \mu_{t-1\rightarrow t} (y_{t}^{i} = 1) \mu_{t\leftarrow t+1} (y_{t+1}^{j} = 1) p(x_{t+1} | y_{t+1}) p(y_{t+1} | x_{t+1})$$

$$\xi_{t}^{i,j} = \alpha_{t}^{i} \beta_{t+1}^{j} a_{i,j} p(x_{t+1} | y_{t+1}^{i} = 1)$$

The matrix-vector form: $B_{t}(i) \stackrel{\text{def}}{=} p(x_{t} | y_{t}^{i} = 1)$ $A(i, j) \stackrel{\text{def}}{=} p(y_{t+1}^{j} = 1 | y_{t}^{i} = 1)$ $\alpha_{t} = \left(A^{T} \alpha_{t-1}\right) \cdot B_{t}$ $\beta_{t} = A\left(\beta_{t+1} \cdot B_{t+1}\right)$ $\xi_{t} = \left(\alpha_{t} \left(\beta_{t+1} \cdot B_{t+1}\right)^{T}\right) \cdot A$ $\gamma_{t} = \alpha_{t} \cdot B_{t}$

 y_t)

Learning HMM



- **Supervised learning**: estimation when the "right answer" is known
 - Examples:
 - GIVEN: a genomic region $x = x_1...x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands
 - GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls
- <u>Unsupervised learning</u>: estimation when the "right answer" is unknown
 - Examples:
 - GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition
 - GIVEN: 10,000 rolls of the casino player, but we don't see when he changes dice
- QUESTION: Update the parameters θ of the model to maximize P(x|θ) -- Maximal likelihood (ML) estimation



Learning HMM: two scenarios

- Supervised learning: if only we knew the true state path then ML parameter estimation would be trivial
 - E.g., recall that for complete observed tabular BN:



- What if y is continuous? We can treat $\{(x_{n,t}, y_{n,t}): t = 1:T, n = 1:N\}$ as $N \times T$ observations of, e.g., a GLIM, and apply learning rules for GLIM ...
- Unsupervised learning: when the true state path is unknown, we can fill in the missing values using inference recursions.
 - The Baum Welch algorithm (i.e., EM)
 - Guaranteed to increase the log likelihood of the model after each iteration
 - Converges to local optimum, depending on initial conditions

The Baum Welch algorithm

• The complete log likelihood

$$\ell_{c}(\mathbf{\theta}; \mathbf{x}, \mathbf{y}) = \log p(\mathbf{x}, \mathbf{y}) = \log \prod_{n} \left(p(y_{n,1}) \prod_{t=2}^{T} p(y_{n,t} \mid y_{n,t-1}) \prod_{t=1}^{T} p(x_{n,t} \mid x_{n,t}) \right)$$

• The expected complete log likelihood

$$\left\langle \boldsymbol{\ell}_{c}(\boldsymbol{\theta};\mathbf{x},\mathbf{y})\right\rangle = \sum_{n} \left(\left\langle y_{n,1}^{i}\right\rangle_{p(y_{n,1}|\mathbf{x}_{n})} \log \pi_{i}\right) + \sum_{n} \sum_{t=2}^{T} \left(\left\langle y_{n,t-1}^{i}y_{n,t}^{j}\right\rangle_{p(y_{n,t-1},y_{n,t}|\mathbf{x}_{n})} \log a_{i,j}\right) + \sum_{n} \sum_{t=1}^{T} \left(x_{n,t}^{k}\left\langle y_{n,t}^{i}\right\rangle_{p(y_{n,t}|\mathbf{x}_{n})} \log b_{i,k}\right)$$

• EM

• The E step

$$\gamma_{n,t}^{i} = \left\langle y_{n,t}^{i} \right\rangle = p(y_{n,t}^{i} = \mathbf{1} | \mathbf{x}_{n})$$

$$\xi_{n,t}^{i,j} = \left\langle y_{n,t-1}^{i} y_{n,t}^{j} \right\rangle = p(y_{n,t-1}^{i} = \mathbf{1}, y_{n,t}^{j} = \mathbf{1} | \mathbf{x}_{n})$$

