Probabilistic Graphical Models in Machine Learning

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Plan of Discussion

- Machine Learning (ML)
 - History and Problem types solved
- Probabilistic Graphical Models (PGMs)
 - Tutorial
 - Specialized models
- Computational Forensics Application
 - Handwriting

What is Machine Learning?

- Automatic construction of programs from examples of input-output behavior
- Marriage of Computer Science and Probability /Statistics
 - 1. Computer Science:
 - Artificial Intelligence
 - Tasks performed by humans not well described algorithmically
 - Data Explosion
 - User and thing generated

2. Statistics:

Methods that learn from data (MLE or Bayesian)

When is Machine Learning Needed

- Problems involving uncertainty
 - Perceptual data (images, text, speech, video)
- Information overload
 - Large Volumes
 - Limitations of time, cognitive ability
- Constantly Changing Data Streams
 - Search engine adaptation
- Principled design
 - High performance systems

Problem Types and Methods

1. Classification

- OCR, Spam Filter (Logistic Regression)
- Text Categorization (SVM)

2. Regression:

LeToR (GP)

3. Collective Classification

- Speech, Handwriting (HMM)
- PoS, NE (MEMM, CRF)

4. Inferring a Probability Distribution

- Computational Forensics (BN, Sampling)
- 5. Clustering Data Mining (EM, BIC)

History of ML





20 x 20 cell Adaptive Wts

- First Generation (1960-1980)
 - Perceptrons, Nearest-neighbor, Naïve Bayes
 - Special Hardware, Limited performance



USPS-MI OCR

- Second Generation (1980-2000)
 - ANNs, Kalman, HMMs, SVMs

Amhesst. **USPS-RCR**

- HW addresses, speech reco, postal words
- Difficult to include domain knowledge
 - Black box models fitted to large data sets
- Third Generation (2000-Present)
 - PGMs, Fully Bayesian (including GP)
 - Image segmentation, Text analytics (NE Tagging)
 - Expert prior knowledge with statistical models

Classification: OCR

Input $x=\{x_1...x_{12}\}$: Image Features Output (y): Class Labels $\{y^0, y^1, y^9\}$





















Wide variability of same numeral

- Handcrafted rules will result in large no of rules and exceptions
- Better to have a machine that learns from a large training set

 x_1 x_3 Handwritten Digits x_4 x_{12}

Features (x_i) :

Values: Proportion of black pixels in each of 12 cells x_i i=1,...,12

$$x_i^0 = 0-10\%$$
 $x_i^1 = 10-20\%$

 $|Val(x_i)| = 10$

No of parameters=10¹²- 1
Or 1 trillion

Per class
No of samples needed=??

1,000 chars/page, 1,000s of pages

Regression: Learning To Rank







In LETOR 4.0 dataset 46 query-document features Maximum of 124 URLs/query





- Great Wall of China, History, Gallery of Pictures, Travel Guide, News ...
- Great Wall of China center on Great Wall history, discovery & research, news, travel guide, articles, and gallery of pictures.
- Great Wall of China, Beijing Great Wall Tours, Great Wall Facts www.travelchinaquide.com/china great wall/ Cached

China Great Wall facts on its history, construction, scenery, tours, photos, protection, wall map and first-hand reviews from travelers who have been there.

The Great Wall of China - 360-degree Virtual Tour, Simatai www.thechinaguide.com/great_wall_of_china/ - Cached

The Great Wall of China was built over more than two thousand years. Construction on the first section began between the 7th and 6th century BC, and the last ...

