CSCE 970 Lecture 8: Structured Prediction

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CSCE 970 Lecture 8: Structured Prediction
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Introduction
Definitions
Applications
Graphical Models
Training

Introduction
Out with the old ...

We now know how to answer the question:
Does this picture contain a cat?

E.g., convolutional layers feeding connected layers feeding softmax

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Introduction
... and in with the new.

What we want to know now is: **Where are the cats?**

No longer a classification problem; need more sophisticated (**structured**) output

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Outline

- Definitions
- Applications
- Graphical modeling of probability distributions
- Training models
- Inference

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Definitions
Structured Outputs

- Most machine learning approaches learn function $f : \mathcal{X} \rightarrow \mathbb{R}$
  - Inputs $\mathcal{X}$ are **any kind of objects**
  - Output y is a **real number** (classification, regression, density estimation, etc.)
- Structured output learning approaches learn function $f : \mathcal{X} \rightarrow \mathcal{Y}$
  - Inputs $\mathcal{X}$ are **any kind of objects**
  - Outputs $y \in \mathcal{Y}$ are **complex (structured) objects** (images, text, audio, etc.)

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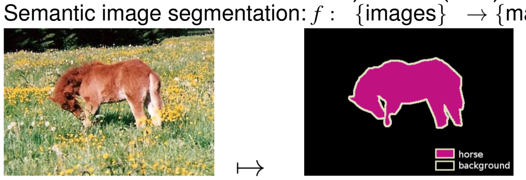
Definitions
Structured Outputs (2)

Can think of structured data as consisting of parts, where each part contains information, as well as how they fit together

- **Text:** Word sequence matters
- **Hypertext:** Links between documents matter
- **Chemical structures:** Relative positions of molecules matter
- **Images:** Relative positions of pixels matter

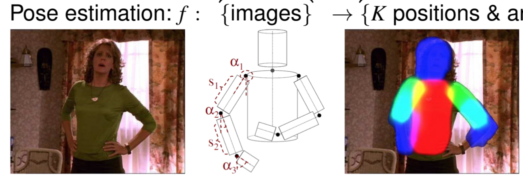
Applications
Image Processing

Semantic image segmentation: $f : \overbrace{\{\text{images}\}}^{\{0,\ldots,255\}^{3(m\times n)}} \rightarrow \overbrace{\{\text{masks}\}}^{\{0,1\}^{m\times n}}$



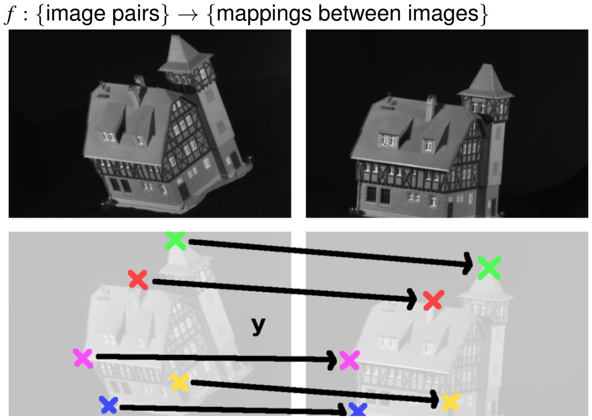
Applications
Image Processing (2)

Pose estimation: $f : \overbrace{\{\text{images}\}}^{\{0,\ldots,255\}^{3(m\times n)}} \rightarrow \overbrace{\{K \text{ positions \& angles}\}}^{\mathbb{R}^{3K}}$



Applications
Image Processing (3)

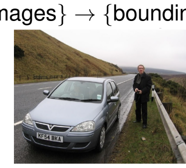
Point matching:
$f : \{\text{image pairs}\} \rightarrow \{\text{mappings between images}\}$



Applications
Image Processing (4)

Object localization
$f : \{\text{images}\} \rightarrow \{\text{bounding box coordinates}\}$

input: image



output: object position ($left, top$ $right, bottom$)

Applications
Others

- Natural language processing (e.g., translation; output is sentences)
- Bioinformatics (e.g., structure prediction; output is graphs)
- Speech processing (e.g., recognition; output is sentences)
- Robotics (e.g., planning; output is action plan)
- Image denoising (output is “clean” version of image)

Graphical Models
Probabilistic Modeling

- To represent structured outputs, we will often employ probabilistic modeling
  - Joint distributions (e.g., $P(A, B, C)$)
  - Conditional distributions (e.g., $P(A \mid B, C)$)
- Can estimate joint and conditional probabilities by counting and normalizing, but have to be careful about representation

Graphical Models
Probabilistic Modeling (2)

- E.g., I have a coin with unknown probability p of heads
- I want to estimate the probability of flipping it ten times and getting the sequence `HHTTHHTTTT`
- One way of representing this joint distribution is a single, big lookup table:
- Each experiment consists of ten coin flips
- For each outcome, increment its counter
- After n experiments, divide `HHTTHHTTTT`'s counter by n to get the estimate
- Will this work?

Outcome	Count
TTHHTTHHTH	1
HHHTHTTTHH	0
HTTTTTHHHT	0
TTHTHTHHTT	1
⋮	⋮

Graphical Models
Probabilistic Modeling (3)

- **Problem:** Number of possible outcomes grows exponentially with number of variables (flips)
  - ⇒ Most outcomes will have count $= 0$, a few with 1, probably none with more
  - ⇒ Lousy probability estimates
- Ten flips is bad enough, but consider 100 ☹
- How would **you** solve this problem?

Graphical Models
Factoring a Distribution

- Of course, we recognize that all flips are independent, so

$$\Pr[\texttt{HHTTHHTTTT}] = p^4 (1-p)^6$$

- So we can count n coin flips to estimate p and use the formula above
- I.e., we **factor** the joint distribution into independent components and multiply the results:

$$\Pr[\texttt{HHTTHHTTTT}] = \Pr[f_1 = \texttt{H}] \Pr[f_2 = \texttt{H}] \Pr[f_3 = \texttt{T}] \cdots \Pr[f_{10} = \texttt{T}]$$

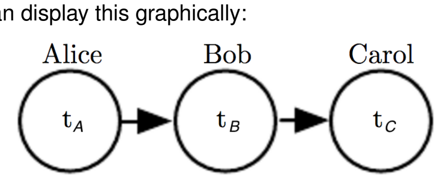
- We greatly reduce the number of parameters to estimate

Graphical Models
Factoring a Distribution (2)

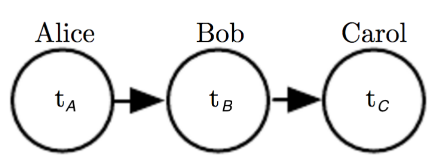
- Another example: **Relay racing team**
- Alice, then Bob, then Carol
- Let t_A = Alice's finish time (in seconds), t_B = Bob's, t_C = Carol's
- Want to model the joint distribution $\Pr[t_A, t_B, t_C]$
- Let $t_C, t_B, t_A \in \{1, \ldots, 1000\}$
- How large would the table be for $\Pr[t_A, t_B, t_C]$?
- How many races must they run to populate the table?

