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) $_3$

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

- First Generation (1960-1980)
	- Perceptrons, Nearest-neighbor, Naïve Bayes
	- Special Hardware, Limited performance
- Second Generation (1980-2000)
	- ANNs, Kalman, HMMs, SVMs
		- 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

USPS-MLOCR

 $Amhex$ USPS-RCR

20 x 20 cell Adaptive Wts

Classification: OCR

Input $x = \{x_1, \ldots, x_{12}\}$: Image Features Output (*y*): Class Labels {*y0, y1,.y9*}

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

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

Features (x_i) :

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

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

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

\n
$$
|Val(x_i)| = 10
$$

\n...

No of parameters*=1012- 1 Or 1 trillion* Per class No of samples needed=??

Regression: Learning To Rank

– Log frequency of query in

(*d* Features of Query-URL pair)

– # of images on page

PageRank of page

URL contains " \sim "

Page length

Regression returns continuous value

-Allows fine-grained ranking of URLs

– URL length

- Point-wise (0,1,2,3)

Input (x_i) :

of (out) links on page

– Query word in color on page

Traditional IR uses TF/IDF

anchor text

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

Discriminative vs Generative Training

Independent variables $x = \{x_1, x_1, x_2\}$ and binary target *y*

1. Generative: estimate CPD parameters

2. Discriminative: estimate CRF parameters w_i

 x_1 x_2 x_{12} *y* Jointly optimize *12* parameters High dimensional estimation but correlations accounted for Can use much richer features: Edges, image patches sharing same pixels **Naïve Markov** $p(y_i | \phi) = y_i(\phi) = \frac{\exp(a_i)}{\sum_{i} y_i}$ $\sum_j \exp(a_j)$ where $a_j = w_j^T \phi$ Potential Functions (log-linear) $\phi_i(x_i, y) = \exp\{w_i x_i \cdot I\{y = I\}\},\$ $\phi_0(y) = \exp\{w_0 I\{y=1\}\}\$ $\tilde{P}(y=1|x) = \exp\left\{w_0 + \sum w_i x_i\right\}$ *i*=1 $\big\{w_0 + \sum^{12}$ $\overline{\mathsf{L}}$ \overline{a} $\left\{ \right\}$ ⎭ $\tilde{P}(y=0 | x) = \exp\{0\} = 1$ $P(y=1 | x) = sigmoid\left\{\mathbf{w}_0 + \sum_{i} \mathbf{w}_i x_i\right\}$ *i*=1 $\big\{w_0 + \sum^{12}$ \overline{a} \overline{a} $\left\{ \right.$ ⎭ where $sigmoid(z) = \frac{e^{z}}{1+z}$ $1+ e^z$ Unnormalized Normalized I has value *1* when $y=1$, else 0 multiclass Logistic Regression

Collective Labeling: Three Models

Both CRF and MEMM are Discriminative Models Directly obtain *P(Y|X)* HMM is generative Needs *P(X,Y)* Sequence of observations *X={X1,..Xk}* Need a joint label $Y=\{Y_1,..Y_k\}$

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

i=1

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

: 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

$$
r \equiv P(S_i = 1 | E_i = 1)
$$

= $P(S_i = 1, E_i = 1) / P(E_i = 1)$
= $P(S_i = 1, E_i = 1, C_i = 0) / P(E_i = 1) + P(S_i = 1, E_i = 1, C_i = 1) / P(E_i = 1)$
= $0 + P(S_i = 1, C_i = 1 | E_i = 1)$ [satisfaction only upon click]
= $P(S_i = 1 | C_i = 1) P(C_i = 1 | E_i = 1)$

Probabilistic Model for Handwriting Style

 $\ell\mathcal{U}$

 H $H\!u$

|*Val(X)|=4* x *5* x *3* x *4* x *4* x *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

BN for "and"

Nine variables No of parameters needed= 809,999

tern

 $ds^5 = \text{no}$

fixed pat-

tern

tern

tern

down

tern

 $as^5 = \text{no}$

fixed pat-

tern

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
=
$$
\sum_{A,T,B,R} P(L)P(A)P(T)P(B|A,L)P(C|T)P(R|B,C)
$$
 From the Graphical Model

Probability of Evidence

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

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

Learning

Learning Problems with PGMs

• Parameter Learning (given structure)

- Structure Learning
	- Search through network space
- Partial Data

Parameter Learning For BN

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

Bayesian Estimate

Bayesian Estimation

Prior

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

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

 $\boldsymbol{\theta} | O \sim \text{Dirichlet}(\alpha'_1, ..., \alpha'_k)$ Posterior

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

25

Parameter Learning for MN

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

 $\ell(\theta) = \sum_{i=1}^k \theta_i \left(\sum_m f_i(\xi[m]) \right)$ $\sum_{i=1}^k \theta_i \bigg(\sum_m f_i(\xi[m]) \bigg)$ $\sum_{i=1}^{k} \theta_i \left(\sum_m f_i(\xi[m]) \right) - M \ln \sum_{\xi} \exp \left(\sum_{i=1}^{k} \theta_i f_i(\xi) \right)$ $\sum_{\xi} \exp \biggl(\sum_{i=1}^k \theta_i f_i(\xi) \biggr)$ Log-likelihood of *M* i.i.d. samples

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

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

Compute γ^2 statistics for all pairwise variables & construct E_p

Structure from Chi-squared Independence

Let $G = \{V, E\}$, $E = \{P\}$, $k = 1$ Compute S_0

- 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)
		- \cdot $\theta_{\rm G}$ are parameters of G

Structure Learning of MNs

Information-theoretic Chow-Liu algorithm

Algorithm for structure learning:

- Estimate empirical probability: 1. $P(X_1 = N) = \frac{\sum_D 1[X_1 = N]}{\sum_D 1}$
- 2. Calculate all marginal entropies:

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

and all pair-joint entropies:

$$
H(X_1, X_2) = -\sum_{X_1, X_2} P(X_1, X_2) \log(P(X_1, X_2)) \bigg|_{\frac{1}{2}}
$$

- $\overline{3}$. Calculate mutual information: $I(X_1, X_2) = H(X_1) + H(X_2) - H(X_1, X_2)$
- Include edges (X_i, X_j) in to the structure 4. if $I(X_1, X_2) \geq threshold$

 $I(XI, X2) \geq$ threshold

Gives graph

Rare and Common Style Inferences from PGMs

Doc: 199a Score : -12 Doc: 409c Score : -12 Doc: 124c Score : -11 Doc: 1434b Score \cdot -11 Doc: $40h$ Score : -4 Doc: 130b Score : -4 Doc: 1007c Score : -4 Doc: 685a Score : -4 Rare Styles : Looped or tented 't', loop of 'h' with both sides curved Common Styles: Single stroke 't', retraced 'h', pointed arch of 'h', baseline of 'h' slanting down, 't' taller, cross of 't' below

All scores in log-likelihood

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