Information theory and coding

Graphical models

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May 2, 2019

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Outline of this lecture

On the qualitative vs. quantitative notion of Independence
- Motivation
- Characterization of independence relations

Graphical models of independence relations
- Motivation
- Undirected graphical models: Markov networks
- Directed graphical models: Bayesian networks

Discussion and further topics
- Relations between UGs and DAGs

Tree structured graphical models

- Objective: Introduce and motivate graphical representation of qualitative and quantitative probabilistic knowledge
    - Qualitative notion of dependence
    - Characterization of desired properties of independence relations
    - Probability calculus as a model of Independence relations
- Two graphical representations of Independence relations
    - Undirected graphs: Markov networks
    - Directed graphs: Bayesian networks
    - Relations between these two types of representations
    - Quantitative aspects/questions
- In depth analysis of tree-structured graphical models
    - Undirected trees and the Chow-Liu algorithm
    - Directed trees and polytrees

***NB**: Extended/original set of slides at* http://www.montefiore.ulg.ac.be/~lwh/Info/chapter3.pdf.

Why do we need a qualitative notion of dependence?

- Making statements about independence (or relevance) is a profound feature of common-sense reasoning, while probability calculus gives a formalization and a safe procedure for testing any (conditional) Independence statements.
- However, this procedure relies on the computation of the probabilities of all combinations of statements, and is essentially intractable in large domains.
- In short, the probability calculus procedure is in itself not an operational model of reasoning about Independence relations, specially hen we don't (yet) have the number.
- We would like to dispose of a kind of 'logic' of Independence, in which we can derive easily new Independence statements from previously established or postulated ones, without resorting to number crunching.

Desired properties of independence relations

Consider a domain characterised by a finite set $\mathbb{U}$ of discrete variables, and let $\mathbb{A}, \mathbb{B}, \mathbb{C}$ denote three disjoint **subsets** of $\mathbb{U}$.

Let us denote by $\mathbb{A} \perp \mathbb{B} | \mathbb{C}$ the statement that

"$\mathbb{A}$ is independent of $\mathbb{B}$, given that we know $\mathbb{C}$",

i.e. when we already know the values of the variables in $\mathbb{C}$, we consider that the knowledge of the values of the variables in $\mathbb{B}$ is irrelevant to our beliefs about the values in $\mathbb{A}$.

We want to derive rules which are characteristics of independence relations, and which allows us to infer in a sound way new independence relations from established ones.
We will first propose a set of four rules and then verify that they are valid inference rules for probabilistic independence relations.

Semi-graphoids (1)

Desired properties of an independence relation:

(1) Symmetry:

$$(\mathbb{X} \perp \mathbb{Y} | \mathbb{Z}) \Leftrightarrow (\mathbb{Y} \perp \mathbb{X} | \mathbb{Z})$$

If $\mathbb{Y}$ tells us nothing about $\mathbb{X}$ (in some context $\mathbb{Z}$), then $\mathbb{X}$ tells us nothing about $\mathbb{Y}$.

(2) Decomposition:

$$(\mathbb{X} \perp (\mathbb{Y} \cup \mathbb{W}) | \mathbb{Z}) \Rightarrow (\mathbb{X} \perp \mathbb{Y} | \mathbb{Z}) \& (\mathbb{X} \perp \mathbb{W} | \mathbb{Z})$$

If two combined items of information $(\mathbb{Y} \cup \mathbb{W})$ are judged irrelevant to $\mathbb{X}$, then each separate item ($\mathbb{Y}$ or $\mathbb{W}$) is irrelevant as well.

Semi-graphoids (2)

(3) Weak union:

$$(\mathbb{X} \perp (\mathbb{Y} \cup \mathbb{W})|\mathbb{Z}) \Rightarrow (\mathbb{X} \perp \mathbb{Y}|(\mathbb{Z} \cup \mathbb{W}))$$

Learning some irrelevant information $\mathbb{W}$ cannot help the other irrelevant information $\mathbb{Y}$ become relevant.

***NB**: "strong" union will be defined later.*

(4) Contraction:

$$(\mathbb{X} \perp \mathbb{Y}|\mathbb{Z}) \& (\mathbb{X} \perp \mathbb{W}|(\mathbb{Z} \cup \mathbb{Y})) \Rightarrow (\mathbb{X} \perp (\mathbb{Y} \cup \mathbb{W})|\mathbb{Z})$$

If we judge $\mathbb{W}$ irrelevant to $\mathbb{X}$ after learning some irrelevant information $\mathbb{Y}$, then $\mathbb{W}$ must also have been irrelevant before we learned $\mathbb{Y}$.