Input (x_i) :

(*d* Features of Query-URL pair)

- Log frequency of query in anchor text
- Query word in color on page
- # of images on page
- # of (out) links on page
- PageRank of page
- URL length
- URL contains "~"
- Page length

Traditional IR uses TF/IDF

Output (y): Relevance Value

Target Variable

- Point-wise (0,1,2,3)
- Regression returns continuous value
 -Allows fine-grained ranking of URLs

Role of PGMs in ML

- Dozens of ML models, Large Data sets
 - PGMs Provide understanding of:
 - model relationships (theory)
 - problem structure (practice)
 - Allow including human knowledge
- Nature of PGMs
 - 1.Represent joint distributions
 - 1. Many variables without full independence
 - 2.Expressive
 - 3.Declarati
 - 2.Inference: Separate model/algorithm errors
 - 3.Learning

Representation

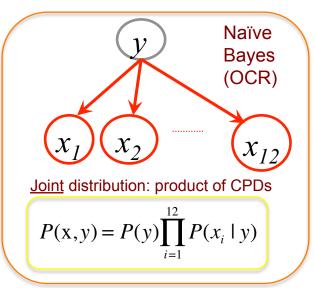
Probabilistic Graphical Models

1. Bayesian Network (BN)

Directed Acyclic Graph

Nodes: variables Edges: direct causality (correlation irrespective of others)

1		CF	PDs		$P(x_i y_i)$,)	у	x_i^0	x_i^l	x_i^2	x_i^3	x_i^4	x_i^5	x_i^6	x_i^7	x_i^{8}	x_i^{g}
	P(y))			•		y^0	0	0	0.1	0.2	0.3	0.2	0.1	0.1	0	0
	y^{θ}	y^1	y^2	y^3	y^4	J	y^{I}										
ŀ									12	CPD	S						
ı	0.1	0.1	0.1	0.1	0.1	(No	of pa	aram	eters	s = 100	0×1	2 = 1.2	200	
L														, ,, ,,	,-		
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							y'										



2. Markov Network (or MRF)

– Edge: influence (non-directional)

CRF: MN for conditional P(y|x)y target x: observed

$$\tilde{P}(y \mid \mathbf{x}) = \prod_{i=1}^{n} \phi_i(x_i, y)$$

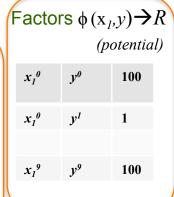
$$P(y \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \tilde{P}(y \mid \mathbf{x})$$

$$Z(\mathbf{x}) = \sum_{\mathbf{y}} \tilde{P}(\mathbf{y} \mid \mathbf{x})$$

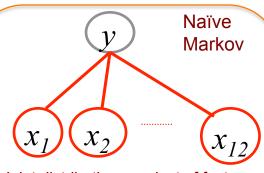
 $\tilde{P}(y \mid x) = \prod_{i=1}^{m} \phi_i(x_i, y)$ $\tilde{P}(y \mid x)$ Is unnormalized

 $P(y \mid x) = \frac{1}{Z(x)} \tilde{P}(y \mid x)$ Z(x) Partition function of x

m=no of factors



Undirected



Joint distribution: product of factors

$$P(x,y) = \frac{1}{Z} \prod_{i=1}^{12} \phi_i(x_i, y)$$

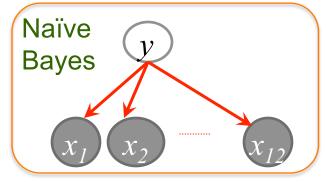
where Z is normalizing constant Partition function

$$Z = \sum_{\mathbf{x}} \prod_{i=1}^{12} \phi_i(x_i, y)$$

Discriminative vs Generative Training

Independent variables $x = \{x_1, ... x_{12}\}$ and binary target y

1. Generative: estimate CPD parameters

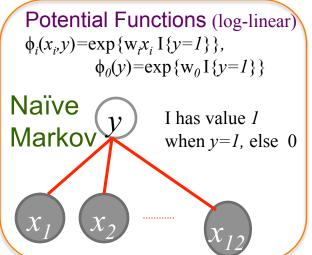


$$P(y,x) = P(y) \prod_{i=1}^{12} P(x_i | y)$$

From joint get required conditional

Low-dimensional estimation independently estimate 12x 10 parameters But pixel independence is false For sparse data generative is better

2. Discriminative: estimate CRF parameters w_i



Normalized

$$\tilde{P}(y = 1 \mid x) = \exp\left\{w_0 + \sum_{i=1}^{12} w_i x_i\right\}$$

$$P(y=1 \mid x) = sigmoid\left\{w_0 + \sum_{i=1}^{12} w_i x_i\right\} \text{ where } sigmoid(z) = \frac{e^z}{1 + e^z}$$