Graphical Models
Factoring a Distribution (3)

- But we can factor this distribution by observing that t_A is independent of t_B and t_C
  - ⇒ Can estimate t_A on its own
- Also, t_B directly depends on t_A, but is independent of t_C
- t_C directly depends on t_B, and indirectly on t_A
- Can display this graphically:



Graphical Models
Factoring a Distribution (4)



- This **directed graphical model** (often called a **Bayesian network** or **Bayes net**) represents conditional dependencies among variables
- Makes factoring easy:

$$\Pr[t_A, t_B, t_C] = \Pr[t_A] \Pr[t_B \mid t_A] \Pr[t_C \mid t_B]$$

Graphical Models
Factoring a Distribution (5)

$$\Pr[t_A, t_B, t_C] = \Pr[t_A]\Pr[t_B \mid t_A]\Pr[t_C \mid t_B]$$

- Table for $\Pr[t_A]$ requires[1] 1000 entries, while $\Pr[t_B \mid t_A]$ requires 10^6, as does $\Pr[t_C \mid t_B]$
  - $\Rightarrow$ Total 2.001×10^6, versus 10^9
- Idea easily extends to continuous distributions by changing discrete probability $\Pr[\cdot]$ to pdf $p(\cdot)$

[1] Technically, we only need 999 entries, since the value of the last one is implied since probabilities must sum to one. However, then the analysis requires the use of a lot of "9"s, and that's not something I'm willing to take on at this point in my life.

Directed Models
Conditional Independence

Definition: X is **conditionally independent** of Y given Z if the probability distribution governing X is independent of the value of Y given the value of Z; that is, if

$$(\forall x_i, y_j, z_k)\ \Pr[X = x_i \mid Y = y_j, Z = z_k] = \Pr[X = x_i \mid Z = z_k]$$

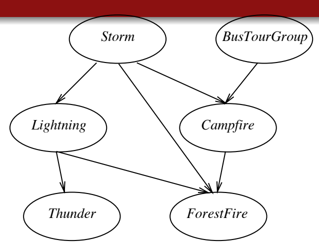
more compactly, we write

$$\Pr[X \mid Y, Z] = \Pr[X \mid Z]$$

Example: *Thunder* is conditionally independent of *Rain*, given *Lightning*

$$\Pr[Thunder \mid Rain, Lightning] = \Pr[Thunder \mid Lightning]$$

Directed Models
Definition



	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8

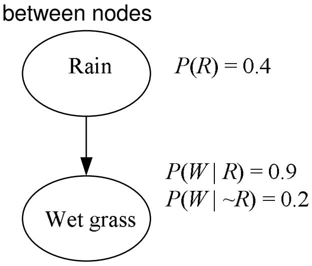
Campfire

Network (directed acyclic graph) represents a set of conditional independence assertions:

- **Each node is asserted to be conditionally independent of its nondescendants, given its immediate predecessors**
- E.g., Given *Storm* and *BusTourGroup*, *Campfire* is CI of *Lightning* and *Thunder*

Directed Models
Causality

Can think of edges in a Bayes net as representing a **causal relationship** between nodes

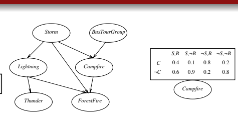


E.g., rain causes wet grass

Probability of wet grass depends on whether there is rain

Directed Models
Generative Models

Represents joint probability distribution over $\langle Y_1, \ldots, Y_n \rangle$, e.g., $\Pr[Storm, BusTourGroup, \ldots, ForestFire]$



- In general, for y_i = value of Y_i

$$\Pr[y_1, \ldots, y_n] = \prod_{i=1}^{n} \Pr[y_i \mid Parents(Y_i)]$$

($Parents(Y_i)$ denotes immediate predecessors of Y_i)

- E.g., $\Pr[S, B, C, \neg L, \neg T, \neg F] =$

$$\Pr[S] \cdot \Pr[B] \cdot \underbrace{\Pr[C \mid B, S]}_{0.4} \cdot \Pr[\neg L \mid S] \cdot \Pr[\neg T \mid \neg L] \cdot \Pr[\neg F \mid S, \neg L, \neg C]$$

- If variables continuous, use pdf $p(\cdot)$ instead of $\Pr[\cdot]$

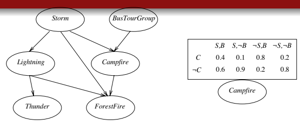
Directed Models
Predicting Most Likely Label

We sometimes call graphical models **generative** (vs **discriminative**) models since they can be used to generate instances $\langle Y_1, \ldots, Y_n \rangle$ according to joint distribution

Can use for classification

- Label r to predict is one of the variables, represented by a node
- If we can determine the most likely value of r given the rest of the nodes, can predict label
- One idea: Go through all possible values of r, and compute joint distribution (previous slide) with that value and other attribute values, then return one that maximizes

Directed Models
Predicting Most Likely Label (cont'd)



E.g., if *Storm* (S) is the label to predict, and we are given values of B, C, $\neg L$, $\neg T$, and $\neg F$, can use formula to compute $\Pr[S, B, C, \neg L, \neg T, \neg F]$ and $\Pr[\neg S, B, C, \neg L, \neg T, \neg F]$, then predict more likely one

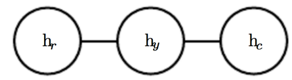
Easily handles unspecified attribute values

Issue: Takes time exponential in number of values of unspecified attributes

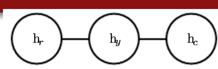
More efficient approach: **Pearl's message passing algorithm** for chains and trees and polytrees (at most one path between any pair of nodes)