Properties of probabilistic independence relation

Notation: If P is a probability distribution defined over the variables in $\mathbb{U}$, we write:

$$(\mathbb{A} \perp_P \mathbb{B} | \mathbb{C}) \Leftrightarrow (\forall a, b, c : P(b, c) > 0 \Rightarrow P(a|b, c) = P(a|c))$$

Theorem (Probabilistic independence)

The probabilistic independence relationship $(\cdot \perp_P \cdot | \cdot)$ induced by any probabilistic model P satisfies the four properties: symmetry (1), decomposition (2), weak union (3) and contraction (4).

Theorem (Intersection property (5))

The probabilistic independence relationship induced by any ***strictly positive*** *probabilistic model P also satisfies*

$$(\mathbb{X} \perp_P \mathbb{Y} | (\mathbb{Z} \cup \mathbb{W}) \& (\mathbb{X} \perp_P \mathbb{W} | (\mathbb{Z} \cup \mathbb{Y})) \Rightarrow (\mathbb{X} \perp_P (\mathbb{Y} \cup \mathbb{W}) | \mathbb{Z})$$

Induced inference rules

- Chaining rule:
$$(\mathbb{X} \perp \mathbb{Z} | \mathbb{Y}) \& ((\mathbb{X} \cup \mathbb{Y}) \perp \mathbb{W} | \mathbb{Z}) \Rightarrow \mathbb{X} \perp \mathbb{W} | \mathbb{Y}$$

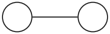
- Mixing rule:
$$(\mathbb{X} \perp (\mathbb{Y} \cup \mathbb{W}) | \mathbb{Z}) \& (\mathbb{Y} \perp \mathbb{W} | \mathbb{Z}) \Rightarrow (\mathbb{X} \cup \mathbb{W}) \perp \mathbb{Y} | \mathbb{Z}$$

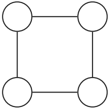
Exercise*: Show that these two rules follow logically from (1) to (4), and hence are valid inference rules for any probabilistic independence relation.*

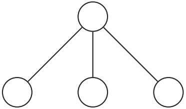
Summary

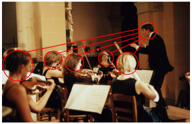
- We have abstracted from the quantitative notion of conditional independence defined by probability theory.
- This abstraction is necessary for efficient manipulation of the notion of independence/irrelevance.
- We have shown, to some extent, that one can axiomatize the notion of independence in a way which remains logically coherent with the same notion defined by probability calculus.
- We have illustrated that such an axiomatization is useful to derive new independencies from postulated ones, and even new inference rules from postulated ones.
- However, we are still lacking an intuitive and efficient way to reason ourselves coherently in this framework.

Why graphical (independence) models?

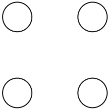




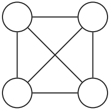




Empty graph



Complete graph



Undirected graphs as independence models

Definitions:

- A (general) graph is denoted by $G = (V, E)$ where V is a finite set of vertices, and $E \subset V \times V$ is the set of edges.
- A path (of length $n > 0$) in G, is a sequence of **different** vertices $v_1, v_2, \ldots, v_{n+1}$ such that

$$(v_i, v_{i+1}) \in E, \quad i = 1, \ldots, n.$$

- An edge $(v, v') \in E$ such that $v = v'$ is called a loop.
- An edge $(v, v') \in E$ such that $v \neq v'$ and $(v', v) \in E$ is called a line.
- An edge which is not a line nor a loop is called an arrow.
- G is an undirected graph if G has no loops and no arrows (i.e. G has only lines).

Vertex separation in undirected graphs

Let us consider an undirected $\mathrm{G} = (\mathbb{U}, \mathrm{E})$.

From local to global vertex separation:

- The absence of a line between variables represents the absence of a **direct** interaction between them.
- All other relations are induced by the notion of separation: *We say that in a graph* G *the sets* $\mathbb{A}$ *and* $\mathbb{B}$ *are separated by* $\mathbb{C}$ *if all paths from* $\mathbb{A}$ *to* $\mathbb{B}$ *traverse* $\mathbb{C}$*.*
  We denote this by $(\mathbb{A}; \mathbb{B} | \mathbb{C})_G$.

