A Tutorial on Graphical Models and How to Learn Them from Data

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Overview

- **Graphical Models: Core Ideas and Notions**
- **A Simple Example: How does it work in principle?**
- **Conditional Independence Graphs**
  - conditional independence and the graphoid axioms
  - separation in (directed and undirected) graphs
  - decomposition/factorization of distributions
- **Evidence Propagation in Graphical Models**
- **Building Graphical Models**
- **Learning Graphical Models from Data**
  - quantitative (parameter) and qualitative (structure) learning
  - evaluation measures and search methods
  - learning by measuring the strength of marginal dependences
  - learning by conditional independence tests
- **Summary**

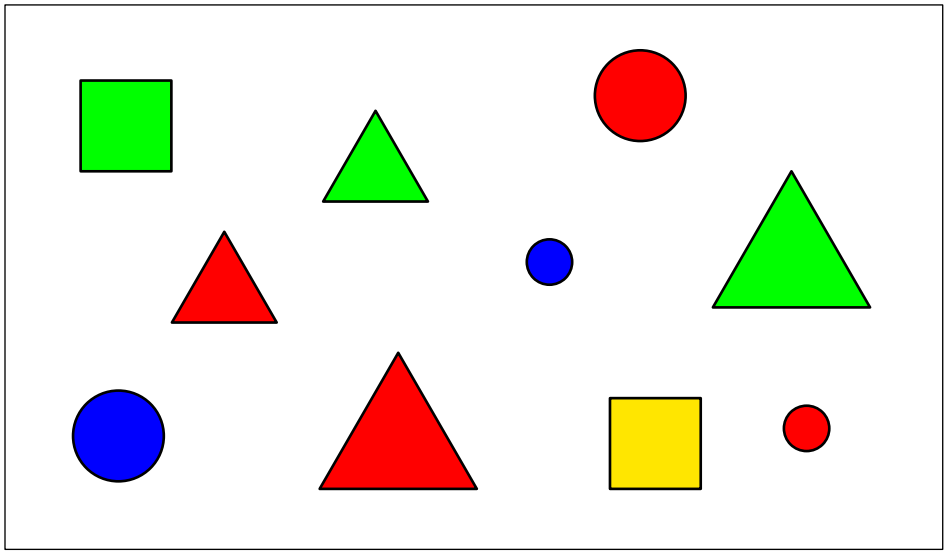
Graphical Models: Core Ideas and Notions

- **Decomposition:** Under certain conditions a distribution δ (e.g. a probability distribution) on a multi-dimensional domain, which encodes *prior* or *generic knowledge* about this domain, can be decomposed into a set $\{\delta_1, \ldots, \delta_s\}$ of (usually overlapping) distributions on lower-dimensional subspaces.
- **Simplified Reasoning:** If such a decomposition is possible, it is sufficient to know the distributions on the subspaces to draw all inferences in the domain under consideration that can be drawn using the original distribution δ.
- Such a decomposition can nicely be represented as a **graph** (in the sense of graph theory), and therefore it is called a **Graphical Model**.
- The graphical representation
  - encodes **conditional independences** that hold in the distribution,
  - describes a **factorization** of the probability distribution,
  - indicates how **evidence propagation** has to be carried out.

A Simple Example:
The Relational Case

A Simple Example

Example Domain

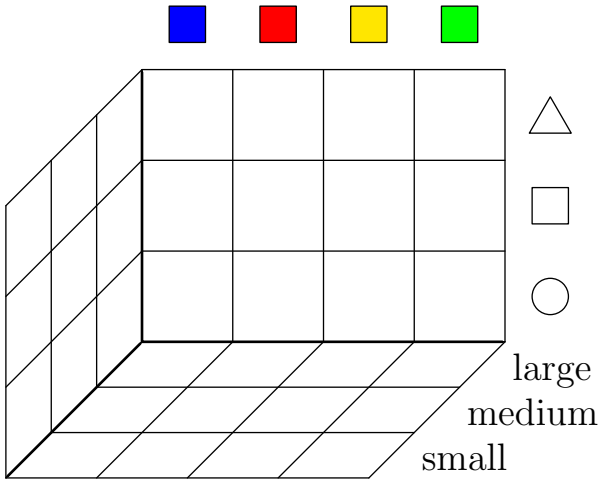


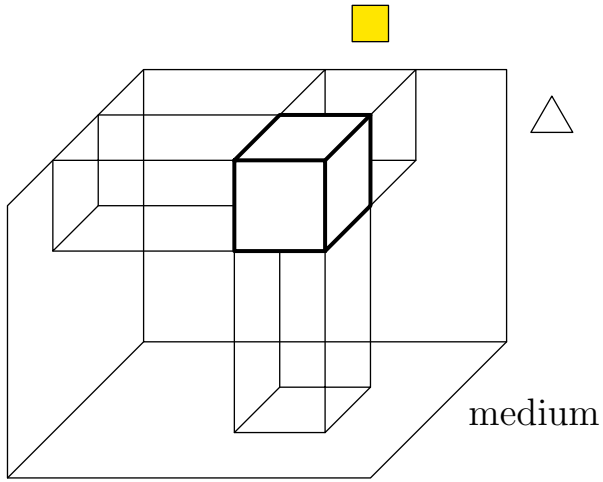
Relation

color	shape	size
■	○	small
■	○	medium
■	○	small
■	○	medium
■	△	medium
■	△	large
■	□	medium
■	□	medium
■	△	medium
■	△	large

- 10 simple geometrical objects, 3 attributes.
- One object is chosen at random and examined.
- Inferences are drawn about the unobserved attributes.