Undirected Models

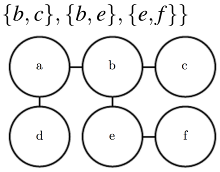
- Since directed edges imply causal relationships, might want to use **undirected** edges if causality not modeled
- E.g., let $h_y = 1$ if you are healthy, 0 if sick
  - h_r same but for your roommate, h_c for coworker
- h_y and h_r directly influence each other, but causality unknown and irrelevant
- h_y and h_c also directly influence each other
- h_r and h_c only indirect influence, via h_y
- Can model $\Pr[h_r, h_y, h_c]$ with **undirected model**, aka **Markov random field** (MRF), aka **Markov network**



Undirected Models
Factors



- In directed models, factors defined by a node's parents: *conditionally indep. of nondescendants given parents*
- In undirected models, factors defined by maximal **cliques** (complete subgraphs): *conditionally indep. of all other variables given neighbors*
- In graph above, cliques are $\{\{h_r, h_y\}, \{h_y, h_c\}\}$
- In graph below, cliques are $\{\{a, d\}, \{a, b\}, \{b, c\}, \{b, e\}, \{e, f\}\}$



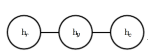
Undirected Models
Factors (2)

- Given clique $\mathcal{C} \in \mathcal{G}$ and $\boldsymbol{y}_{\mathcal{C}}$ = values on nodes in $\mathcal{C}$, **factor** $\phi_{\mathcal{C}}(\boldsymbol{y}_{\mathcal{C}})$ describes how likely they will co-exist
- Not quite a probability; need to **normalize** it first
- First go through all cliques $\mathcal{C}$, compute factor on $\mathcal{C}$ using values from $\boldsymbol{y}$:
$$\tilde{P}(\boldsymbol{y}) = \prod_{\mathcal{C} \in \mathcal{G}} \phi_{\mathcal{C}}(\boldsymbol{y}_{\mathcal{C}})$$
- Can convert this to a probability of $\boldsymbol{y}$ by normalizing:
$$\Pr[\boldsymbol{y}] = \tilde{P}(\boldsymbol{y})/Z \ ,$$
where $Z = \sum_{\boldsymbol{y} \in \mathcal{Y}} \tilde{P}(\boldsymbol{y})$ comes from summing (or integrating) over all possible values across all nodes
- Z doesn't change if model doesn't

Undirected Models
Factors (3)

Model:

$\phi(\mathcal{C}_{ry})$	$h_y = 0$	$h_y = 1$
$h_r = 0$	2	1
$h_r = 1$	1	10



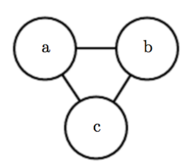
$\phi(\mathcal{C}_{yc})$	$h_y = 0$	$h_y = 1$
$h_c = 0$	5	1
$h_c = 1$	2	15

Distribution:

h_r	h_y	h_c	$\phi(\mathcal{C}_{ry})$	$\phi(\mathcal{C}_{yc})$	$\tilde{P}(\boldsymbol{y})$	$\Pr[\boldsymbol{y}]$
0	0	0	2	5	10	0.051
0	0	1	2	2	4	0.020
0	1	0	1	1	1	0.005
0	1	1	1	15	15	0.076
1	0	0	1	5	5	0.025
1	0	1	1	2	2	0.010
1	1	0	10	1	10	0.051
1	1	1	10	15	150	0.762
					$Z = 197$	1.0

What is time complexity of brute-force approach?

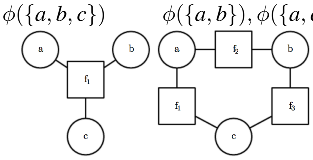
Undirected Models
Factor Graphs



- How do we interpret this MRF?
- Could be one factor: $\phi(\{a, b, c\})$
- Or, is it three: $\phi(\{a, b\}), \phi(\{a, c\}), \phi(\{b, c\})$

A **factor graph** makes explicit the scope of each factor ϕ

$\phi(\{a, b, c\})$ $\phi(\{a, b\}), \phi(\{a, c\}), \phi(\{b, c\})$



Bipartite graph, so no circles or squares connected

Undirected Models
Factor Graphs (2)

- Formally, a factor graph is a bipartite graph $(V, \mathcal{F}, \mathcal{E})$, where V = **variable nodes**, $\mathcal{F}$ = **factor nodes** and edges $\mathcal{E} \subseteq V \times \mathcal{F}$ with one endpoint V and one in $\mathcal{F}$
- The **scope** $N : \mathcal{F} \to 2^V$ of factor $f \in \mathcal{F}$ is the set of neighboring variables:

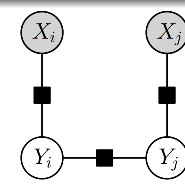
$$N(f) = \{i \in V : (i, f) \in \mathcal{E}\}$$

- Now compute distribution similar to before:

$$\Pr[\boldsymbol{y}] = \frac{1}{Z} \prod_{f \in \mathcal{F}} \phi_f(\boldsymbol{y}_{N(f)})$$

Undirected Models
Conditional Random Fields

- A **conditional random field** (CRF) is a factor graph used to directly model a conditional distribution $\Pr[Y = \boldsymbol{y} \mid X = \boldsymbol{x}]$
- E.g., probability that a specific pixel y is part of a cat given the **observation** (input image) $\boldsymbol{x}$



$$\Pr[Y_i = y_i, Y_j = y_j \mid X_i = x_i, X_j = x_j] = \frac{1}{Z(x_i, x_j)} \phi_i(y_i; x_i)\phi_j(y_j; x_j)\phi_{i,j}(y_i, y_j)$$

$$\Pr[Y = \boldsymbol{y} \mid X = \boldsymbol{x}] = \frac{1}{Z(\boldsymbol{x})} \prod_{f \in \mathcal{F}} \phi_f(\boldsymbol{y}_f; \boldsymbol{x}_f)$$

Z now depends on $\boldsymbol{x}$

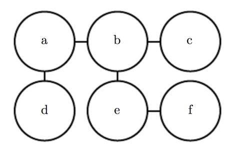
Undirected Models
Energy-Based Functions

