Learning Graphical Models for Hypothesis Testing

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Introduction

- **Motivation**: Can sparse graphical models be learnt better if intended purpose is known?
- **Contribution**: Given training data from 2 distributions, we learn models to be used **specifically** for hypothesis testing.

The Problem

The Hypothesis Testing Problem

$X = (X_1, \dots X_n)$ is a length-n vector of finite-valued random variables, generated from one of two hypotheses

$$H_0 : X \sim p \quad \text{or} \quad H_1 : X \sim q \tag{1}$$

p, q are not available *a priori*.

Given: Labeled training sets $\mathcal{T}_0, \mathcal{T}_1$, consisting of K samples each that are generated IID according to p, q respectively.

Task: Given a new test sample x, decide between H_0 and H_1.

Natural Solutions

1. Generate empiricals p_e from $\mathcal{T}_0$ and q_e from $\mathcal{T}_1$ and do a Likelihood Ratio Test (LRT) using p_e, q_e.

   Problem: When n is large, the number of possible sample vectors is large. For e.g. if each X_i is binary, this number is 2^n. Unless K is of the order 2^n, p_e, q_e will be poor approximations of p, q, and be inefficient at classification.

2. Learn sparse models $\widehat{p}$ from $\mathcal{T}_0$ and $\widehat{q}$ from $\mathcal{T}_1$. Then do a LRT.

   Problem: Each model uses information about only of the two hypotheses.

Our Approach

We learn $\widehat{p}, \widehat{q}$ each using **both** $\mathcal{T}_0$ and $\mathcal{T}_1$ and then do a LRT.

$$\widehat{p}(x) \underset{\text{declare } H_1}{\overset{\text{declare } H_0}{\gtrless}} \widehat{q}(x) \tag{2}$$

Learning Graphical Models Specifically for Hypothesis Testing

Ideally, we would like to learn $\widehat{p}, \widehat{q}$ to minimize $\Pr(err)$, given by

$$P(e_0) = P(\text{declare } H_1 | H_0) = \sum_x p(x)\, \mathbf{1}_{\{\widehat{q}(x) \geq \widehat{p}(x)\}} \tag{3}$$

and $P(e_0)$. But we do not know p, q so instead we minimize

$$P(\tilde{e}_0) = \sum_x p_e(x)\, \mathbf{1}_{\{\widehat{q}(x) \geq \widehat{p}(x)\}} \tag{4}$$

and $P(\tilde{e}_1)$. $P(\tilde{e}_0)$ counts the fraction of samples in $\mathcal{T}_0$ that are misclassified. Learning $\widehat{p}, \widehat{q}$ involves

1. Learning the **graph structure** of models $\widehat{p}, \widehat{q}$.
2. Learning the **parameters** of the models.

Learning Graph Structure

We first concentrate on learning the graph structures G_0, G_1 of the models $\widehat{p}, \widehat{q}$. The **projection** p_{G_0} of p onto G_0 is the closest distribution (in KL-divergence) to p that is Markov on G_0.

$$D(p \,||\, p_{G_0}) \leq D(p \,||\, p') \tag{5}$$

for all p' that is Markov on G_0. For structure learning, for any given G_0 assume that $\widehat{p}$ is projection of p_e onto G_0.

For low $P(\tilde{e}_0)$ and $P(\tilde{e}_1)$, we would like $\log\left(\widehat{p}(x)/\widehat{q}(x)\right) > 0$ if $p_e(x) > q_e(x)$ and < 0 otherwise. Thus, **choose G_0 and G_1 to maximize**

$$\sum_x (p_e(x) - q_e(x)) \log\left(\frac{\widehat{p}(x)}{\widehat{q}(x)}\right) \tag{6}$$

This decomposes into two independent objectives with the first maximization problem being:

$$\max_{G_0} \left\{ \sum_x (p_e(x) - q_e(x)) \log \widehat{p}(x) \right\} \equiv \min_{G_0} \left\{ D(p_e||p_{G_0}) - D(q_e||p_{G_0}) \right\}. \tag{7}$$

This is similar to $\min_{G_0} D(p||p_{G_0})$ in the classical objective. So **any** classical learning method may be adapted to this objective. In this work, $\widehat{p}$ and $\widehat{q}$ are **Markov on trees**. Objective (7) becomes a **Max-Weight Spanning Tree** (MWST) problem with edge weights

$$w_{ij} = \sum_{(x_i, x_j)} (p_e(x_i, x_j) - q_e(x_i, x_j)) \log\left(\frac{p_e(x_i, x_j)}{p_e(x_i) p_e(x_j)}\right). \tag{8}$$

The space and time **complexity** of the tree-finding procedure is the **same** as the Chow-Liu procedure [1].