In particular:

- The sets $\mathbb{A}$ and $\mathbb{B}$ are separated if there is no path from $\mathbb{A}$ to $\mathbb{B}$.
- If there is no line connecting $\mathbb{A}$ to $\mathbb{B}$, then $(\mathbb{A}; \mathbb{B} | \mathbb{U} \setminus (\mathbb{A} \cup \mathbb{B}))_G$.

Undirected graphs as independence models

Can we use undirected graphs (UGs) as independence models?

The good news:

- The vertex separation relation satisfies properties (1)-(5).
  Exercise: *Check this.*
- Vertex separation is easy to check (polynomial time).

Questions:

- Is vertex separation compatible with probabilistic independence?
- How general is vertex separation w.r.t. probabilistic independence?
- What kind of independence relations can be exactly represented by vertex separation?

Notions of dependency, independency and perfect maps

Let us consider a distribution P and an undirected graph G over $\mathbb{U}$.

Definition (D-map (independent subsets are indeed separated))
G *is a D-map of* P *if for any three disjoint* $\mathbb{A}, \mathbb{B}, \mathbb{C} \subset \mathbb{U}$ *we have*

$$(\mathbb{A} \perp_P \mathbb{B} | \mathbb{C}) \Rightarrow (\mathbb{A}; \mathbb{B} | \mathbb{C})_G$$

Definition (I-map (separated subsets are indeed independent))
G *is a I-map of* P *if for any three disjoint* $\mathbb{A}, \mathbb{B}, \mathbb{C} \subset \mathbb{U}$ *we have*

$$(\mathbb{A} \perp_P \mathbb{B} | \mathbb{C}) \Leftarrow (\mathbb{A}; \mathbb{B} | \mathbb{C})_G$$

Definition (Perfect map (equivalence between "$\perp_P$" and ";"))
G *is a perfect map of* P *if it is a D-map **and** an I-map of* P.

Representation power of undirected graphs

Preliminary comments:

- Any P has at least a D-map (e.g. the empty graph)
- Any P has at least an I-map (e.g. the complete graph)
- Some P have not perfect-map (e.g. two coins and a bell)

There is thus a need to delineate more precisely

- those dependency models that have perfect maps, and
- those graphical models which are perfect maps of a dependency model
- provide constructive algorithms to switch between P and G.

We say that a dependency model M (i.e. a rule that assigns truth values to a three-place relation $(\mathbb{A} \perp_M \mathbb{B}|\mathbb{C})$ over disjoint subsets of some $\mathbb{U}$) is graph-isomorph if there exists an undirected graph $(\mathbb{U}, E)$ which is a perfect map of M.

Goal: characterize graph-isomorph probabilistic models.

On the structure of the set of UGs over some $\mathbb{U}$

Lattice structure:

- For a fixed $\mathbb{U}$, we can identify an undirected graph $G = (\mathbb{U}, E)$ with its set of edges E.
- The set of edges can itself be identified with a subset of the set of pairs $\{v, v'\} \in \mathbb{U}$.
- For any $G = (\mathbb{U}, E)$ and $G' = (\mathbb{U}, E')$, let us write $G \subset G'$ if $E \subset E'$.

Monotonicity w.r.t. addition or removal of edges:

- if G is a D-map of P, any $G' \subset G$ is also a D-map of P,
- if G is an I-map of P, any $G' \supset G$ is also an I-map of P.

Extreme maps:

- G is a maximal D-map, if there is no $G' \supset G$ (other than G itself) which is also a D-map.
- G is a minimal I-map, if there is no $G' \subset G$ (other than G itself) which is also an I-map.

Characterization of graph-isomorph dependency model

Theorem (Graph isomorph dependency model M)

A necessary and sufficient condition for a dependency model $\mathbb{M}$ *over some* $\mathbb{U}$ *to be graph-isomorph, is that it satisfies Symmetry (1), Decomposition (2), Intersection (5), Strong union and Transitivity,*

where Strong union means that

$$(\mathbb{X} \perp_M \mathbb{Y} | \mathbb{Z}) \Rightarrow (\mathbb{X} \perp_M \mathbb{Y} | (\mathbb{Z} \cup \mathbb{W}))$$

and Transitivity means that:

$$(\mathbb{X} \perp_M \mathbb{Y} | \mathbb{Z}) \Rightarrow \forall \gamma \in \mathbb{U} : (\mathbb{X} \perp_M \{\gamma\} | \mathbb{Z}) \text{ or } (\{\gamma\} \perp_M \mathbb{Y} | \mathbb{Z}).$$

NB: $\{\gamma\}$ *denotes a singleton subset of* $\mathbb{U}$.