Logistic Regression

$$\tilde{P}(y=0 \mid x) = \exp\{0\} = 1$$
where $sigmoid(z) = \frac{e^z}{1+e^z}$

Jointly optimize 12 parameters

High dimensional estimation but correlations accounted for Can use much richer features:

Edges, image patches sharing same pixels

multiclass

$$p(y_i \mid \phi) = y_i(\phi) = \frac{\exp(a_i)}{\sum_{j} \exp(a_j)}$$

where $a_j = \mathbf{w}_j^T \boldsymbol{\phi}$

Collective Labeling: Three Models

Sequence of observations $X = \{X_1, ... X_k\}$ Need a joint label $Y = \{Y_1, ... Y_k\}$ Both CRF and MEMM are Discriminative Models Directly obtain P(Y|X)HMM is generative Needs P(X,Y)

Model Trade-offs in expressive power and learnability

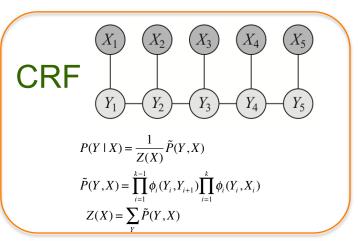
- 1.MEMM and HMM are more easily learned
 - Directed models: ML parameter estimates have closed-form
 - CRF requires expensive iterative gradient-based approach

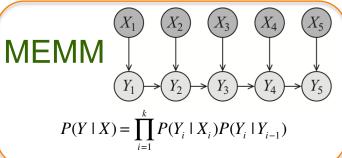
2. Ability to use rich feature sets

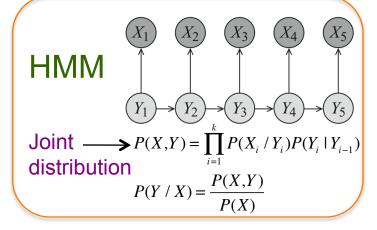
- HMM needs explicit modeling over features
- CRF and MEMM are discriminative models and avoid this

3.Independence Assumptions made

- MEMM assumes Y_i independent of X_2 not given Y_2
- Later observation has no effect on current state
 - In <u>activity recognition</u> in video sequence,
 Frames labelled as running/walking.
 Earlier frames may be blurry but later ones clearer
 Model incapable of going back







Dynamic BN: Training Data for LeToR

- Dynamic BN can model Time Trajectory
- LeToR relevance values are assigned by human editors
 - Expensive
 - Can change over time
- Click Logs:
 - provide implicit feedback
 - cheap proxy for editorial labels

 E_{i-1} E_{i} C_{i} C_{i} C_{i}

 C_i : Click on i^{th} URL in retrieved list

Hidden Variables:

 E_i : did the user examine the url?

 A_i : was the user attracted by the url?

 S_i : was the user satisfied by the landing page?

Inference: posterior probabilities of E_i , A_i and S_i

$$r \equiv P(S_{i} = 1 \mid E_{i} = 1)$$

$$= P(S_{i} = 1, E_{i} = 1) / P(E_{i} = 1)$$

$$= P(S_{i} = 1, E_{i} = 1, C_{i} = 0) / P(E_{i} = 1) + P(S_{i} = 1, E_{i} = 1, C_{i} = 1) / P(E_{i} = 1)$$

$$= 0 + P(S_{i} = 1, C_{i} = 1 \mid E_{i} = 1)$$
 [satisfaction only upon click]
$$= P(S_{i} = 1 \mid C_{i} = 1) P(C_{i} = 1 \mid E_{i} = 1)$$