- We now know how to factor the distribution graphically, but what form will $\phi(\cdot)$ take?
- Want to learn them to infer a distribution
- Need $\tilde{p}(\boldsymbol{x}) > 0$ for all $\boldsymbol{x}$ in order to get a distribution
- Define an **energy function** $E_f : \mathcal{Y}_{N(f)} \to \mathbb{R}$ for factor f
- Then define $\phi_f = \exp(-E_f(y_f)) > 0$ and get

$$\begin{aligned} p(Y = \boldsymbol{y}) &= \frac{1}{Z} \prod_{f \in \mathcal{F}} \phi_f(y_f) = \frac{1}{Z} \prod_{f \in \mathcal{F}} \exp\left(-E_f(y_f)\right) \\ &= \frac{1}{Z} \exp\left(-\sum_{f \in \mathcal{F}} E_f(y_f)\right) \end{aligned}$$

Undirected Models
Energy-Based Functions (2)

Using this form of ϕ allows us to factor our energy function as well!



$$E(a, b, c, d, e, f) = E_{a,b}(a, b) + E_{b,c}(b, c) + E_{a,d}(a, d) + E_{b,e}(b, e) + E_{e,f}(e, f)$$

Undirected Models
Energy-Based Functions (3)

- Still need a form for $E(\cdot)$ to parameterize and learn
- Define $E_f(\boldsymbol{y}_f; \boldsymbol{w})$ to depend on weight vector $\boldsymbol{w} \in \mathbb{R}^d$:

$$E_f : \mathcal{Y}_{N(f)} \times \mathbb{R}^d \to \mathbb{R}$$

- E.g., say we are doing binary image segmentation
  - Want adjacent pixes to try to take same value, so define $E_f : \{0, 1\} \times \{0, 1\} \times \mathbb{R}^2 \to \mathbb{R}$ as

$$E_f(0, 0; \boldsymbol{w}) = E_f(1, 1; \boldsymbol{w}) = w_1$$
$$E_f(0, 1; \boldsymbol{w}) = E_f(0, 1; \boldsymbol{w}) = w_2$$

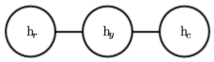
  - We learn w_1 and w_2 from training data, expecting $w_1 > w_2$
  - More on this later

Separation and D-Separation

- An edge between two nodes indicates a direct interaction between the variables
- Paths between nodes indicate **indirect** interactions
- Observing (instantiating) some variables change the interactions between others
- Useful to know which subsets of variables are conditionally independent from each other, given values of other variables
- Say that set of variables $\mathbb{A}$ is **separated** (if undirected model) or **d-separated** (if directed) from set $\mathbb{B}$ given set $\mathbb{S}$ if the graph implies that $\mathbb{A}$ and $\mathbb{B}$ are conditionally independent given $\mathbb{S}$

Separation and D-Separation
Example

Recall example on health of you, roommate, and coworker

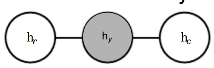


h_r	$\Pr[h_c = 0 \mid h_r]$
0	$(10+1)/(10+4+1+15) = 11/30$
1	$(5+10)/(5+2+10+150) = 15/167$

$\Rightarrow \Pr[h_c = 0]$ influenced by h_r

h_r	h_y	h_c	$\tilde{P}(\mathbf{y})$
0	0	0	10
0	0	1	4
0	1	0	1
0	1	1	15
1	0	0	5
1	0	1	2
1	1	0	10
1	1	1	150

What if we **know** that you are healthy ($h_y = 1$)?



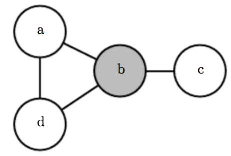
h_r	$\Pr[h_c = 0 \mid h_y = 1, h_r]$
0	$1/(1+15) = 1/16$
1	$10/(10+150) = 10/160 = 1/16$

$\Rightarrow$ Given h_y, h_c is CI from h_r

h_r	h_y	h_c	$\tilde{P}(\mathbf{y})$
0	0	0	10
0	0	1	4
0	1	0	1
0	1	1	15
1	0	0	5
1	0	1	2
1	1	0	10
1	1	1	150

Separation and D-Separation
Separation in Undirected Models

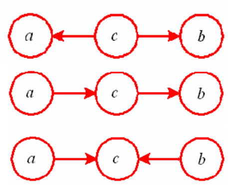
- If a variable is observed, it **blocks** all paths through it
- In an undirected model, two nodes are separated if all paths between them are blocked



- E.g., a and c are blocked, as are d and c, but not a and d (even though one of their paths is blocked)

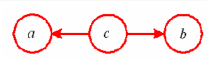
Separation and D-Separation
D-Separation in Directed Models

- In directed models, d-separation is more complicated
- Depends on the direction of the edges involved
- When considering nodes a and b connected via c, can classify connection as **tail-to-tail**, **head-to-tail**, and **head-to-head**



- For each case, assuming no other path exists (ignoring edge direction) between a and b, we will determine if a and b are independent, or conditionally independent given c

Separation and D-Separation
D-Separation in Directed Models: Tail-to-Tail



E.g., a = car won't start, b = lights work, c = battery low

$\Pr[c = 1] = 1/2$

c	$\Pr[a = 1 \mid c]$
0	1/3
1	1/2

c	$\Pr[b = 1 \mid c]$
0	4/5
1	1/10

- Factorization:

$$\Pr[a, b, c] = \Pr[a \mid c] \Pr[b \mid c] \Pr[c]$$

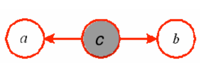
- When c unknown, get $\Pr[a, b]$ by marginalizing:

$$\Pr[a, b] = \sum_c \Pr[a \mid c] \Pr[b \mid c] \Pr[c] \ ,$$

which generally does not equal $\Pr[a] \Pr[b]$
$\Rightarrow$ a and b not independent

- E.g., $\Pr[a = 1, b = 1] = 0.292 \neq 0.321 = (0.583)(0.550) = \Pr[a = 1] \Pr[b = 1]$

Separation and D-Separation
D-Separation in Directed Models: Tail-to-Tail (2)



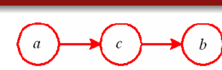
E.g., $c = 1$ (battery low)

- When conditioning on c:

$$\Pr[a, b \mid c] = \frac{\Pr[a, b, c]}{\Pr[c]} = \frac{\Pr[c] \Pr[a \mid c] \Pr[b \mid c]}{\Pr[c]} = \Pr[a \mid c] \Pr[b \mid c]$$

- Thus a and b conditionally independent given c (car not starting independent of lights working)
- Say that connection between a and b is **blocked** by c when it is observed and **unblocked** when unobserved
- Always true for uncoupled tail-to-tail connections (where there's no edge between a and b)