• The M step ("symbolically" identical to MLE)

$$\pi_{i}^{ML} = \frac{\sum_{n} \gamma_{n,1}^{i}}{N} \qquad \qquad a_{ij}^{ML} = \frac{\sum_{n} \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_{n} \sum_{t=1}^{T-1} \gamma_{n,t}^{i}}$$



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Shortcomings of Hidden Markov Model (1): locality of features



- HMM models capture dependences between each state and only its corresponding observation
 - NLP example: In a sentence segmentation task, each segmental state may depend not just on a single word (and the adjacent segmental stages), but also on the (non-local) features of the whole line such as line length, indentation, amount of white space, etc.
- Mismatch between learning objective function and prediction objective function
 - HMM learns a joint distribution of states and observations P(Y, X), but in a prediction task, we need the conditional probability P(Y|X)

Solution: Maximum Entropy Markov Model (MEMM)



- Models dependence between each state and the full observation sequence explicitly
 - More expressive than HMMs
- Discriminative model
 - Completely ignores modeling P(X): saves modeling effort
 - Learning objective function consistent with predictive function: P(Y|X)

Then, shortcomings of MEMM (and HMM) (2): the Label bias problem



What the local transition probabilities say:

- State 1 almost always prefers to go to state 2
- State 2 almost always prefer to stay in state 2

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• $0.4 \times 0.45 \times 0.5 = 0.09$



Probability of path 2->2->2 :

 $\bullet 0.2 \times 0.3 \times 0.3 = 0.018$

State 1

State 2

State 3

State 4

State 5

Other paths: 1-> 1-> 1-> 1: 0.09







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• Although locally it seems state 1 wants to go to state 2 and state 2 wants to remain in state 2.

• why?



Most Likely Path: 1-> 1-> 1-> 1

- State 1 has only two transitions but state 2 has 5:
 - Average transition probability from state 2 is lower

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Label bias problem in MEMM:

• Preference of states with lower number of transitions over others

Solution: Do not normalize probabilities locally





From local probabilities

Solution: Do not normalize probabilities locally





From local probabilities to local potentials

• States with lower transitions do not have an unfair advantage!

From MEMM





From MEMM to CRF



$$P(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n})} \prod_{i=1}^{n} \phi(y_i, y_{i-1}, \mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n}, \mathbf{w})} \prod_{i=1}^{n} \exp(\mathbf{w}^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_{1:n}))$$

- CRF is a partially directed model
 - Discriminative model like MEMM
 - Usage of global normalizer Z(x) overcomes the label bias problem of MEMM
 - Models the dependence between each state and the entire observation sequence (like MEMM)

Conditional Random Fields

• General parametric form:



$$P(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp(\sum_{i=1}^{n} (\sum_{k} \lambda_{k} f_{k}(y_{i}, y_{i-1}, \mathbf{x}) + \sum_{l} \mu_{l} g_{l}(y_{i}, \mathbf{x})))$$
$$= \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp(\sum_{i=1}^{n} (\lambda^{T} \mathbf{f}(y_{i}, y_{i-1}, \mathbf{x}) + \mu^{T} \mathbf{g}(y_{i}, \mathbf{x})))$$

where
$$Z(\mathbf{x}, \lambda, \mu) = \sum_{\mathbf{y}} \exp(\sum_{i=1}^{n} (\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x})))$$

CRFs: Inference



• Given CRF parameters λ and μ , find the \mathbf{y}^* that maximizes $P(\mathbf{y}|\mathbf{x})$ $\mathbf{y}^* = \arg \max \exp(\sum_{n=1}^{n} (\lambda^T \mathbf{f}(u; u; \mathbf{x}) + \mu^T \mathbf{g}(u; \mathbf{x})))$

$$\mathbf{y}^* = \arg \max_{\mathbf{y}} \exp(\sum_{i=1} (\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x})))$$

- Can ignore Z(x) because it is not a function of y
- Run the max-product algorithm on the junction-tree of CRF:



• Given $\{(\mathbf{x}_d, \mathbf{y}_d)\}_{d=1}^N$, find λ^* , μ^* such that

$$\lambda *, \mu * = \arg \max_{\lambda,\mu} L(\lambda,\mu) = \arg \max_{\lambda,\mu} \prod_{d=1}^{N} P(\mathbf{y}_d | \mathbf{x}_d, \lambda, \mu)$$

$$= \arg \max_{\lambda,\mu} \prod_{d=1}^{N} \frac{1}{Z(\mathbf{x}_{d},\lambda,\mu)} \exp(\sum_{i=1}^{n} (\lambda^{T} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_{d}) + \mu^{T} \mathbf{g}(y_{d,i}, \mathbf{x}_{d})))$$

$$= \arg \max_{\lambda,\mu} \sum_{d=1} \left(\sum_{i=1} (\lambda^T \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) + \mu^T \mathbf{g}(y_{d,i}, \mathbf{x}_d)) - \log Z(\mathbf{x}_d, \lambda, \mu) \right)$$

• Computing the gradient w.r.t λ :

Gradient of the log-partition function in an exponential family is the expectation of the sufficient statistics.

$$\nabla_{\lambda} L(\lambda, \mu) = \sum_{d=1}^{N} \left(\sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) - \sum_{\mathbf{y}} \left(P(\mathbf{y} | \mathbf{x}_d) \sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) \right) \right)$$

$$\nabla_{\lambda} L(\lambda, \mu) = \sum_{d=1}^{N} \left(\sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) - \sum_{\mathbf{y}} \left(P(\mathbf{y} | \mathbf{x}_d) \sum_{i=1}^{n} \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) \right) \right)$$

- Computing the model expectations:
 - Requires exponentially large number of summations: Is it intractable?

$$\sum_{\mathbf{y}} (P(\mathbf{y}|\mathbf{x}_d) \sum_{i=1}^n \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d)) = \sum_{i=1}^n (\sum_{\mathbf{y}} \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) P(\mathbf{y}|\mathbf{x}_d))$$
$$= \sum_{i=1}^n \sum_{y_i, y_{i-1}} \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) P(y_i, y_{i-1}|\mathbf{x}_d)$$
Expectation of **f** over the corresponding marginal probability of neighboring nodes!!

- Tractable!
 - Can compute marginals using the sum-product algorithm on the chain



• Computing marginals using junction-tree calibration:





• Computing feature expectations using calibrated potentials:

$$\sum_{y_i, y_{i-1}} \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) P(y_i, y_{i-1} | \mathbf{x}_d) = \sum_{y_i, y_{i-1}} \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) \alpha'(y_i, y_{i-1})$$

• Now we know how to compute $r_{\lambda}L(\lambda,\mu)$:

$$\nabla_{\lambda} L(\lambda, \mu) = \sum_{d=1}^{N} \left(\sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_{d}) - \sum_{\mathbf{y}} \left(P(\mathbf{y} | \mathbf{x}_{\mathbf{d}}) \sum_{i=1}^{n} \mathbf{f}(y_{i}, y_{i-1}, \mathbf{x}_{d}) \right) \right)$$

=
$$\sum_{d=1}^{N} \left(\sum_{i=1}^{n} \left(\mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_{d}) - \sum_{y_{i}, y_{i-1}} \alpha'(y_{i}, y_{i-1}) \mathbf{f}(y_{i}, y_{i-1}, \mathbf{x}_{d}) \right) \right)$$

• Learning can now be done using gradient ascent:

$$\lambda^{(t+1)} = \lambda^{(t)} + \eta \nabla_{\lambda} L(\lambda^{(t)}, \mu^{(t)})$$

$$\mu^{(t+1)} = \mu^{(t)} + \eta \nabla_{\mu} L(\lambda^{(t)}, \mu^{(t)})$$

• In practice, we use a Gaussian Regularizer for the parameter vector to improve generalizability

$$\lambda_{*,\mu*} = \arg \max_{\lambda,\mu} \sum_{d=1}^{N} \log P(\mathbf{y}_{d} | \mathbf{x}_{d}, \lambda, \mu) - \frac{1}{2\sigma^{2}} (\lambda^{T} \lambda + \mu^{T} \mu)$$