Unusualness of Handwriting

Probabilistic Model for Handwriting Style

the the the the the the

QDE Features

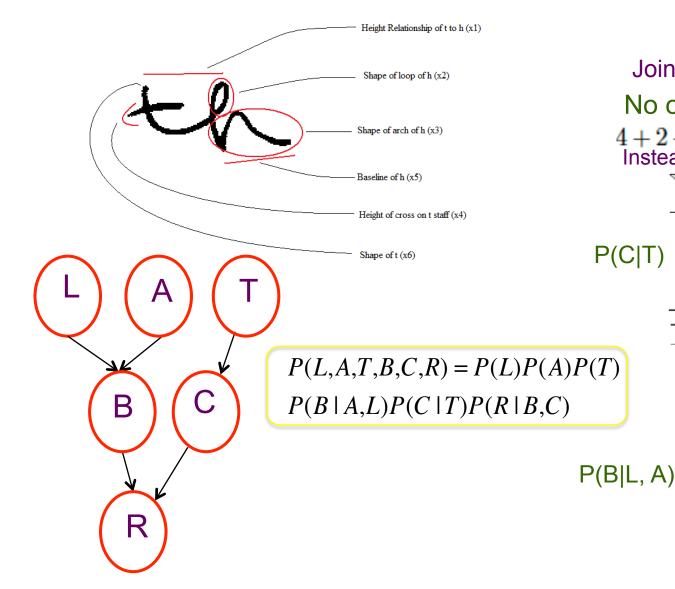
P(R,L,A,C,B,T)

		_			
R = Height Rela-	L = Shape of Loop	A = Shape of	C = Height of	B = Baseline of h	S = Shape of t
tionship of t to h	of h	Arch of h	Cross on t staff		
$r^0 = t$ shorter than h	$l^0 = \text{retraced}$	a^0 = rounded	$c^0 = \text{upper half of}$	$b^0 = \text{slanting up}$	$s^0 = \text{tented}$
		arch	staff	ward	
$r^1 = t$ even with h	$l^1 = $ curved right side	$a^1 = \text{pointed}$	$c^1 = lower half of$	b^1 = slanting	$s^1 = \text{single stroke}$
	and straight left side		staff	downward	
$r^2 = t$ taller than h	$l^2 = \text{curved left side}$	a^2 =no set pat-	c^2 = above staff	b^2 = baseline even	$s^2 = looped$
): [and straight right side	tern			
r^3 = no set pattern	l^3 = both sides		$c^3 = \text{no fixed pat-}$	$b^3 = \text{no set pattern}$	$s^3 = closed$
	curved		tern		
	l^4 = no fixed pattern				s^4 = mixture of
					shapes

$$|Val(X)| = 4 \times 5 \times 3 \times 4 \times 4 \times 5 = 4,800$$

No of parameters = 4,799

BN for "th"



Joint Probability

No of parameters=

$$4+2+59+4+19+63=151$$
 Instead of 4,800

X4 a	b	c (d
a 0.80	a 0.80 0.08 0.04 b 0.47 0.37 0.01	0.04	0.08
D(OIT) b 0.47	0.37	0.01	0.15
P(C T) c 0.59	0.29	0.06	0.06
d 0.76	0.12	0.03	0.09
e 0.45	0.18	0.02	0.36

X5	а	b	С	d
$x_2 = a, x_3 = a$	0.097	0.091	0.59	0.22
$x_2 = a_1 x_3 = b$	0.11	0.13	0.47	0.29
$x_2 = a, x_3 = c$	0.09	0.16	0.31	0.43
$x_2=b,x_3=a$	0.22	0.11	0.44	0.22
$x_2 = b, x_3 = b$	0.29	0.16	0.33	0.21
$x_2 = b, x_3 = c$	0.14	0.14	0.43	0.29
$x_2 = c, x_3 = a$	0.33	0.17	0.17	0.33
$x_2 = c, x_3 = b$	0.25	0.25	0.25	0.25
$x_2 = c, x_3 = c$	0.20	0.20	0.40	0.20
$x_2 = d_1 x_3 = a$	0.12	0.12	0.41	0.35
$x_2 = d_1 x_3 = b$	0.18	0.15	0.51	0.15
$x_2 = d, x_3 = c$	0.17	0.17	0.33	0.33
$x_2 = e_1 x_3 = a$	0.04	0.11	0.61	0.25
$x_2 = e_1 x_3 = b$	0.24	0.12	0.24	0.39