Separation and D-Separation
D-Separation in Directed Models: Head-to-Tail



E.g., a = leave on time, b = on time for work, c = catch the ferry

$\Pr[a = 1] = 1/2$

a	$\Pr[c = 1 \mid a]$
0	1/3
1	1/2

c	$\Pr[b = 1 \mid c]$
0	1/5
1	9/10

- Factorization:

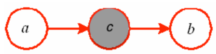
$$\Pr[a, b, c] = \Pr[a] \Pr[c \mid a] \Pr[b \mid c]$$

- When c unknown, get $\Pr[a, b]$ by marginalizing:

$$\Pr[a, b] = \Pr[a] \sum_c \Pr[c \mid a] \Pr[b \mid c] = \Pr[a] \Pr[b \mid a] \ ,$$

which generally does not equal $\Pr[a] \Pr[b]$
$\Rightarrow$ a and b not independent

Separation and D-Separation
D-Separation in Directed Models: Head-to-Tail (2)



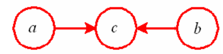
E.g., $c = 1$ (catch ferry)

- When conditioning on c:

$$\Pr[a, b \mid c] = \frac{\Pr[a, b, c]}{\Pr[c]} = \frac{\Pr[a] \Pr[c \mid a] \Pr[b \mid c]}{\Pr[c]} = \Pr[a \mid c] \Pr[b \mid c]$$

- Thus a and b conditionally independent given c (on time for work independent of leaving on time)
- Say that connection between a and b is blocked by c when it is observed and unblocked when unobserved
- Always true for uncoupled head-to-tail connections

Separation and D-Separation
D-Separation in Directed Models: Head-to-Head



E.g., a = rain, b = sprinkler, c = wet grass

$\Pr[a = 1] = 1/4$, $\Pr[b = 1] = 1/3$

a	b	$\Pr[c = 1 \mid a, b]$
0	0	1/10
0	1	6/10
1	0	4/5
1	1	10/11

- Factorization:

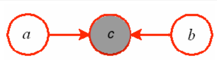
$$P(a, b, c) = P(a)P(b)P(c \mid a, b)$$

- When c unknown, get $P(a, b)$ by marginalizing:

$$P(a, b) = P(a)P(b) \sum_c P(c \mid a, b) = P(a)P(b)$$

$\Rightarrow$ a and b are independent

Separation and D-Separation
D-Separation in Directed Models: Head-to-Head (2)



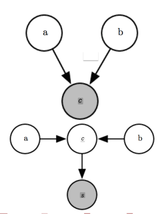
E.g., $c = 1$ (grass wet)

- When conditioning on c:

$$\Pr[a, b \mid c] = \frac{\Pr[a, b, c]}{\Pr[c]} = \frac{\Pr[a] \Pr[b] \Pr[c \mid a, b]}{\Pr[c]} ,$$

which generally does not equal $\Pr[a \mid c] \Pr[b \mid c]$

- a-b connection blocked by c when c **unobserved** and unblocked when observed (also unblocks if one of c's **descendants** observed)
- E.g., if grass wet and not raining, $\Pr[b = 1]$ increases
- Always true for uncoupled head-to-head connections



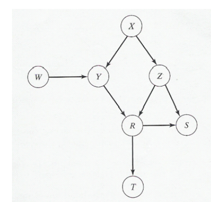
Separation and D-Separation
D-Separation in Directed Models: Example

W and T:

- $[W, Y, R, T]$ blocked by Y or R
- $[W, Y, X, Z, R, T]$ blocked by X or Z or R
- $[W, Y, X, Z, S, R, T]$ blocked by X or Z or R but **not** by S since observing S unblocks the chain

Y and T:

- $[Y, R, T]$ blocked by R
- $[Y, X, Z, R, T]$ blocked by X or Z or R
- $[Y, X, Z, S, R, T]$ blocked by X or Z or R



Separation and D-Separation
D-Separation in Directed Models: Example (2)

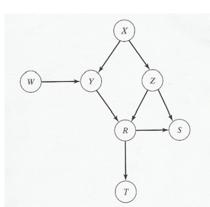
W and S:

- $[W, Y, R, S]$ blocked by Y or R
- $[W, Y, X, Z, R, S]$ blocked by X or Z or R
- $[W, Y, X, Z, S]$ blocked by X or Z
- $[W, Y, R, Z, S]$ blocked by Y or Z

Y and S:

- $[Y, R, S]$ blocked by R
- $[Y, R, Z, S]$ blocked by Z
- $[Y, X, Z, R, S]$ blocked by X or Z or R
- $[Y, X, Z, S]$ blocked by X or Z

Thus $\{W, Y\}$ and $\{S, T\}$ are CI given $\{R, Z\}$

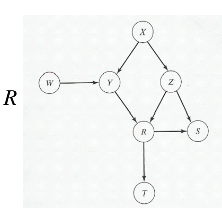


Separation and D-Separation
D-Separation in Directed Models: Example (2)

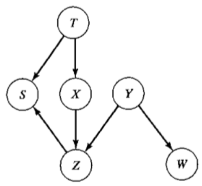
W and X:

- Chain $[W, Y, X]$ blocked by Y when not observed
- Chain $[W, Y, R, Z, X]$ blocked by R when not observed
- Chain $[W, Y, R, S, Z, X]$ blocked by S when not observed

Thus W and X are independent



Markov Blankets



- Let $\mathcal{V}$ be a set of random variables (nodes), and $X \in \mathcal{V}$. A **Markov blanket** $\mathcal{M}_X$ of X is any set of variables such that X is CI of all other variables given $\mathcal{M}_X$
- If no proper subset of $\mathcal{M}_X$ is a Markov blanket, then $\mathcal{M}_X$ is a **Markov boundary**
- **Theorem:** The set of X's parents, children, and co-parents (other parents of X's children) form a Markov blanket of X
- Node X has Markov blanket $\{T, Y, Z\}$

Learning Graphical Models
Conditional Random Fields

- Learning a CRF with input $\boldsymbol{x}$, parameterized by weight vector $\boldsymbol{w}$:

$$\Pr[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}] = \frac{1}{Z(\boldsymbol{x}, \boldsymbol{w})} \exp\left(-E(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{w})\right)$$

  where $Z(\boldsymbol{x}, \boldsymbol{w}) = \sum_{\boldsymbol{y} \in \mathcal{Y}} \exp\left(-E(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{w})\right)$
- Let energy function $E(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{w}) = \langle \boldsymbol{w}, \varphi(\boldsymbol{x}, \boldsymbol{y}) \rangle$
  - I.e., a weighted sum of features produced by **feature function** $\varphi(\boldsymbol{x}, \boldsymbol{y})$
  - $\varphi(\boldsymbol{x}, \boldsymbol{y})$ could be a deep network, possibly trained earlier
  - $\boldsymbol{w}$ is trained to get $\Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]$ "close" to the true distribution $\Pr_D[\boldsymbol{y} \mid \boldsymbol{x}]$