The Reasoning Space





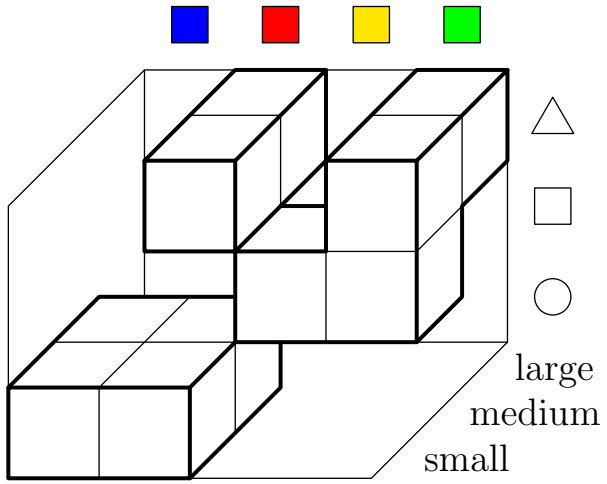
- The reasoning space consists of a finite set Ω of states.
- The states are described by a set of n attributes A_i, $i = 1, \ldots, n$, whose domains $\{a_1^{(i)}, \ldots, a_{n_i}^{(i)}\}$ can be seen as sets of propositions or events.
- The events in a domain are mutually exclusive and exhaustive.
- The reasoning space is assumed to contain the true, but unknown state ω_0.

The Relation in the Reasoning Space

Relation

color	shape	size
■	○	small
■	○	medium
■	○	small
■	○	medium
■	△	medium
■	△	large
■	□	medium
■	□	medium
■	△	medium
■	△	large

Relation in the Reasoning Space

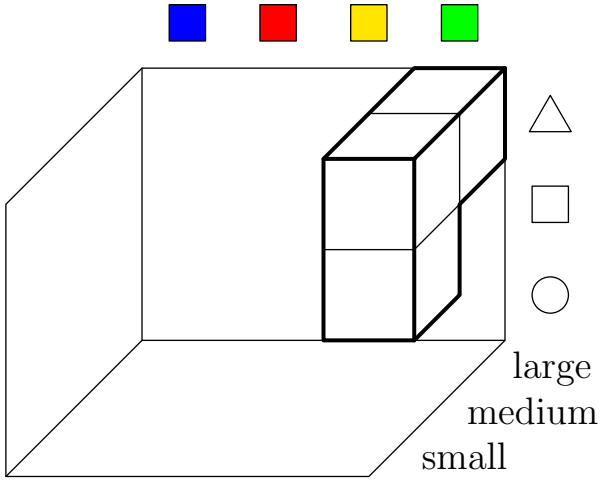


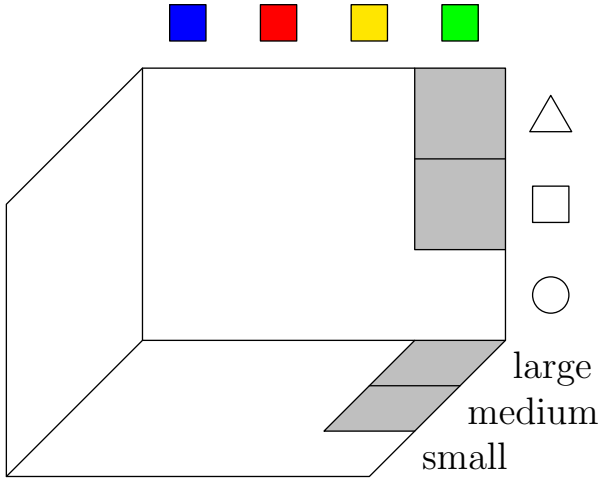
Each cube represents one tuple.

- The spatial representation helps to understand the decomposition mechanism.