0.03

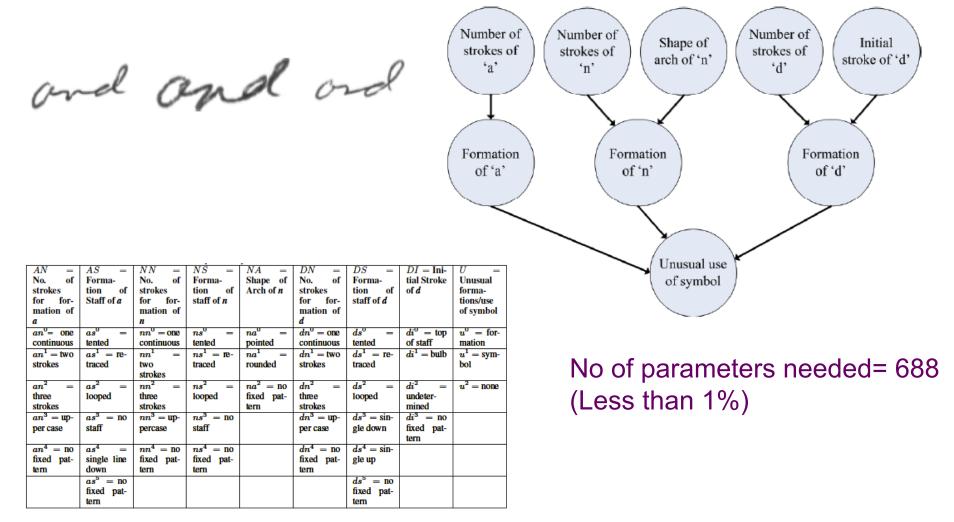
0.42

0.45

0.09

 $x_2 = e, x_3 = c$

BN for "and"



Nine variables
No of parameters needed= 809,999

Inference

Inference and Queries with PGMs

- Inference: Probabilistic Models used to answer queries
- Query Types
 - 1. Probability Queries
 - Query has two parts
 - Evidence: a subset E of variables and their instantiation e
 - Query Variables: a subset Y of random variables in network

2. MAP Queries

- Maximum a posteriori probability
- Also called MPE (Most Probable Explanation)

Inferring the Probability of Evidence

Probability Distribution of Evidence

$$P(L,C) = \sum_{A,T,B,R} P(L,A,T,B,C,R)$$
 Sum Rule of Probability
$$= \sum_{A,T,B,R} P(L)P(A)P(T)P(B \mid A,L)P(C \mid T)P(R \mid B,C)$$
 From the Graphical Model

Probability of Evidence

$$P(L = l^{0}, C = c^{1}) = \sum_{A,T,B,R} P(L = l^{0}) P(A) P(T) P(B \mid A, L) P(C = c^{1} \mid T) P(R \mid B, C = c^{1})$$

More Generally

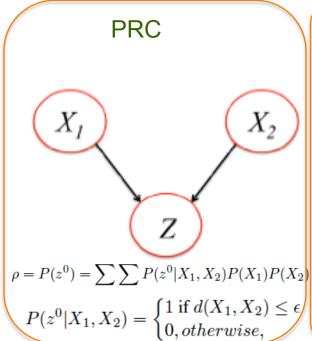
$$P(E = e) = \sum_{X \setminus E} \prod_{i=1}^{n} P(X_i \mid pa(X_i)) |_{E=e}$$

- An intractable problem
 - #P complete

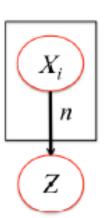
P: solution in polynomial time NP: verified in polynomial time #P complete: how many solutions

- Tractable when tree-width is less than 25
- Approximations are usually sufficient (hence sampling)
 - When P(Y=y|E=e)=0.29292, approximation yields 0.3

Inference: Rarity







$$\rho[n] = 1 - (1 - \rho)^{\frac{n}{2}}$$

n

Conditional nPRC

$$\rho[n] = 1 - (1 - \rho)^{\frac{n(n-1)}{2}}$$
 $p(Z = 1|X_s) = \sum_{\mathbf{X}} p(Z = 1|X_s, \mathbf{X})p(\mathbf{X})$