- In practice, gradient ascent has very slow convergence
 - Alternatives:
 - Conjugate Gradient method
 - Limited Memory Quasi-Newton Methods

CRFs: some empirical results



Comparison of error rates on synthetic data

60

MEMM error

10





Data is increasingly higher order in the direction of arrow

> CRFs achieve the lowest error rate for higher order data



CRFs: some empirical results

• Parts of Speech tagging

| model | error | oov error |
|------------------|-------|-----------|
| HMM | 5.69% | 45.99% |
| MEMM | 6.37% | 54.61% |
| CRF | 5.55% | 48.05% |
| MEMM+ | 4.81% | 26.99% |
| CRF ⁺ | 4.27% | 23.76% |

⁺Using spelling features

- Using same set of features: HMM >=< CRF > MEMM
- Using additional overlapping features: CRF⁺ > MEMM⁺ >> HMM

Other CRFs

- So far we have discussed only 1dimensional chain CRFs
 - Inference and learning: exact
- We could also have CRFs for arbitrary graph structure
 - E.g: Grid CRFs
 - Inference and learning no longer tractable
 - Approximate techniques used
 - MCMC Sampling
 - Variational Inference
 - Loopy Belief Propagation
 - We will discuss these techniques soon





Image Segmentation



- Images are noisy.
- Objects occupy continuous regions in an image.



Input image



Pixel-wise separate optimal labeling



Locally-consistent joint optimal labeling

[Nowozin,Lampert 2012]

Y: labelsX: data (features)S: pixelsN_i: neighbors of pixel i

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Undirected Graphical Models (with an Image Labeling Example)

- Image can be represented by 4-connected 2D grid.
- MRF / CRF with image labeling problem
 - $X = \{x_i\}_{i \in S}$: observed data of an image.
 - x_i: data at *i*-th site (pixel or block) of the image set S
 - $Y = \{y_i\}_{i \in S}$: (hidden) labels at *i*-th site. $y_i \in \{1, \dots, L\}$.



• Object: maximize the conditional probability $Y^*=\operatorname{argmax}_Y P(Y|X)$





MRF (Markov Random Field)

• Definition: $Y = \{y_i\}_{i \in S}$ is called Markov Random Field on the set S, with respect to neighborhood system N, iff for all $i \in S$,

 $\mathsf{P}(y_i|y_{S-\{i\}}) = \mathsf{P}(y_i|y_{Ni}).$

- The posterior probability is $P(Y | X) = \frac{P(X, Y)}{P(X)} \propto P(X | Y)P(Y) = \prod_{i \in S} P(x_i | y_i) \cdot P(Y)$ (2)
 - (1) Very strict independence assumptions for tractability: Label of each site is a function of data only at that site.
 - (2) P(Y) is modeled as a MRF

$$P(Y) = \frac{1}{Z} \prod_{c \in C} \psi_c(y_c)$$

 X_i

CRF



• Definition: Let G = (S, E), then (X, Y) is said to be a Conditional Random Field (CRF) if, when conditioned on *X*, the random variables y_i obey the Markov property with respect to the graph

 $P(y_i|X, y_{S-\{i\}}) = P(y_i|X, y_{Ni})$ MRF: $P(y_i|y_{S-\{i\}}) = P(y_i|y_{Ni})$

• Globally conditioned on the observation X





CRF vs MRF

• MRF: two-step generative model

- Infer likelihood P(X|Y) and prior P(Y)
- Use Bayes theorem to determine posterior P(Y|X)

MRF $P(Y|X) = \frac{1}{Z} \exp(\sum_{i \in S} \log p(x_i | y_i) + \sum_{i \in S} \sum_{i' \in N_i} V_2(y_i, y_{i'}))$