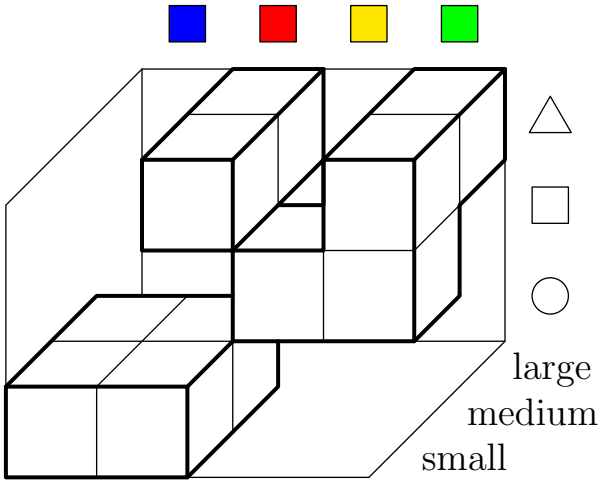
Reasoning

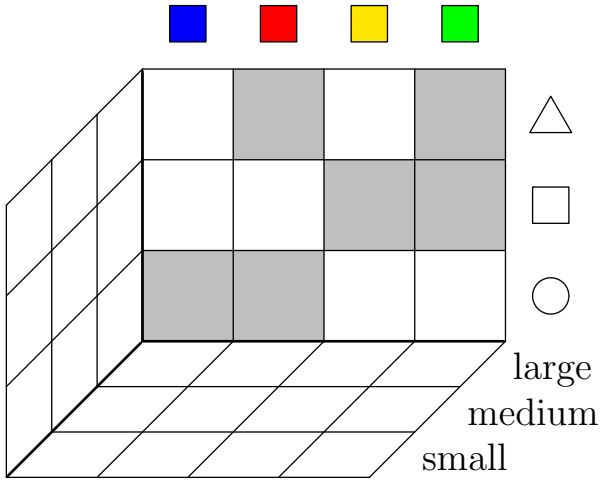
- Let it be known (e.g. from an observation) that the given object is green.
  This information considerably reduces the space of possible value combinations.
- From the prior knowledge it follows that the given object must be
  - either a triangle or a square and
  - either medium or large.