For identical match $1 - (1 - P(X_s))^n$

Rare

thithth

 $nPRC=1.17 \times 10^{-5}$

AND AND AND

$$nPRC=2.14 \times 10^{-8}$$

Common

ththth

nPRC = 0.156

and and ord

Learning

Learning Problems with PGMs

Parameter Learning (given structure)

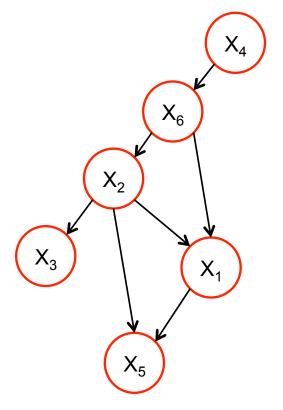
Bayesian Networks	Markov Networks
Local normalization within each CPD	Global normalization constant (the partition function)
Estimate local groups of parameters separately	Global parameter coupling across the network (even MLE has no closed form)

- Structure Learning
 - Search through network space
- Partial Data
 - -EM

Data Collection



Parameter Learning For BN



Max Likelihood Est $P(x_5|x_1,x_2)$

	<i>X</i> ₅ = 0	X ₅ = 1	X ₅ = 2	X ₅ = 3
$X_1 = 0, X_2 = 0$	0.50	0	0	0.50
$X_1 = 0, X_2 = 1$	0	1.00	0	0
$X_1 = 0, X_2 = 2$	0.18	0.36	0.27	0.18
$X_1 = 0, X_2 = 3$	0.27	0.40	0.30	0.03
$X_1 = 0, X_2 = 4$	0.22	0.45	0.28	0.05
$X_1 = 1, X_2 = 0$	0.43	0	0.28	0.29
$X_1 = 1, X_2 = 1$	NaN	NaN	NaN	NaN
$X_1 = 1, X_2 = 2$	0.39	0.06	0.33	0.22
$X_1 = 1, X_2 = 3$	0.33	0.17	0.33	0.17
$X_1 = 1, X_2 = 4$	0.42	0.11	0.29	0.18

Bayesian Estimate

	<i>X</i> ₅ = 0	<i>X</i> ₅ = 1	<i>X</i> ₅ = 2	<i>X</i> ₅ = 3
$X_1 = 0, X_2 = 0$	0.29	0.14	0.29	0.29
$X_1 = 0, X_2 = 1$	0.25	0.25	0.25	0.25
$X_1 = 0, X_2 = 2$	0.25	0.38	0.25	0.12
$X_1 = 0, X_2 = 3$	0.22	0.41	0.31	0.06
$X_1 = 0, X_2 = 4$	0.16	0.52	0.25	0.07
$X_1 = 1, X_2 = 0$	0.29	0.14	0.29	0.29
$X_1 = 1, X_2 = 1$	0.25	0.25	0.25	0.25
$X_1 = 1, X_2 = 2$	0.37	0.05	0.47	0.11
$X_1 = 1, X_2 = 3$	0.33	0.22	0.33	0.11
$X_1 = 1, X_2 = 4$	0.38	0.13	0.29	0.20

Bayesian Estimation

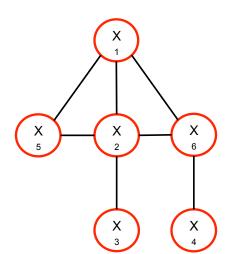
Prior $\boldsymbol{\theta} \sim \text{Dirichlet}(\alpha_1, ..., \alpha_k) \ \alpha_1 = ... = \alpha_k = 1$

Likelihood $O = \{o_1, ..., o_k\} \sim \text{Multinomial}(\theta_1, ..., \theta_k)$

Posterior $\boldsymbol{\theta}|O \sim \text{Dirichlet}(\alpha_1', ..., \alpha_k')$

$$\alpha'_i = \alpha_i + o_i$$
, for $i = 1, ..., k$

Parameter Learning for MN



Joint distribution for pairwise MN

$$p(X) = \frac{1}{Z} \phi_1(X_1, X_2) \cdot \phi_2(X_1, X_5) \cdot \phi_3(X_1, X_6)$$
$$\cdot \phi_4(X_2, X_5) \cdot \phi_5(X_2, X_6) \cdot \phi_6(X_2, X_3) \cdot \phi_7(X_4, X_6)$$
$$\cdot \phi_1(X_1) \cdot \phi_2(X_2) \cdot \phi_3(X_3) \cdot \phi_4(X_4) \cdot \phi_5(X_5) \cdot \phi_6(X_6)$$