Construction of a minimal I-map

Goal *: Given P, construct a minimal I-map G of P.*

Motivation: A minimal I-map is a graph displaying a maximal number of independencies without false-positives.

Theorem (Existence, unicity, construction of minimal I-map)
Every dependency model M which satisfies symmetry, decomposition and intersection, has a unique minimal I-map $G_0 = (\mathbb{U}, E_0)$ produced by connecting only those pairs (v, v') for which $(\{v\} \perp_M \{v'\} | \mathbb{U} \setminus \{v, v'\})$ is FALSE.

Goal *: Check whether G is an I-map of P.*
If P is strictly positive, we can check whether G is an I-map, by constructing first a minimal I-map G_0 of P (in polynomial time) and then checking whether $G_0 \subset G$.

NB: *See more details in the extended set of slides.*

Markov networks, blankets and boundaries

Definitions:

- *Given* P *(resp.* M*), we say that* G *is a* *Markov network* *of* P *(resp.* M*) if it is a minimal I-map of* P *(resp.* M*).*
- *A* *Markov blanket* $\mathrm{BL}_M(v)$ *of* $v \in \mathbb{U}$ *is any subset* $\mathbb{S} \subset \mathbb{U}$ *for which* $(\{v\} \perp_M \mathbb{U} \setminus (\{v\} \cup \mathbb{S}) | \mathbb{S})$*.*
- *A* *Markov boundary* $\mathrm{B}_M(v)$ *of* $v \in \mathbb{U}$ *is a minimal Markov blanket.*

Theorem (Unicity and construction of Markov boundaries)

Every element v *of a dependency model* M *which satisfies symmetry, decomposition, intersection and weak union, has a* *unique* *Markov boundary, and this corresponds with the set of vertices adjacent to* v *in the minimal I-map* G_0 *of* M

Summary of UG models

- We have seen that we can make use of undirected models to represent useful independencies, in a way compatible with the definition of probabilistic conditional independence.
- Not all independence structures may be represented by UGs.
- But we can commit with the idea of building the most refined model of them in the form of a minimal I-map.
- Futher topic of relevance:

  For any G is there a P such that its G is a perfect map? (answer is yes, with a few hypotheses)

Directed acyclic graphs (DAGs)

Definitions:

- A directed graph $D = (V, E)$ is a graph with only arrows, i.e. no loops and no lines or, in other words, $(v, v') \in E \Rightarrow v \neq v' \& (v', v) \notin E$.
- A cycle of length $n > 0$, in a graph $G = (V, E)$, is a sequence $v_1, \ldots, v_{n+1}$ such that $(v_i, v_{i+1}) \in E$ & $v_1 = v_{n+1}$.
- The cycle is said to be simple (or proper) if all nodes except v_1 and v_{n+1} are different.
- A DAG is a directed graph without any cycle.

NB:*This definition of DAG is equivalent to saying:*

- *that a DAG is a directed graph without any simple cycle, or*
- *that a DAG is a graph without any cycle.*

D-separation in DAGs

Definition (D-separation)

If $\mathbb{X}, \mathbb{Y}, \mathbb{Z}$ are three disjoint sets of vertices in a DAG D, then $\mathbb{Z}$ is said to d-separate $\mathbb{X}$ from $\mathbb{Y}$, denoted by $(\mathbb{X}; \mathbb{Y}|\mathbb{Z})_D$, if there is no path between a vertex in $\mathbb{X}$ and a vertex in $\mathbb{Y}$ along which the following two conditions hold:

(i) *every node with converging arrows is in $\mathbb{Z}$ or has a descendant in $\mathbb{Z}$ and*

(ii) *every other node is outside of $\mathbb{Z}$.*

- If a path satisfies the above condition, it is said to be active; otherwise it is said to be blocked.
- A DAG is an I-map of P if all its d-separations correspond to conditional independencies satisfied in P.
- It is a minimal I-map, or a Bayesian network of P, if none of its arrows can be deleted without destroying its I-mapness.