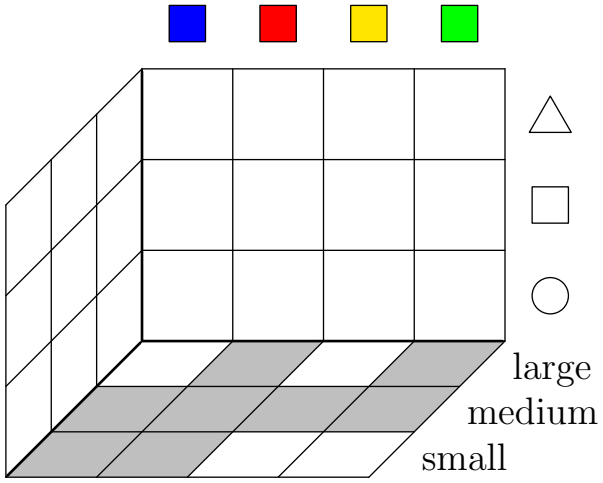


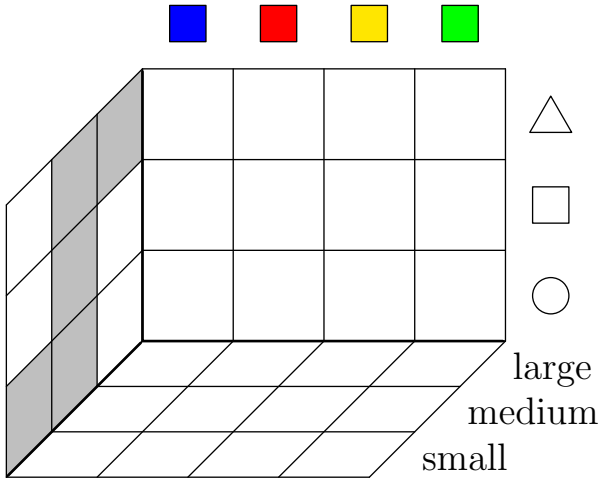


Prior Knowledge and Its Projections

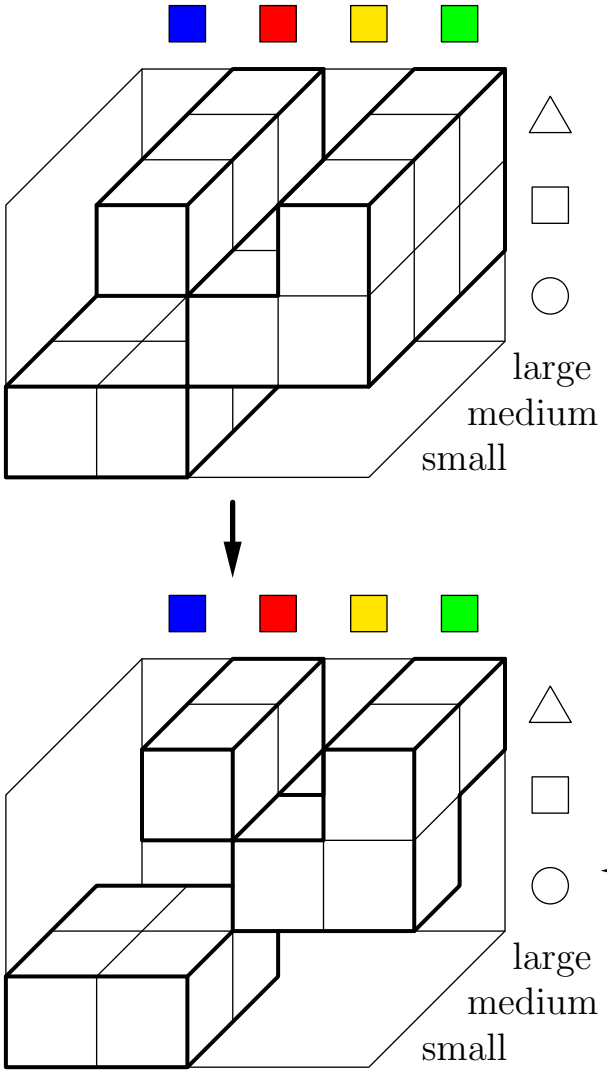








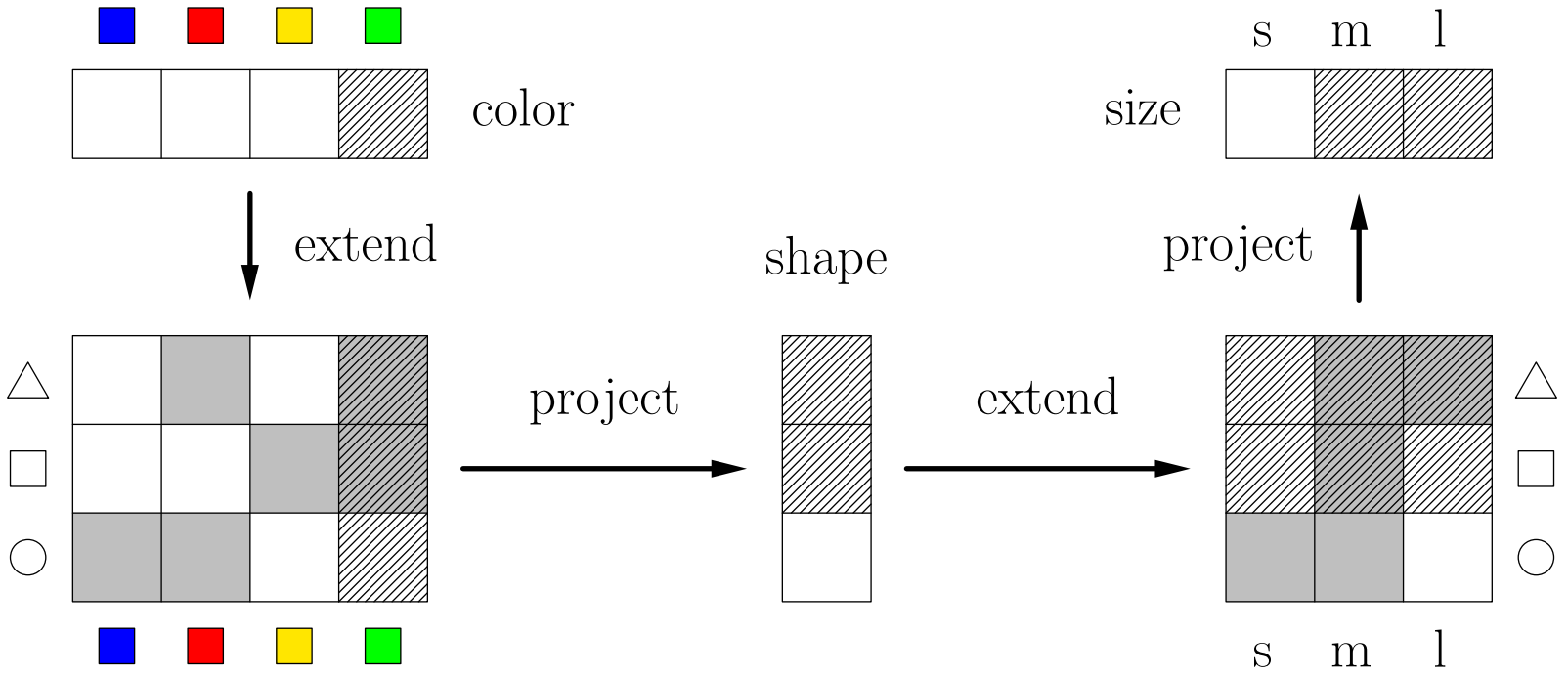
Cylindrical Extensions and Their Intersection



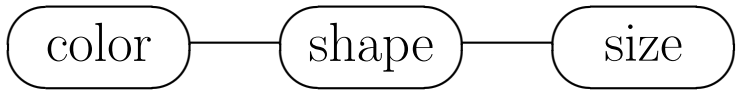
Intersecting the cylindrical extensions of the projection to the subspace spanned by color and shape and of the projection to the subspace spanned by shape and size yields the original three-dimensional relation.

