The Chow-Liu Algorithm

C. K. Chow and C. N. Liu. Approximating discrete probability distributions with dependence trees. IEEE Transactions of Information Theory, IT-14(3), 1968.

The Goal

Given a finite set of samples in a dataset, estimate the underlying n-dimensional discrete probability distribution using a tree model.

Trees

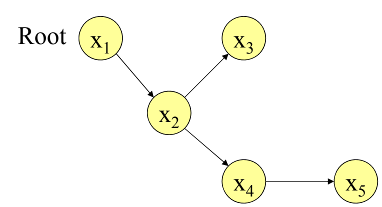
What is a tree?

- The variables in the dataset are the vertices V
- There are edges in the set E that connect the vertices
- We'll assume the edges are undirected for now
- A graph (V,E) is a tree if it is connected and has no cycles

Technical point: We will allow our trees to be a forest ie. the tree model we learn may be disconnected

Trees

- In a directed tree, we pick a vertex as the root
- We then turn the edges into directed edges and orient the edges away from the root
- This means that each vertex has at most one parent (but may have more than one child)



Tree Models

Notation:

- $\boldsymbol{x}$ (as in bold x) is an n-dimensional vector ie. $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$
- Each x_i in $\boldsymbol{x}$ is a variable
- $P(\boldsymbol{x})$ is a joint probability distribution of n discrete variables $x_1, x_2, \ldots, x_n$

5

Tree Models

- We want to approximate the true joint probability distribution using tree models of the form:

$$P_t(x) = \prod_{i=1}^{n} P(x_i | x_{\pi(i)})$$

- $\pi(i)$ means "parent of variable i"
- If i is the root then $\pi(i)$ is the empty set: $P(x_i | x_{\pi(i)}) = P(x_i)$

6

Tree Models

$$P_t(x) = \prod_{i=1}^{n} \underbrace{P(x_i | x_{\pi(i)})}$$

- Tree models consider the pairwise relationships between variables in the dataset
- It is an improvement over just treating the variables independently of each other

7

Closeness of approximation

- Let P($\mathbf{x}$) and $P_t(\boldsymbol{x})$ be two probability distributions of n discrete variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$.
- Let

$$KL(P, P_t) = \sum_{\boldsymbol{x}} P(\boldsymbol{x}) log \frac{P(\boldsymbol{x})}{P_t(\boldsymbol{x})}$$

Note: This summation is over all configurations of $(x_1, x_2, \ldots, x_n)$

The formula for $KL(P, P_t)$ is called the Kullback-Leibler divergence (or KL divergence for short)

8

Kullback-Leibler Divergence

- We'll rewrite the KL divergence as:

$$KL(P,P_t) = \sum_{\boldsymbol{x}} P(\boldsymbol{x}) \log P(\boldsymbol{x}) - \sum_{\boldsymbol{x}} P(\boldsymbol{x}) log P_t(\boldsymbol{x})$$

- The first term doesn't depend on P_t.
- The second term is known as the cross-entropy between P and P_t.
- Properties of KL divergence:
  - $KL(P,P_t) \geq 0$
  - $KL(P,P_t) = 0$ if and only if $P(\boldsymbol{x}) \equiv P_t(\boldsymbol{x})$ for all $\boldsymbol{x}$

9

A Minimization Problem

Given:

- An nth-order probability distribution $P(x_1, x_2, \ldots, x_n)$ with x_i being discrete
- T_n- The set of all possible first-order dependence trees

Find the optimal first-order dependence tree τ such that $\mathrm{KL}(P, P_\tau) \leq KL(P, P_t)$ for all $t \epsilon T_n$.

10

Exhaustive Search

- Why not just search over all possible trees?
- Not feasible -- there are $n^{(n-2)}$ possible trees with n vertices (from Cayley's formula)
- We will turn the search into a maximum weight spanning tree (MWST) problem

11

Mutual Information

- Define the mutual information $I(x_i, x_j)$ between two variables x_i and x_j to be:

$$I(x_i, x_j) = \sum_{x_i, x_j} P(x_i, x_j) log\left(\frac{P(x_i, x_j)}{P(x_i)P(x_j)}\right)$$

- Key insight: a probability distribution of tree dependence $P_t(\boldsymbol{x})$ is an optimum approximation to $P(\boldsymbol{x})$ iff its tree model has maximum weight
- Proof to follow

12

Proof

$$KL(P,P_t) = \sum_{\boldsymbol{x}} P(\boldsymbol{x}) log P(\boldsymbol{x}) - \sum_{\boldsymbol{x}} P(\boldsymbol{x}) \sum_{i=1}^{n} log P\big(x_i | x_{\pi(i)}\big)$$

$$= \sum_{\boldsymbol{x}} P(\boldsymbol{x}) log P(\boldsymbol{x}) - \sum_{\boldsymbol{x}} P(\boldsymbol{x}) \sum_{i=1,\neq root}^{n} log \frac{P\big(x_i, x_{\pi(i)}\big)}{P\big(x_{\pi(i)}\big)}$$

$$= \sum_{\boldsymbol{x}} P(\boldsymbol{x}) log P(\boldsymbol{x}) - \sum_{\boldsymbol{x}} P(\boldsymbol{x}) \sum_{i=1,\neq root}^{n} log \frac{P\big(x_i, x_{\pi(i)}\big)}{P(x_i) P\big(x_{\pi(i)}\big)}$$

$$- \sum_{\boldsymbol{x}} P(\boldsymbol{x}) \sum_{i=1}^{n} log P(x_i)$$

Proof (continued)