Learning Graphical Models
Conditional Random Fields (2)

- Want $\boldsymbol{w}$ such that $\Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]$ is close to the true distribution $\Pr_D[\boldsymbol{y} \mid \boldsymbol{x}]$
- Measure distance via **Kullback-Leibler (KL) divergence**: for any $\boldsymbol{x} \in \mathcal{X}$ we have

$$\mathrm{KL}(P \| D) = \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_D[\boldsymbol{y} \mid \boldsymbol{x}] \log \frac{\Pr_D[\boldsymbol{y} \mid \boldsymbol{x}]}{\Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]}$$

- By marginalizing over all $\boldsymbol{x} \in \mathcal{X}$ we get

$$\mathrm{KL}_{tot}(P \| D) = \sum_{\boldsymbol{x} \in \mathcal{X}} \Pr_D[\boldsymbol{x}] \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_D[\boldsymbol{y} \mid \boldsymbol{x}] \log \frac{\Pr_D[\boldsymbol{y} \mid \boldsymbol{x}]}{\Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]}$$

Learning Graphical Models
Conditional Random Fields (3)

- Goal is to find weights yielding close distribution, so

$$\begin{aligned}
\boldsymbol{w}^* &= \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^d} \mathrm{KL}_{tot}(P \| D) \\
&= \operatorname*{argmax}_{\boldsymbol{w} \in \mathbb{R}^d} \sum_{\boldsymbol{x} \in \mathcal{X}} \Pr_D[\boldsymbol{x}] \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_D[\boldsymbol{y} \mid \boldsymbol{x}] \log \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}] \\
&= \operatorname*{argmax}_{\boldsymbol{w} \in \mathbb{R}^d} \sum_{\boldsymbol{x} \in \mathcal{X}} \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_D[\boldsymbol{x}] \Pr_D[\boldsymbol{y} \mid \boldsymbol{x}] \log \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}] \\
&= \operatorname*{argmax}_{\boldsymbol{w} \in \mathbb{R}^d} \sum_{\boldsymbol{x} \in \mathcal{X}} \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_D[\boldsymbol{x}, \boldsymbol{y}] \log \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}] \\
&= \operatorname*{argmax}_{\boldsymbol{w} \in \mathbb{R}^d} \mathsf{E}_{(\boldsymbol{x}, \boldsymbol{y}) \sim D} \left[\log \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]\right] \\
&\approx \operatorname*{argmax}_{\boldsymbol{w} \in \mathbb{R}^d} \sum_{(\boldsymbol{x}^n, \boldsymbol{y}^n) \in \mathcal{D}} \log \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}]
\end{aligned}$$

  for training data $\mathcal{D}$

Learning Graphical Models
Conditional Random Fields: RMCL

- I.e., we choose a model ($\boldsymbol{w}^*$) that **maximizes the conditional log likelihood** of the data
  - If all $(\boldsymbol{x}, \boldsymbol{y})$ instances are drawn iid, then $\boldsymbol{w}^*$ maximizes the probability of seeing all the $\boldsymbol{y}$s given all the $\boldsymbol{x}$s
- Throw in a regularizer for good measure
- **Definition:** Let $\Pr[\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{w}] = \frac{1}{Z(\boldsymbol{x}, \boldsymbol{w})} \exp\left(-\langle \boldsymbol{w}, \varphi(\boldsymbol{x}, \boldsymbol{y}) \rangle\right)$ be a probability distribution parameterized by $\boldsymbol{w} \in \mathbb{R}^d$ and let $\mathcal{D} = \{(\boldsymbol{x}^n, \boldsymbol{y}^n)\}_{n=1,\ldots,N}$ be a set of training examples. For any $\lambda > 0$, **regularized maximum conditional likelihood (RMCL)** training chooses

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^d} \lambda \|\boldsymbol{w}\|^2 + \sum_{n=1}^{N} \langle \boldsymbol{w}, \varphi(\boldsymbol{x}^n, \boldsymbol{y}^n) \rangle + \sum_{n=1}^{N} \log Z(\boldsymbol{x}^n, \boldsymbol{w})$$

Learning Graphical Models
Conditional Random Fields: RMCL (2)

Goal: find $\boldsymbol{w}$ minimizing

$$\mathcal{L}(\boldsymbol{w}) = \lambda \|\boldsymbol{w}\|^2 + \sum_{n=1}^{N} \langle \boldsymbol{w}, \varphi(\boldsymbol{x}^n, \boldsymbol{y}^n) \rangle + \sum_{n=1}^{N} \log Z(\boldsymbol{x}^n, \boldsymbol{w})$$

Compute the gradient:

$$\begin{aligned}
\nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) &= 2\lambda \boldsymbol{w} + \sum_{n=1}^{N} \left[\varphi(\boldsymbol{x}^n, \boldsymbol{y}^n) - \sum_{\boldsymbol{y} \in \mathcal{Y}} \left(\frac{\exp(-\langle \boldsymbol{w}, \varphi(\boldsymbol{x}^n, \boldsymbol{y}) \rangle)}{\sum_{\boldsymbol{y}' \in \mathcal{Y}} \exp(-\langle \boldsymbol{w}, \varphi(\boldsymbol{x}^n, \boldsymbol{y}') \rangle)} \right) \varphi(\boldsymbol{x}^n, \boldsymbol{y}) \right] \\
&= 2\lambda \boldsymbol{w} + \sum_{n=1}^{N} \left[\varphi(\boldsymbol{x}^n, \boldsymbol{y}^n) - \sum_{\boldsymbol{y} \in \mathcal{Y}} \Pr_P[\boldsymbol{y} \mid \boldsymbol{x}^n, \boldsymbol{w}] \varphi(\boldsymbol{x}^n, \boldsymbol{y}) \right] \\
&= \boxed{2\lambda \boldsymbol{w} + \sum_{n=1}^{N} \left[\varphi(\boldsymbol{x}^n, \boldsymbol{y}^n) - \mathsf{E}_{\boldsymbol{y} \sim P(\boldsymbol{y} \mid \boldsymbol{x}^n, \boldsymbol{w})} \left[\varphi(\boldsymbol{x}^n, \boldsymbol{y}) \right] \right]}
\end{aligned}$$