Reasoning with Projections

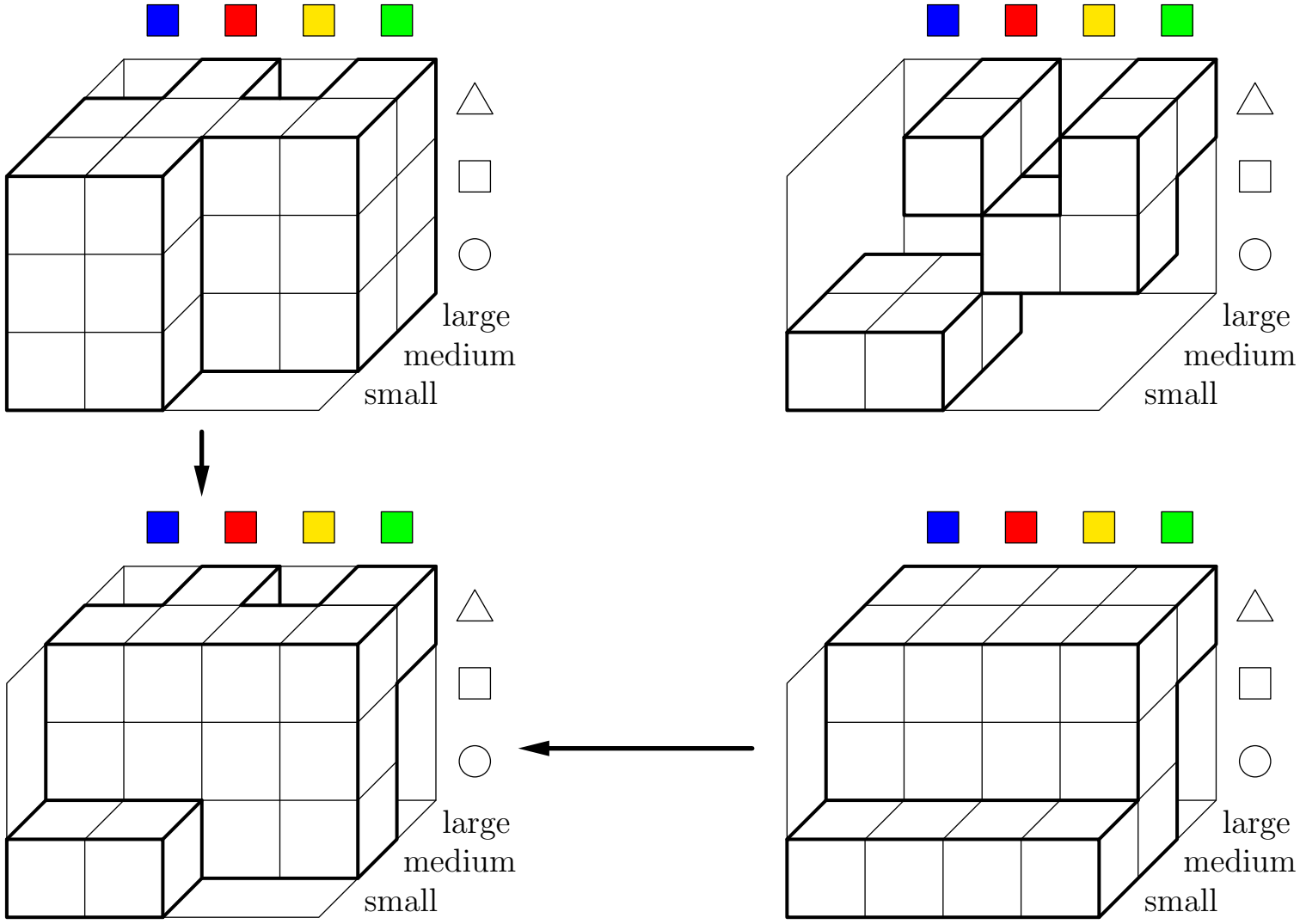
The same result can be obtained using only the projections to the subspaces without reconstructing the original three-dimensional relation:



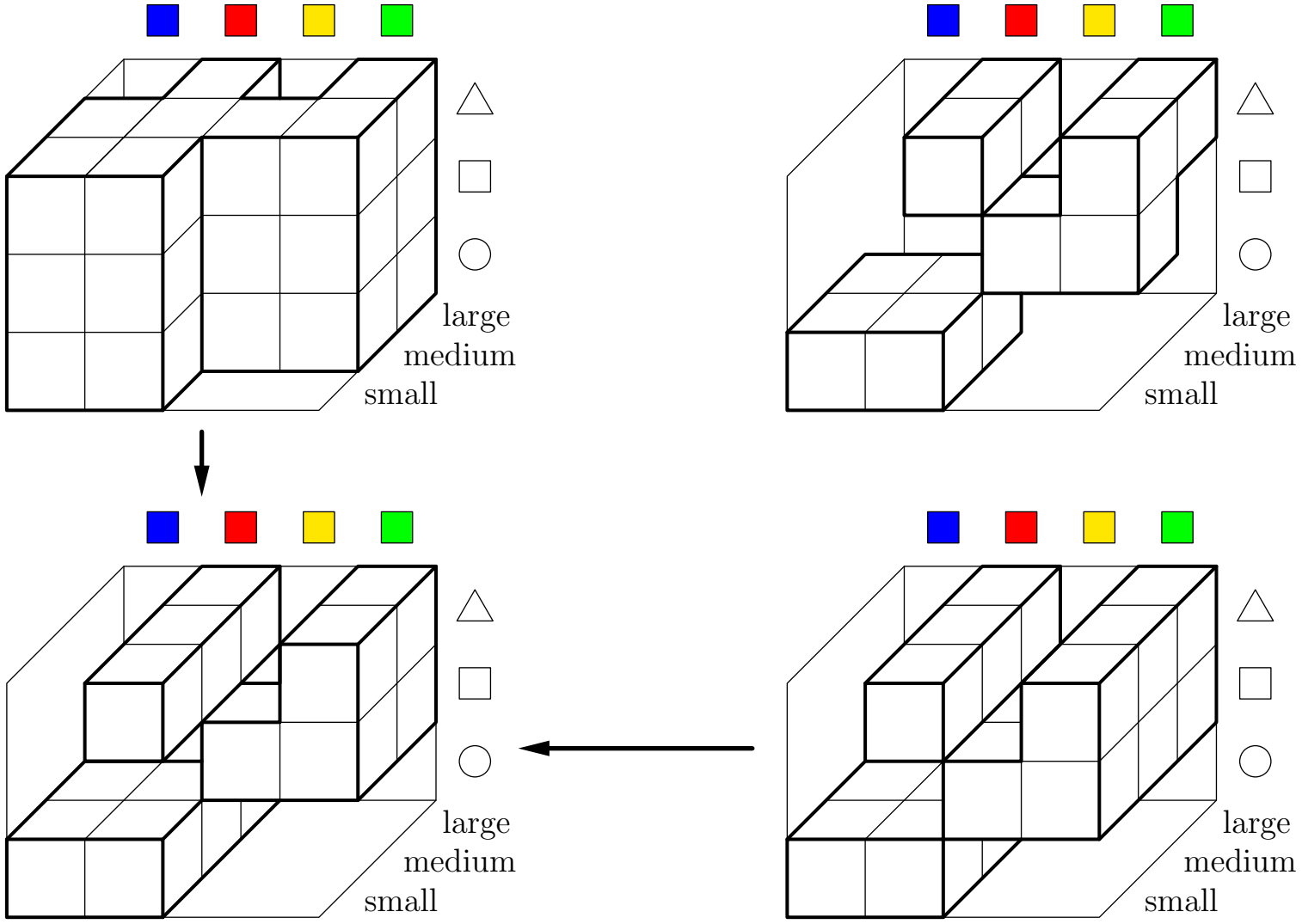
This justifies a graph representation:



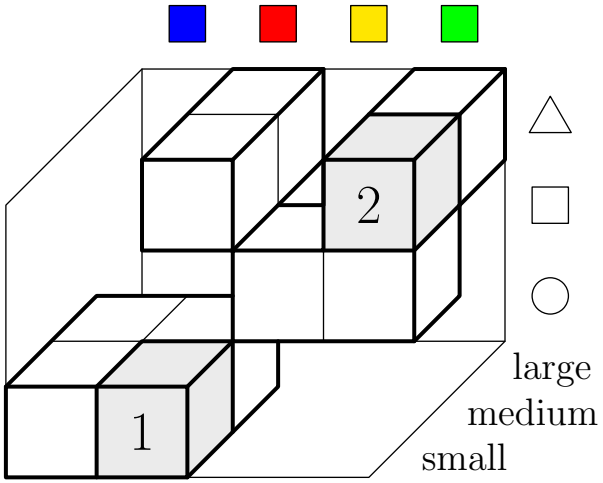
Using other Projections 1

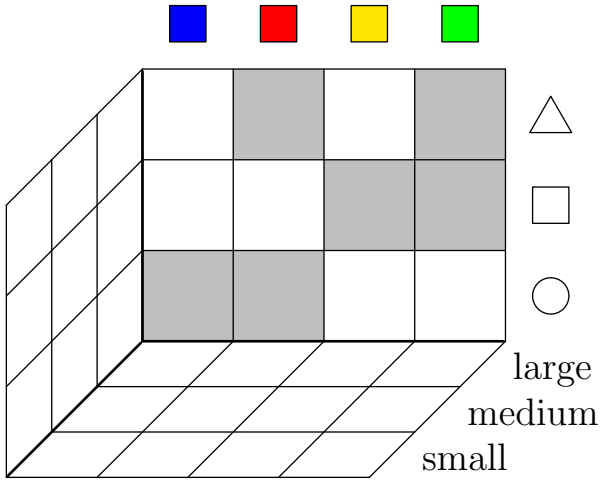


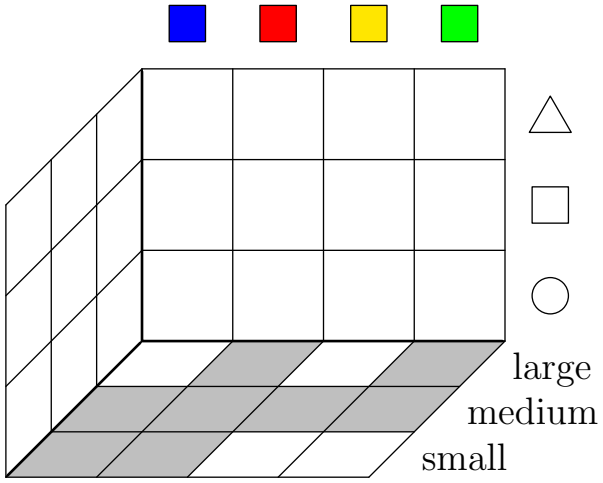
Using other Projections 2

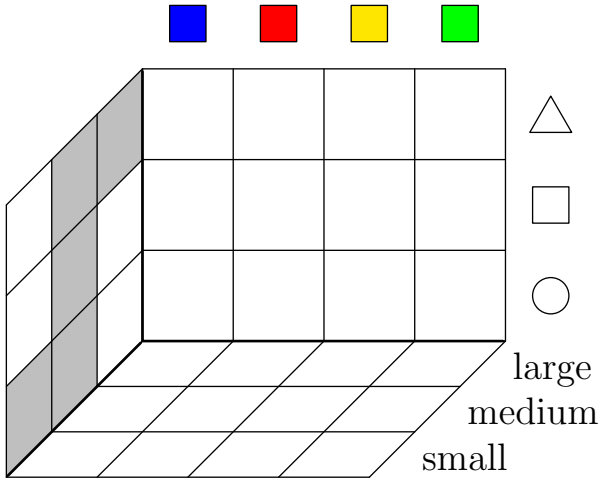


Is Decomposition Always Possible?









Relational Graphical Models: Formalization

Possibility-Based Formalization

Definition: Let Ω be a (finite) sample space.
A **discrete possibility measure** R on Ω is a function $R : 2^\Omega \to \{0, 1\}$ satisfying

1. $R(\emptyset) = 0$ and
2. $\forall E_1, E_2 \subseteq \Omega : R(E_1 \cup E_2) = \max\{R(E_1), R(E_2)\}$.

- Similar to Kolmogorov's axioms of probability theory.
- If an event E can occur (if it is possible), then $R(E) = 1$,
  otherwise (if E cannot occur/is impossible) then $R(E) = 0$.
- $R(\Omega) = 1$ is not required, because this would exclude the empty relation.
- From the axioms it follows $R(E_1 \cap E_2) \leq \min\{R(E_1), R(E_2)\}$.
- Attributes are introduced as random variables (as in probability theory).
- $R(A = a)$ and $P(a)$ are abbreviations of $R(\{\omega \mid A(\omega) = a\})$.

Possibility-Based Formalization (continued)

Definition: Let $U = \{A_1, \ldots, A_n\}$ be a set of attributes defined on a (finite) sample space Ω with respective domains $\mathrm{dom}(A_i)$, $i = 1, \ldots, n$. A **relation** r_U over U is the restriction of a discrete possibility measure R on Ω to the set of all events that can be defined by stating values for all attributes in U. That is, $r_U = R|_{\mathcal{E}_U}$, where

$$\begin{aligned}
\mathcal{E}_U &= \Big\{ E \in 2^\Omega \;\Big|\; \exists a_1 \in \mathrm{dom}(A_1) : \ldots \exists a_n \in \mathrm{dom}(A_n) : \\
&\qquad\qquad E \mathrel{\widehat{=}} \bigwedge_{A_j \in U} A_j = a_j \Big\} \\
&= \Big\{ E \in 2^\Omega \;\Big|\; \exists a_1 \in \mathrm{dom}(A_1) : \ldots \exists a_n \in \mathrm{dom}(A_n) : \\
&\qquad\qquad E = \Big\{ \omega \in \Omega \;\Big|\; \bigwedge_{A_j \in U} A_j(\omega) = a_j \Big\} \Big\}.
\end{aligned}$$

- Corresponds to the notion of a probability distribution.
- Advantage of this formalization: No index transformation functions are needed for projections, there are just fewer terms in the conjunctions.