No of Parameters θ_i :

$$20 + 16 + 20 + 20 + 25 + 15 + 20 + 4 + 5 + 3 + 4 + 4 + 5 = 161$$

e.g.,
$$\theta_{21} = \log \phi_1(X_1 = 0, X_5 = 0)$$
$$\theta_{22} = \log \phi_1(X_1 = 0, X_5 = 1)$$
$$\vdots$$
$$\theta_{36} = \log \phi_1(X_1 = 3, X_5 = 3)$$

Log-linear model

$$P(x_1,...,x_n:\theta) = \frac{1}{Z(\theta)} \exp\left\{\sum_{i=1}^k \theta_i f_i(D_i)\right\}$$

n: # variables, k: # cliques θ_i : parameters

Log-likelihood of *M* i.i.d. samples

$$\ell(\theta) = \sum_{i=1}^{k} \theta_i \left(\sum_{m} f_i(\xi[m]) \right) - M \ln \sum_{\xi} \exp \left(\sum_{i=1}^{k} \theta_i f_i(\xi) \right)$$

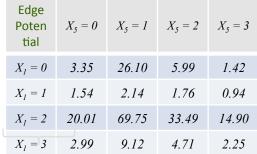
Gradient of log-likelihood

$$\frac{\partial}{\partial \theta_i} \frac{1}{M} \ell(\theta) = \frac{\sum_{m} f_i(\xi[m])}{M} - \frac{\sum_{\xi} f_i(\xi) \exp\left(\sum_{i=1}^k \theta_i f_i(\xi)\right)}{\sum_{\xi} \exp\left(\sum_{i=1}^k \theta_i f_i(\xi)\right)}$$

Concave, **BUT** no analytical maximum => Use iterative gradient ascent

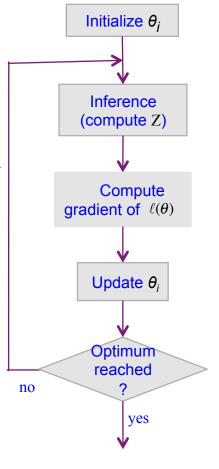
Estimated edge potential for

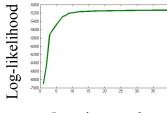
Edge Poten tial	$X_5 = 0$	$X_5 = 1$	$X_5 = 2$	$X_5 = 3$
$X_I = 0$	3.35	26.10	5.99	1.42
$X_I = 1$	1.54	2.14	1.76	0.94
$X_I = 2$	20.01	69.75	33.49	14.90
$X_I = 3$	2.99	9.12	4.71	2.25



Inference step for Z: Computes unnormalized prob for every setting of X => expensive

- Approximate inference
 - particle-based methods (MCMC sampling)
 - global algorithm (belief prop, mean-field)
- Approximate objective
 - Not as much inference
 - Pseudo-likelihood, maxent





Iteration number

Structure Learning of BNs

Problem: Many perfect maps for distribution P*

Goal: Asymptotically recover G*'s equivalence class

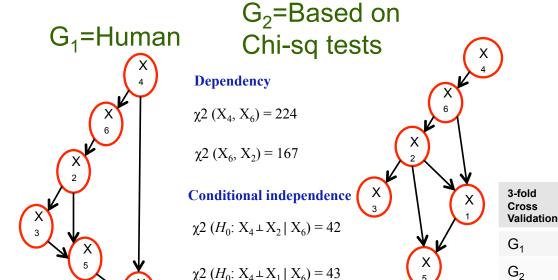
Search through space of BNs

Score function for each BN

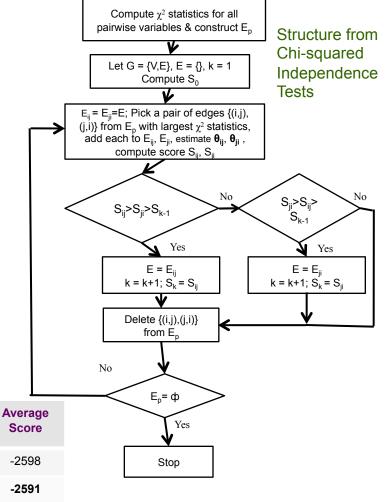
- Score_L (G : D) = log-likelihood (θ_G : D)