Learning Model Parameters

LRT can be done with $\widehat{p}, \widehat{q}$ being the projections of the p_e, q_e onto G_0, G_1. However, further reductions of $P(\tilde{e}_0)$ and $P(\tilde{e}_1)$ are possible by optimizing the **parameters** of $\widehat{p}$ and $\widehat{q}$ so that they remain Markov on the same graphs G_0, G_1. For this, we upper bound

$$P(\tilde{e}_0) \leq \min_{\lambda \geq 0} \sum_x p_e(x) \left(\frac{\widehat{q}(x)}{\widehat{p}(x)}\right)^{\lambda}. \tag{9}$$

Consider $\widehat{p}$ and $\widehat{q}$ to be members of **exponential families**:

$$\widehat{p}(x\,;\, \theta_{\widehat{p}}) = \exp\left[\langle \theta_{\widehat{p}}, \phi_p(x) \rangle - \Phi(\theta_{\widehat{p}})\right], \tag{10}$$

where $\phi_p(x), \phi_q(x)$ are the (fixed) features of G_0, G_1 and determine the family. $\theta_{\widehat{p}}, \theta_{\widehat{q}}$ are the **exponential parameters** to which we optimize using **convex programming**. $\Phi(\cdot)$ is the log-partition function.

Lemma 1 *Let* $A_0(\theta_{\widehat{p}}, \theta_{\widehat{q}}, \lambda) \stackrel{\triangle}{=} \sum_x p_e(x) \left(\frac{\widehat{q}(x)}{\widehat{p}(x)}\right)^{\lambda}$, *then*

1. *A_0 is convex in $\theta_{\widehat{p}}$ for fixed $(\theta_{\widehat{q}}, \lambda)$.*
2. *A_0 is convex in λ for fixed $(\theta_{\widehat{p}}, \theta_{\widehat{q}})$.*

We use an alternating minimizing procedure parameterized by a discrete set of λ's (from 0 to 1) to find the optimal $\theta^*_{\widehat{p}}, \theta^*_{\widehat{q}}$.

For each value of λ, $\theta_{\widehat{p}}, \theta_{\widehat{q}}$ are initialized by transforming the mean parameters of p_e, q_e to exponential parameters. Finally, $\theta^*_{\widehat{p}}, \theta^*_{\widehat{q}}$ are chosen as the pair that **minimize the sum**:

$$A(\theta_{\widehat{p}}, \theta_{\widehat{q}}, \lambda) = A_0(\theta_{\widehat{p}}, \theta_{\widehat{q}}, \lambda) + A_1(\theta_{\widehat{p}}, \theta_{\widehat{q}}, 1 - \lambda). \tag{11}$$

Alternating-Minimization Algorithm

for $\lambda \leftarrow 0$ to 1 **do**
  Evaluate $\theta^{(\lambda)}_{\widehat{p}}, \theta^{(\lambda)}_{\widehat{q}}$ as follows ;
  repeat
    $\theta_{\widehat{p}} = \text{argmin}_{\theta_{\widehat{p}}}\ A_0\left(\theta_{\widehat{p}}, \theta_{\widehat{q}}, \lambda\right)$;
    $\theta_{\widehat{q}} = \text{argmin}_{\theta_{\widehat{q}}}\ A_1\left(\theta_{\widehat{p}}, \theta_{\widehat{q}}, 1 - \lambda\right)$;
  until convergence;
endFor
$\lambda_{\min} = \text{argmin}_{\lambda} \left[A_0\left(\theta^{(\lambda)}_{\widehat{p}}, \theta^{(\lambda)}_{\widehat{q}}, \lambda\right) + A_1\left(\theta^{(\lambda)}_{\widehat{p}}, \theta^{(\lambda)}_{\widehat{q}}, 1 - \lambda\right)\right]$;
$\theta^*_{\widehat{p}} = \theta^{(\lambda_{\min})}_{\widehat{p}}$;
$\theta^*_{\widehat{q}} = \theta^{(\lambda_{\min})}_{\widehat{q}}$;

Connection to Error Exponents

The parameter learning procedure above is related to the **error exponent** [2] of the hypothesis test. Suppose we are given M new samples. Let e_0^M be the (conditional) error event that H_1 is declared when the truth was H_0. The error exponent is:

$$E_0(\widehat{p}, \widehat{q}) = \lim_{M \to \infty} -\frac{1}{M} P(e_0^M). \tag{12}$$

Lemma 2 $E_0(\widehat{p}, \widehat{q}) = \max_{\lambda \geq 0} -\log\left[\sum_x p(x) \left(\frac{\widehat{q}(x)}{\widehat{p}(x)}\right)^{\lambda}\right]$.