Learning Graphical Models
Conditional Random Fields: RMCL (3)

- The gradient has a nice, compact form, and is **convex**
  - ⇒ Any local optimum is a global one
- **Problem:** Computing expectation requires summing over exponentially many combinations of values of $\boldsymbol{y}$
- We can factor energy function, and therefore its derivative, and therefore the expectation of its derivative
- Let's focus on an individual factor f:

$$\mathsf{E}_{\boldsymbol{y}_f \sim P(\boldsymbol{y}_f | \boldsymbol{x}^n, \boldsymbol{w})} \left[\varphi_f(\boldsymbol{x}^n, \boldsymbol{y}_f) \right] = \sum_{\boldsymbol{y}_f \in \mathcal{Y}_f} \Pr_P(\boldsymbol{y}_f \mid \boldsymbol{x}, \boldsymbol{w}) \varphi_f(\boldsymbol{x}^n, \boldsymbol{y}_f)$$

- Summation still has exponentially many terms, but instead of $K^{|V|}$ now it's $K^{|N(f)|}$ (more manageable)
- Still need to compute each factor's marginal probability

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Learning Graphical Models
Inference

- Efficient **inference** of marginal probabilities and Z in a graphical model is itself a major research area
- Depends on the structural model we're using
- Start with **belief propagation** in acyclic models
- Then approximate **loopy belief propagation** for cyclic models

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Learning Graphical Models
Inference: Sum-Product Algorithm

- **Belief propagation** is a general approach to inference in directed and undirected graphical models
- Generally, some node i sends a message to another node j regarding i's belief about variable y
  - i informs j its belief about marginal probability $\Pr[y]$
  - E.g., message value high ⇒ belief is $\Pr[y]$ also high
  - Each node messages each of its neighbors about its belief for each value of the random variable
- **Sum-Product Algorithm** uses belief propagation to find marginal probabilities and Z in **tree-structured** factor graphs (connected and acyclic)
- Each edge $(i,f) \in \mathcal{E} \subseteq V \times \mathcal{F}$ has
  1. $q_{Y_i \to f} \in \mathbb{R}^{|\mathcal{Y}_i|}$ is a **variable-to-factor** message
  2. $r_{f \to Y_i} \in \mathbb{R}^{|\mathcal{Y}_i|}$ is a **factor-to-variable** message
- Note they are vector quantities, one component per value of Y_i

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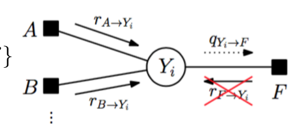
Learning Graphical Models
Inference: Sum-Product Algorithm (2)

Variable-to-Factor Message

- For variable $i \in V$, let

$$M(i) = \{f \in \mathcal{F} : (i,f) \in \mathcal{E}\}$$

be the set of factors adjacent to i



- For each value y_i of variable i, variable-to-factor message is

$$q_{Y_i \to f}(y_i) = \sum_{f' \in M(i) \setminus \{f\}} r_{f' \to Y_i}(y_i)$$

- Variable node i sums up all factor-to-variable messages from all factors except f and transmits result to f

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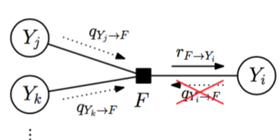
Learning Graphical Models
Inference: Sum-Product Algorithm (3)

Factor-to-Variable Message

- For factor $f \in \mathcal{F}$, recall

$$N(f) = \{i \in V : (i,f) \in \mathcal{E}\}$$

is the set of variables adjacent to f



- For each value y_i of variable i, factor-to-variable message is

$$r_{f \to Y_i}(y_i) = \log \sum_{\substack{y'_f \in \mathcal{Y}_f, \\ y'_i = y_i}} \exp \left(-E_f(y'_f) + \sum_{j \in N(f) \setminus \{i\}} q_{Y_j \to f'}(y'_i) \right)$$

- Factor node f sums up all variable-to-factor messages from all variables except i and transmits result to i

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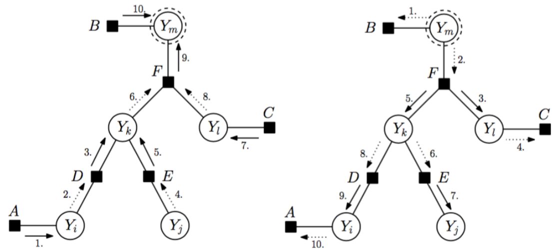
Learning Graphical Models
Inference: Sum-Product Algorithm (4)

- Since we have a tree structure, there is always at least one variable adjacent to only one factor or one factor adjacent to one variable
- These messages depend on nothing, so start there
- Then order the other message computations via precedence graph
- Designate an arbitrary variable node to be the root
- Two phases of algorithm:
  1. **Leaf-to-root** phase: start at leaves and compute messages toward root
  2. **Root-to-leaf** phase: start at root and compute messages toward leaves

Learning Graphical Models
Inference: Sum-Product Algorithm (5)



After two phases, all messages computed

Learning Graphical Models
Inference: Sum-Product Algorithm (6)

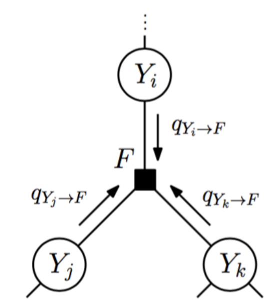
To **compute** Z, sum over factor-to-variable messages directed to root Y_r:

$$\log Z = \log \sum_{y_r \in \mathcal{Y}_r} \exp \left(\sum_{f \in M(r)} r_{f \to Y_r}(y_r) \right)$$

Learning Graphical Models
Inference: Sum-Product Algorithm (7)

To **compute factor marginals:**

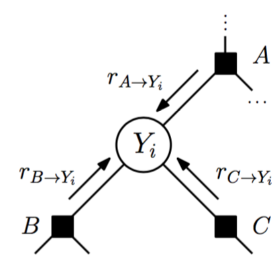
$$\mu_f(\boldsymbol{y}_f) = \Pr[Y_f = \boldsymbol{y}_f] = \exp \left(-E_f(\boldsymbol{y}_f) + \sum_{i \in N(f)} q_{Y_i \to f}(y_i) - \log Z \right)$$