• θ_G are parameters of G

X ₁	X_2	X_3	X_4	X_5	X_6
Height Relation	Shape of loop of 'h'	Shape of arch of 'h'	Height of 't' cross	Baseline of 'h'	Shape of 't'



 $\chi^{2}(D) = \sum_{i,j} \frac{\text{(Observed count of } [x_{i}, y_{j}] - \text{Expected count of } [x_{i}, y_{j}])^{2}}{\text{Expected count of } [x_{i}, y_{j}]}$



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Structure Learning of MNs

Information-theoretic Chow-Liu algorithm

Algorithm for structure learning:

1. Estimate empirical probability:

$$P(X_1 = N) = \frac{\sum_{D} 1[X_1 = N]}{\sum_{D} 1}$$

2. Calculate all marginal entropies:

$$H(X_1) = -\sum_{X_1} P(X_1) \log(P(X_1))$$

and all pair-joint entropies:

$$H(X_1, X_2) = -\sum_{X_1, X_2} P(X_1, X_2) \log(P(X_1, X_2))$$

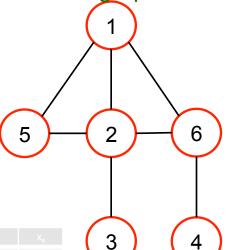
3. Calculate mutual information:

$$I(X_1, X_2) = H(X_1) + H(X_2) - H(X_1, X_2)$$

4. Include edges (X_i, X_j) in to the structure if $I(X_1, X_2) \ge threshold$

0	0.20	0.05	0.10	0.00	0.29	0.17
1	0.16	0.00	0.62	0.36	0.24	0.04
2	0.37	0.12	0.28	0.30	0.30	0.07
3	0.27	0.08		0.34	0.17	0.71
4		0.75				0.00

$I(X1,X2) \ge$	threshold
Gives gra	ph



	X_1	1.34	2.14	2.20	2.41	2.65	2.17
	X_2	2.14	0.84	1.69	1.92	2.16	1.66
1	X_3	2.20	1.69	0.89	1.99	2.23	1.74
	X_4	2.42	1.92	1.99	1.10	2.44	1.89
١	X_5	2.66	2.16	2.23	2.44	1.36	2.21
,	X_6	2.17	1.66	1.75	1.89	2.20	0.87

X ₁	1.33	0.03	0.02	0.02	0.03	0.04
X_2	0.03	0.83	0.03	0.01	0.03	0.05
X_3	0.02	0.03	0.89	0.01	0.02	0.02
X_4	0.02	0.01	0.01	1.10	0.02	0.09
X_5	0.03	0.03	0.02	0.02	1.36	0.03
X_6	0.04	0.05	0.02	0.08	0.03	0.87

Rare and Common Style Inferences from PGMs

Rare Styles: Looped or tented 't', loop of 'h' with both sides curved

Doc: 199a Score : -12 Doc: 409c Score : -12

Doc: 124c Score : -11 Doc: 1434b Score : -11

Common Styles: Single stroke 't', retraced 'h', pointed arch of 'h', baseline of 'h' slanting down, 't' taller, cross of 't' below

Doc: 40b

Score: -4

Doc: 130b

Score: -4

Doc: 1007c

Score: -4

Doc: 685a Score : -4

Summary and Conclusion

- Machine Learning
 - Several generations, with beginnings in DAR field
 - Necessary for changing high volume data
 - To classify, regress, infer, collectively label
- PGMs able to handle complexity
 - BN and MN are expressive
 - Allow incorporating domain knowledge
 - Provide relationships between models
- Computational Forensics Application
 - Handwriting rarity is inferred from PGMs