CRF $P(Y|X) = \frac{1}{Z} \exp(-\sum_{i \in S} V_1(y_i|X) + \sum_{i \in S} \sum_{i' \in N_i} V_2(y_i, y_i|X))$

$$P(Y | X) = \frac{P(X, Y)}{P(X)} \propto P(X | Y) P(Y) = \prod_{i \in S} P(x_i | y_i) \cdot \frac{1}{Z} \prod_{c \in C} \psi_c(y_c)$$

- CRF: one-step discriminative model
 - Directly Infer posterior P(Y|X)
- Popular Formulation

Assumption

Potts model for P(*Y*) with only pairwise potential

Only up to pairwise clique potentials



Example of CRF – DRF

- A special type of CRF
 - The unary and pairwise potentials are designed using local discriminative classifiers.
 - Posterior

$$P(Y | X) = \frac{1}{Z} \exp(\sum_{i \in S} A_i(y_i, X) + \sum_{i \in S} \sum_{j \in N_i} I_{ij}(y_i, y_j, X))$$

- Association Potential
 - Local discriminative model for site *i*: using logistic link with GLM.

$$A_i(y_i, X) = \log P(y_i | f_i(X)) \qquad P(y_i = 1 | f_i(X)) = \frac{1}{1 + \exp(-(w^T f_i(X)))} = \sigma(w^T f_i(X))$$

- Interaction Potential
 - Measure of how likely site *i* and *j* have the same label given X

$$I_{ij}(y_i, y_j, X) = k y_i y_j + (1 - k)(2\sigma(y_i y_j \mu_{ij}(X)) - 1))$$

(1) Data-independent smoothing term (2) Data-dependent pairwise logistic function

S. Kumar and M. Hebert. Discriminative Random Fields. IJCV, 2006. © Eric Xing @ CMU, 2005-2014

Example of CRF – DRF Results

- Task: Detecting man-made structure in natural scenes.
 - Each image is divided in non-overlapping 16x16 tile blocks.
- An example



- Input image Logistic • Logistic: No smoothness in the labels
 - MRF: Smoothed False positive. Lack of neighborhood interaction of the data

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Example of CRF –Body Pose Estimation

- Task: Estimate a body pose.
 - Need to detect parts of human body
 - Appearance + Geometric configuration.
 - A large number of DOFs
- Use CRF to model a human body
 - Nodes: Parts (head, torso, upper/ lower left/right arms). $L=(l_1,..., l_6), l_i = [x_i, y_i, \theta_i].$
 - Edges: Pairwise linkage between parts
 - Tree vs. Graph



V. Ferrari et al. Progressive search space reduction for human pose estimation. CVPR 2008.

D. Ramanan. Learning to Parse Images of Articulated Bodies." NIPS 2006.

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[Zisserman 2010]



Example of CRF –**Body Pose Estimation**

Posterior of configuration

$$P(L | I) \propto \exp(\sum \Phi(l_i) + \sum \Psi(l_i, l_j))$$

- $(i, j) \in E$ $\psi(l_i l_i)$: relative position with geometric constraints
- $\phi(l_i)$: local image evidence for a part in a particular location
- If E is a tree, exact inference is efficiently performed by BP.
- Example of unary and pairwise terms
 - Unary term: appearance feature



Pairwise term: kinematic layout

Example of CRF – Results of Body Pose Estimation

initial parse

head

ll–leø



• Examples of results



[Ramanan 2006]

missing arm torso



[Ferrari et al. 2008]

- Datasets and codes are available.
 - http://www.ics.uci.edu/~dramanan/papers/parse/

ru-arm

http://www.robots.ox.ac.uk/~vgg/research/pose_estimation/

Summary

- Conditional Random Fields are partially directed discriminative models
- They overcome the label bias problem of MEMMs by using a global normalizer
- Inference for 1-D chain CRFs is exact
 - Same as Max-product or Viterbi decoding
- Learning also is exact
 - globally optimum parameters can be learned
 - Requires using sum-product or forward-backward algorithm
- CRFs involving arbitrary graph structure are intractable in general
 - E.g.: Grid CRFs
 - Inference and learning require approximation techniques
 - MCMC sampling
 - Variational methods
 - Loopy BP