Note the close similarity between the above expression and that of A_0 in Lemma 1. If we replace p with p_e, then the right hand side is exactly $-\log A_0(\theta_{\widehat{p}}, \theta_{\widehat{q}}, \lambda)$. Thus **minimizing** A_0 is equivalent to **maximizing** (an empirical version of) the error exponent.

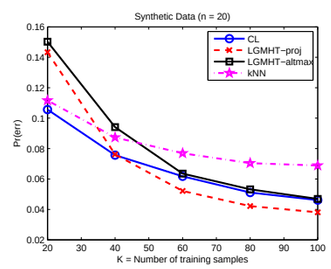
Numerical results

We perform simulations on synthetic examples and on a handwritten digit dataset. Each figure shows 4 curves.

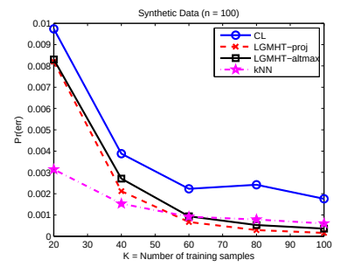
1. **CL**: Learning models according to the Chow-Liu [1] algorithm. ($\widehat{p}$ is learnt only from $\mathcal{T}_0$ and $\widehat{q}$ only from $\mathcal{T}_1$.)
2. **LGMHT-proj**: $\widehat{p}, \widehat{q}$ are simply the projections of p_e, q_e onto G_0, G_1 respectively.
3. **LGMHT-altmax**: $\theta_{\widehat{p}}, \theta_{\widehat{q}}$ are further optimized.
4. **kNN**: Using k-Nearest Neighbours with $k = 11$.

Synthetic examples

X is a **binary** vector of length n. The true distributions p and q are randomly chosen **tree-structured distributions**. Tree structures enable easy generation of training samples $\mathcal{T}_0, \mathcal{T}_1$.

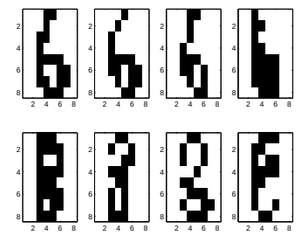


The $\Pr(err)$ is plotted as a function of K for a $n = 20$ node synthetic example.

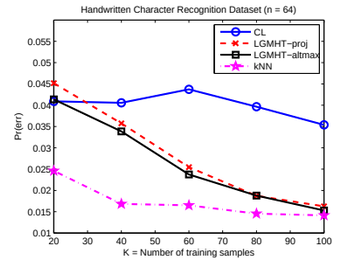


The $\Pr(err)$ is plotted as a function of K for a $n = 100$ node synthetic example.

Handwritten Digits dataset



We used the MNIST handwritten digit dataset and classified the feature vectors corresponding to class labels 6 and 8. The pixel values are quantized to binary levels.



The 8×8 **images** are concatenated into length $n = 64$ vectors the $\Pr(err)$ is plotted as a function of K.

Conclusion

- In general, learning the reduced-order distributions $\widehat{p}, \widehat{q}$ from both datasets $\mathcal{T}_0, \mathcal{T}_1$ (instead of learning $\widehat{p}$ from $\mathcal{T}_0$ only as in CL) results in **lower** $\Pr(err)$, especially on the handwritten digits dataset.
- The parameter optimization procedure gives lower $\Pr(err)$ for the handwritten digits dataset but seems to be overfitting the synthetic datasets.
- In general, kNN performs better than CL and LGMHT but kNN requires distances to be calculated for **each** new test sample. LGMHT computes both distributions $\widehat{p}, \widehat{q}$ offline.
- **Future work**: Examine how the idea of learning graphical models from both datasets can be applied to dimensionality reduction together with classification/clustering.

References

[1] C. K. Chow and C. N. Liu. Approximating discrete probability distributions with dependence trees. *IEEE Transactions on Information Theory*, 14(3):462–7, May 1968.

[2] T. M. Cover and J. A. Thomas. *Elements of Information Theory*. Wiley-Interscience, 2nd edition, 2006.