Note that: $-\sum_{\boldsymbol{x}} P(\boldsymbol{x}) \log P(x_i) = -\sum_{x_i} P(x_i) log P(x_i)$

To see this, suppose $\boldsymbol{x} = (x_1, x_2)$, let all variables are binary, let *i=1*

$$-\sum_{\boldsymbol{x}} P(\boldsymbol{x}) \log P(x_i)$$

$$= -[P(x_1 = 0, x_2 = 0) \log P(x_1 = 0) + P(x_1 = 0, x_2 = 1) \log P(x_1 = 0) +$$
$$P(x_1 = 1, x_2 = 0) \log P(x_1 = 1) + P(x_1 = 1, x_2 = 1) \log P(x_1 = 1)]$$

$$= -[P(x_1 = 0) \log P(x_1 = 0) + P(x_1 = 1) \log P(x_1 = 1)]$$

$$= -\sum_{x_1} P(x_1) \log P(x_1) = -\sum_{x_i} P(x_i) \log P(x_i)$$

Proof (continued)

In the same way:

$$\sum_{x} P(x) log \frac{P\big(x_i, x_{\pi(i)}\big)}{P(x_i) P\big(x_{\pi(i)}\big)}$$

$$= \sum_{x_i, x_{\pi(i)}} P\big(x_i, x_{\pi(i)}\big) log \frac{P\big(x_i, x_{\pi(i)}\big)}{P(x_i) P\big(x_{\pi(i)}\big)} = I\big(x_i, x_{\pi(i)}\big)$$

Proof (continued)

One more piece of notation:

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

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

Substituting the expressions above and from pg 12 into the last line of pg 13:

$$KL(P,P_t) = -\sum_{i=1}^{n} I\big(x_i, x_{\pi(i)}\big) + \sum_{i=1}^{n} H(x_i) - H(\boldsymbol{x})$$

Proof

$$KL(P, P_t) = -\sum_{i=1}^{n} I(x_i, x_{\pi(i)}) + \sum_{i=1}^{n} H(x_i) - H(\boldsymbol{x})$$

Mutual information is always ≥ 0

Independent of the dependence tree

Minimizing $I(P, P_t)$ is the same as maximizing the total branch weight:

$$\sum_{i=1}^{n} I(x_i, x_{\pi(i)})$$

17

The algorithm

- First calculate all n(n-1)/2 pairwise mutual information measures
- Use Kruskal's algorithm to construct maximum weight spanning tree:
  - Construct tree one edge at a time, in decreasing order of the weights
  - If all weights are > 0, you get one connected component
  - Running time is $O(n^2)$ for n variables because you have to consider all n(n-1)/2 edges

18

Estimation

- But in order to calculate mutual information $I(x_i, x_j)$, you need the probability distribution $P(\boldsymbol{x})$
- Need to estimate the mutual information from a finite set of samples using maximum likelihood estimation

19

Estimation

Suppose you are given s independent samples $\boldsymbol{x}^1, \boldsymbol{x}^2, \ldots, \boldsymbol{x}^s$ of a discrete variable $\boldsymbol{x}$. Each sample is an n-component vector ie. $\mathbf{x}^k = (x^k_1, x^k_2, \ldots, x^k_n)$.

Define:

$$n_{uv}(i, j) = \#\text{ of samples with } x_i = u \text{ and } x_j = v$$

$$f_{uv}(i, j) = \frac{n_{uv}(i, j)}{\sum_{u,v} n_{uv}(i, j)}$$

Maximum Likelihood Estimator for $P(x_i = u, x_j = v)$

$$f_u(i) = \sum_{v} f_{uv}(i, j)$$

Maximum Likelihood Estimator for $P(x_i = u)$

20

Estimation

Calculate:

$$\hat{I}(x_i, x_j) = \sum_{u,v} f_{uv}(i,j) \log \frac{f_{uv}(i,j)}{f_u(i) f_v(j)}$$

Use $\hat{I}(x_i, x_j)$ in Kruskal's algorithm instead of $I(x_i, x_j)$

21

The entire algorithm

1. Compute marginal counts $f_u(i)$ and pairwise counts $f_{uv}(i,j)$
2. Compute mutual information $\hat{I}(x_i, x_j)$ for all pairs x_i and x_j
3. Compute MWST using Kruskal's algorithm. Pick a root, orient edges away from the root.
4. Set the parameters in the CPTs for each node to be their maximum likelihood estimates:

$$P(x_i \mid x_{\pi(i)}) = \frac{f_{uv}(i, \pi(j))}{f_u(i)}$$

22

The entire algorithm

1. Compute marginal counts $f_u(i)$ and pairwise counts $f_{uv}(i,j)$
2. Compute mutual information $\hat{I}(x_i, x_j)$ for all pairs x_i and x_j
3. Compute MWST using Kruskal's algorithm. Pick a root, orient edges away from the root.

Steps 1-3 dominate the complexity – they all take $O(n^2)$ time

23

References

- Chow, C. K. and Liu, C. N. "Approximating Discrete Probability Distributions with Dependence Trees".
- Meila-Predoviciu, M. Learning with Mixtures of Trees, PhD Thesis, MIT, 1999.

24