Bayesian networks (BNs)

- Construction of Bayesian networks for a distribution P involves the notion of boundary DAG of M relative to a vertex ordering.
- DAGs as minimal I-maps of Semi-graphoids.

  Main result: *For any semi-graphoid* M *(in particular, for any* P *induced independence model) and any ordering* d*, any corresponding boundary DAG is a minimal I-map of* M*.*
- Corollary of the main result:

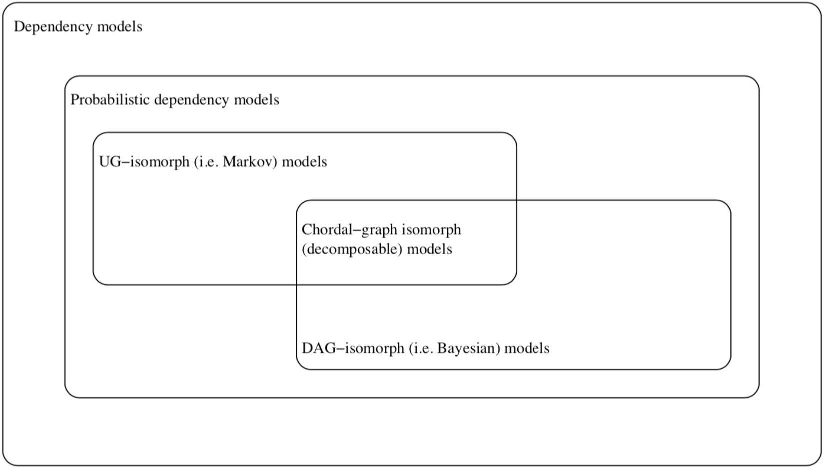
  A necessary and sufficient condition for a DAG D to be a Bayesian network of P is that each variable X be conditionally independent of all its non-descendants, given its parents Π_X, and that no proper subsets of Π_X satisfies this condition.

NB: *See more details about BNs in the extended set of slides.*

Summary of DAG models

- We have seen that we can make use of directed acyclic graphical models to represent useful independencies, in a way compatible with the definition of probabilistic conditional independence.
- Not all independence structures may be represented exactly by DAGs.
- But we can commit with the idea of building the most refined model of them in the form of a minimal I-map.
- As with UGs, we can infer independencies by inspection of the graph, in polynomial time.

The global picture



Quantitative aspects

- What do we need to add to a minimal I-map graphical structure to describe fully a given P?
  - UGs: parametrization via potential (or compatibility) functions over cliques.
  - DAGs: parametrization via conditional distributions over families.
- How can we compute with parametrized DAG or UG P-models?
  - Exact computations: reduce du CG and use (generalized) forward-backward algorithm.
  - Approximations: turn problem into a tractable optimization problem (subject of current research).
- How can we infer UG or DAG models from data?

Tree structured graphical models

Motivations

- Tree structured models offer simple interpretations
- Efficient inference algorithms
- Efficient learning algorithms

Two classes

- Undirected trees and their equivalent directed version
- Polytrees : DAGs whose skeleton is a tree

NB: *See more details about shaded points in the extended set of slides.*

A few additional definitions from graph theory

- Skeleton of a DAG: *UG obtained by replacing all arrows by lines.*
- Directing an UG: *DAG obtained by replacing every line by an arrow, under the constraint of producing a DAG.*
- Induced subgraph : *(of* $G = (V, E)$*) by* $V' \subset V$ *is the graph* $G(V') = (V', E \cap V' \times V')$.

  Note*: induced subgraphs of UGs (resp. DAGs) are UGs (resp. DAGs).*
- Clique of an UG : *a clique of* $G = (V, E)$ *is an induced subgraph* $G(V')$ *such that* $\forall v, v' \in V' : v \neq v' \Rightarrow (v, v') \in E$.
- Maximal clique: *a clique which can not be augmented while maintaining the property of being a clique, i.e. a maximal subgraph whose vertices are all adjacent to each other in* G.