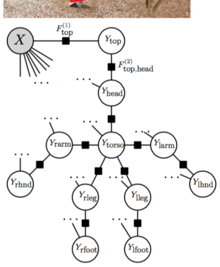
Learning Graphical Models
Inference: Sum-Product Algorithm (8)

To **compute variable marginals:**

$$\Pr[Y_i = y_i] = \exp \left(\sum_{f \in M(i)} r_{f \to Y_i}(y_i) - \log Z \right)$$



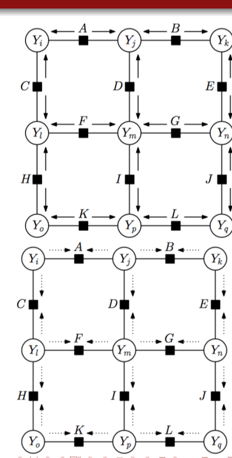
Learning Graphical Models
Inference: Sum-Product Algorithm: **Pictorial Structures** Example



- E.g., $E_{f^{(1)}_{\text{top}}}(y_{\text{top}}; \boldsymbol{x})$ is energy function for factor f_{top} representing top of person
- $\boldsymbol{x}$ is observed image and Y_{top} is tuple (a, b, s, θ) where (a, b) are coordinates, s is scale, and θ is rotation
- $E_{f^{(2)}_{\text{top,head}}}(y_{\text{top}}, y_{\text{head}})$ relates adjecnt pairs of variables

Learning Graphical Models
Inference: Loopy Belief Propagation

- When graph has a cycle, can still perform message passing to **approximate** Z and marginal probabilities
- Initialize messages to fixed value
- Perform updates in random order until convergence
- Factor-to-variable messages $r_{f \to Y_i}$ computed as before
- Variable-to-factor messages computed differently



Learning Graphical Models
Inference: Loopy Belief Propagation (2)

Variable-to-factor messages:

$$\bar{q}_{Y_i \to f}(y_i) = \sum_{f' \in M(i) \setminus \{f\}} r_{f' \to Y_i}(y_i)$$

$$\delta = \log \sum_{y_i \in \mathcal{Y}_i} \exp\left(\bar{q}_{Y_i \to f}(y_i)\right)$$

$$q_{Y_i \to f}(y_i) = \bar{q}_{Y_i \to f}(y_i) - \delta$$

Learning Graphical Models
Inference: Loopy Belief Propagation (3)

To **compute factor marginals:**

$$\bar{\mu}_f(\mathbf{y}_f) = -E_f(\mathbf{y}_f) + \sum_{j \in N(f)} q_{Y_j \to f}(y_j)$$

$$z_f = \log \sum_{\mathbf{y}_f \in \mathcal{Y}_f} \exp(\bar{\mu}_f(\mathbf{y}_f))$$

$$\mu_f(\mathbf{y}_f) = \exp\left(\bar{\mu}_f(\mathbf{y}_f) - z_f\right)$$

Learning Graphical Models
Inference: Loopy Belief Propagation (4)

To **compute variable marginals:**

$$\bar{\mu}_i(y_i) = \sum_{f' \in M(i)} r_{f' \to Y_i}(y_i)$$

$$z_i = \log \sum_{y_i \in \mathcal{Y}_i} \exp(\bar{\mu}_i(y_i))$$

$$\mu_i(y_i) = \exp\left(\bar{\mu}_i(y_i) - z_i\right)$$

Learning Graphical Models
Inference: Loopy Belief Propagation (5)

To **compute Z:**

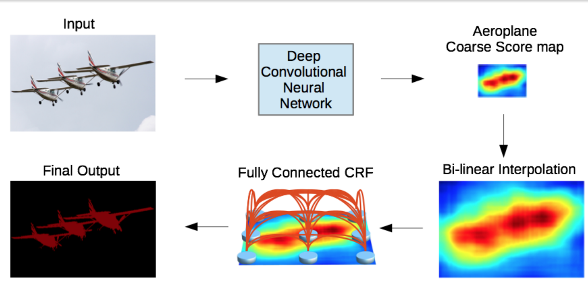
$$\log Z = \sum_{i \in V} (|M(i) - 1|) \left[\sum_{y_i \in \mathcal{Y}_i} \mu_i(y_i) \log \mu_i(y_i) \right] - \sum_{f \in \mathcal{F}} \sum_{\mathbf{y}_f \in \mathcal{Y}_f} \mu_f(\mathbf{y}_f) \left(E_f(\mathbf{y}_f) + \log \mu_f(\mathbf{y}_f) \right)$$

Learning Graphical Models
Conditional Random Fields: Case Study

Chen et al. (2015): Semantic Image Segmentation with Deep Convolutional Nets and Fully Connected CRFs

- Adapted DCNN ResNet-101 (trained for image classification) to the task of semantic segmentation
- Replaced connected layer with a “de-convolution” layer to upscale to original resolution for segmented image
- Result effective, but segment edges blurred
- Used CRF to sharpen

Learning Graphical Models
Conditional Random Fields: Case Study (2): Overview



- Score map generated as output of DCNN interpolated to input resolution
- Right area, but boundary of high-scoring region is fuzzy
- CRF sharpens to final output

- Energy function:

$$E(\mathbf{y}) = \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{ij}(y_i, y_j)$$

  where $y_i \in \{0, 1\}$ is label assignment for pixel i
- Use $\theta_i(y_i) = -\log P(y_i)$ and

$$\theta_{ij}(y_i, y_j) = \mu(y_i, y_j) \left[w_1 \exp\left(-\frac{\|p_i - p_j\|^2}{2\sigma_\alpha^2} - \frac{\|I_i - I_j\|^2}{2\sigma_\beta^2} \right) + w_2 \exp\left(-\frac{\|p_i - p_j\|^2}{2\sigma_\gamma^2} \right) \right]$$

  where
  - $\mu(y_i, y_j) = 1$ iff $y_i \neq y_j$ (different labels)
  - $p_i =$ position of pixel i
  - $I_i =$ RGB color of pixel i
  - $\sigma =$ parameters
- Inference via specialized algorithms for Gaussian-based functions

CSCE 970 Lecture 8: Structured Prediction
Stephen Scott and Vinod Variyam
Introduction
Definitions
Applications
Graphical Models
Training

Image/G.T. | DCNN output | CRF Iteration 1 | CRF Iteration 2 | CRF Iteration 10