Parameterizing UGs: example of the Markov chain $X - Y - Z$

- Cliques: $X - Y$ and $Y - Z$
- Compatibility functions: $g_1(x, y)$ and $g_2(y, z)$
- Suppose we know $P(X, Y, Z)$: how to derive the g_i from P?
  - $g_1(x, y) = P(X, y) = P(X)P(y|x)$ and $g_2(y, z) = P(z|y)$, which corresponds to the parameterization of the DAG $X \rightarrow Y \rightarrow Z$;
  - or $g_2(y, z) = P(y, z) = P(z|y)P(y)$ and $g_1 = P(x|y)$ which corresponds to $X \leftarrow Y \rightarrow Z$;
  - or $g_2(y, z) = P(z)P(y|z)$ and $g_1 = P(x|y)$ which corresponds to $X \leftarrow Y \leftarrow Z$.
  - But, we could not take the parameterization of the DAG $X \rightarrow Y \leftarrow Z$.

    The three first parameterizations correspond to directed version of the UG which do not introduce a v-structure; while the fourth one introduces a v-structure.

Markov trees

- We use indifferently the term Markov tree, tree, or tree-structured UG, to denote UGs without any cycles.
- Typically, we assume in addition that these trees are singly connected, i.e. such that there is a path from any vertex to any other vertex, and use the term 'forest' to denote the case where not all nodes are connected.
- In a singly connected tree over n vertices, we always have exactly $n - 1$ edges.
- In a forest over n vertices, we have $n - c$ edges, where c is the number of connected components.

***NB**: See more details about the procedure for parameterizing Markov trees in the extended set of slides.*

I-map preserving direction of tree-structured UGs

Theorem

Any directed version of a tree-structured UG which has no v-structure produces a DAG which represents exactly the same set of independencies as the original undirected tree.

Corollary: tree-structured UGs may be parameterized by first directing them without introducing any v-structure, and then parameterizing the resulting DAG.

Algorithm: to direct a tree-structured UG in such a way that no v-structures are introduced

1. Choose first a root of the tree: any node of the UG
2. Direct its arcs 'away' from the root
3. Proceed recusively by directing the yet not direct arcs of the successors 'away' from them.

Summary of tree-structured graphical models

- Like DAGs, tree structured UGs may be parameterized 'easily' to represent a P which satisfies the independencies encoded by the UG, by first directing the tree structured UG without introducing v-structures (which maintains the encoded independencies (Why?), and by then using the DAG parameterization procedure to attach conditional distributions to nodes.

NB*: See more details about the chordal graphs in the extended set of slides.*

Learning structure from data (Chapter 8 of Pearl)

- Main question: how to infer the graph structure from the information at hand?
- We will limit ourselves to tree structures
- We will decompose the question in this context into three successive questions:
  - Given a $P(x)$ known to factorize according to a tree structured graph, how to efficiently recover its tree-structured perfect map?
  - Given a general $P(x)$, can we recover the best approximation of $P(x)$ in the form of a parametrization of a tree structured graph?
  - Given only a sample from a generative distribution, how to answer the two preceding questions?

NB: *These questions will only be declined with tree structured UGs. For general tree structured DAGs (polytree), see the extended set of slides.*

Intuition about structure inference

- Consider the case of three variables X, Y, Z, and suppose that we known that they form a Markov chain, but that we don't known in which order.
- In other words, we hesitate between the three following structures: $X - Y - Z$, $Y - X - Z$, $X - Z - Y$.
- Suppose that we are able to compute $\mathrm{I}(X; Y)$, $\mathrm{I}(Y; Z)$ and $\mathrm{I}(X; Z)$:
  - Can we infer from these three quantities a correct structure?
  - The answer is YES.
  - Sort the quantities $\mathrm{I}(X; Y)$, $\mathrm{I}(Y; Z)$ and $\mathrm{I}(X; Z)$ by decreasing order of numerical value, take the two first and create an UG with lines among the corresponding two pairs of variables.
  - Explanation: data processing inequality!

Chow and Liu algorithm: generalization to P which factorize according to tree-structured UG.

- We want to represent graphically the independencies of a distribution $P(X_1, \ldots, X_n)$ known to be Markov w.r.t. to a tree-structured UG (but we do not know the structure).
- Algorithm (Chow and Liu, 1968)
    1. Compute the pairwise mutual informations $I(X_i; X_j), \forall i \neq j$.
    2. Assign a line between the variables corresponding to the largest mutual information.
    3. Examine the next largest information and assign a line, unless it creates a cycle in the graph.
    4. Repeat step 3, until $n - 1$ branches have been assigned.
- Select an arbitraty node as root, direct the UG from it (without introducing v-structures) and to each X_i assign $P(X_i | X_{p(i)})$ where $p(i)$ addresses the (sole) parent of X_i.

Comments about the Chow and Liu algorithm

- When we want to infer a tree-structured UG (or a directed version of it without v-structures) for a target distribution, and dispose of means to compute pairwise quantities from the target distribution, in the form of mutual informations among variables and conditional distributions of one variable given another, we dispose of an 'efficient' algorithm for generating a Markov network (order n^2, roughly).
- The Chow Liu algorithm is an instance of the 'maximum weight spanning tree ' algorithm of graph theory (MWST).

NB*: In the algorithm, we may in principle be led to situations where the* $I(X_i; X_j)$ *of the next line to assign is equal to zero; if this is the case we can immediately stop the procedure (leading to a 'forest' model, i.e. a model where some subsets of variables are disconnected).*

Approximation of probability distributions

- In many practical situations, we do not dispose of precise information about the probability distribution at hand.
- In particular, in such contexts, we are not able to verify in a definite way independencies such as $(X_i \perp X_j | X_k)$.
- In other words, we can only estimate/approximate quantities such as $I(X_i; X_j)$ or $P(X_i | X_{p(i)})$.
- Then : How to infer precise probabilistic models from imprecise data?
- Approach:
  - Defined a space of target probability distributions (model).
  - Define a measure of discrepancy between distributions.
  - Choose the probability distribution in the target space which is as 'compatible as possible' with the information at hand.

Measuring the compatibility among two distributions

Kullback-Leibler divergence:

$$D(P, P') = \sum_x P(x) \log \frac{P(x)}{P'(x)}$$

- tends to zero when $P \to P'$.
- has the likelihood interpretation, when P is inferred from a sample.

Furthermore, to minimize D over the space of trees, we can simply use Chow Liu based on information quantities derived from P.

***NB**: See more details on the KL-divergence, the D-projection and the relevant results in the extended set of slides.*

Comments about the Chow and Liu algorithm

- Given any probability distribution P and the means to compute pairwise mutual informations and pairwise conditional distributions in P, this algorithm allows to infer (in quadratic time), a tree structured approximation of P.
- The resulting distribution P' is the one, among all that factorize along UG trees, that is closest according to the distance measure $\mathrm{D}(\mathrm{P}, \mathrm{P}')$.
- In particular, if P is Markov w.r.t. an UG tree, then the resulting P' will be equal to P.

Learning from observations drawn from P (1)

Let us consider a sample of observations $S = (x^1, \ldots, x^N)$ drawn i.i.d. from a target distribution $P(x)$ (where each x^i is actually an n-tuple, having one element for each variable X_j.

- Given any other distribution P' defined over the same set of variables, we define the sample log-likelihood, by

$$\mathrm{IL}(S, P') = \sum_{i=1}^{N} \log P'(x^i) = \log \left(\prod_{i=1}^{N} P'(x^i) \right).$$

- Given a space $\mathcal{P}$ of candidate distributions, a classical criterion use in statistics, is to choose the one which maximizes the sample likelihood.

Learning from observations drawn from P (2)

Let us consider a configuration x, and denote by $N(x)$ the number of observations in our sample which correspond to that configuration and by $F(x) = N(x)/N$ their relative frequency among the N observations.

- We can rewrite the log-likelihood of the sample w.r.t. P' as
$$\mathrm{IL}(S, P') = N \sum_{x} F(x) \log P'(x)$$
- We then immediately see that maximizing the log-likelihood of the sample by choosing P' is equivalent to choosing P' so as to minimize the KL-divergence $\sum_x F(x) \log \frac{F(x)}{P'(x)}$. Indeed,
$$\sum_{x} F(x) \frac{F(x)}{P'(x)} = -\frac{1}{N} \mathrm{IL}(S, P') + \sum_{x} F(x) \log F(x).$$

Learning a Markov tree approximation from a sample

- Goal: find a tree structure and a parameterization such that the sample likelihood is maximal (over all possible trees and parameterizations of them).
- Solution: use sample to estimate mutual informations, by replacing probabilities by relative frequencies derived from the sample, then apply Chow-Liu to get MWST, then choose a root, then use again sample to estimate the conditional probabilities needed for each vertex.