Possibility-Based Formalization (continued)

Definition: Let $U = \{A_1, \ldots, A_n\}$ be a set of attributes and r_U a relation over U. Furthermore, let $\mathcal{M} = \{M_1, \ldots, M_m\} \subseteq 2^U$ be a set of nonempty (but not necessarily disjoint) subsets of U satisfying

$$\bigcup_{M \in \mathcal{M}} M = U.$$

r_U is called **decomposable** w.r.t. $\mathcal{M}$ iff

$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$r_U\Big(\bigwedge_{A_i \in U} A_i = a_i\Big) = \min_{M \in \mathcal{M}} \Big\{ r_M\Big(\bigwedge_{A_i \in M} A_i = a_i\Big)\Big\}.$$

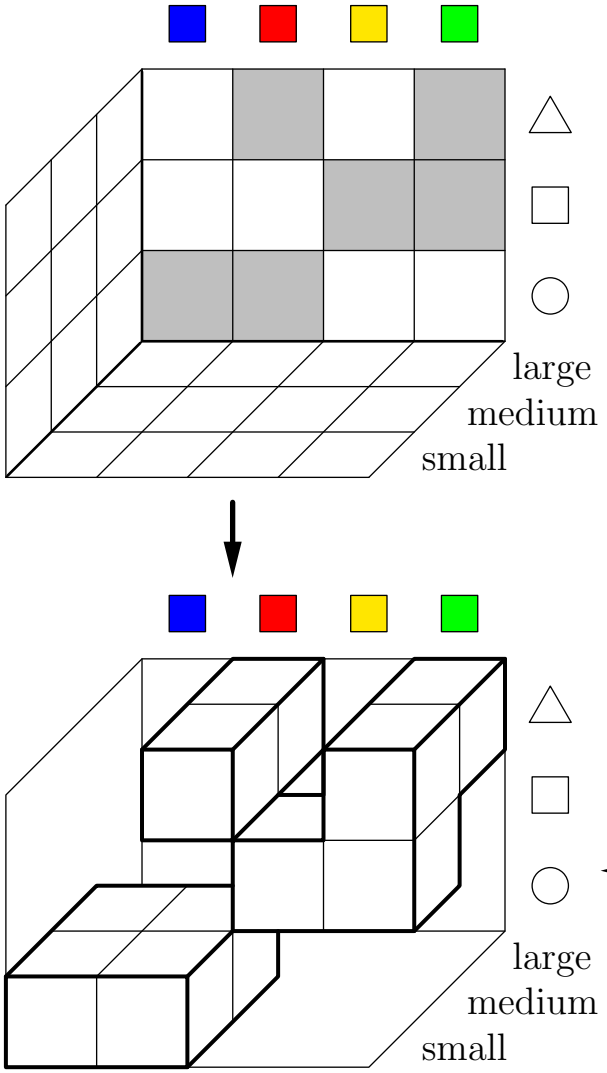
If r_U is decomposable w.r.t. $\mathcal{M}$, the set of relations

$$\mathcal{R}_{\mathcal{M}} = \{r_{M_1}, \ldots, r_{M_m}\} = \{r_M \mid M \in \mathcal{M}\}$$

is called the **decomposition** of r_U.

- Equivalent to **join decomposability** in database theory (natural join).

Relational Decomposition: Simple Example



Taking the minimum of the projection to the subspace spanned by color and shape and of the projection to the subspace spanned by shape and size yields the original three-dimensional relation.

Conditional Possibility and Independence

Definition: Let Ω be a (finite) sample space, R a discrete possibility measure on Ω, and $E_1, E_2 \subseteq \Omega$ events. Then

$$R(E_1 \mid E_2) = R(E_1 \cap E_2)$$

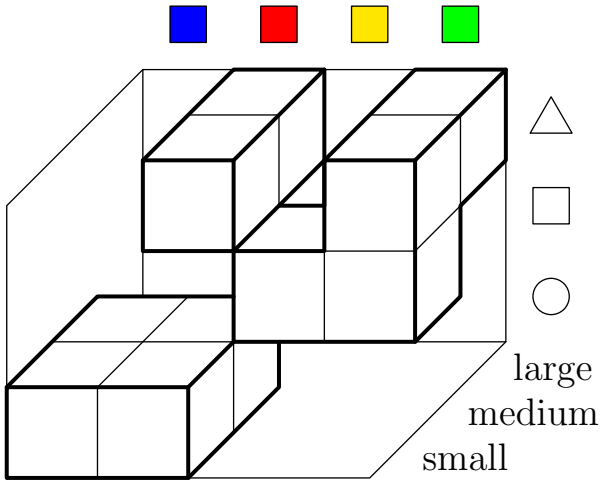
is called the **conditional possibility** of E_1 given E_2.

Definition: Let Ω be a (finite) sample space, R a discrete possibility measure on Ω, and A, B, and C attributes with respective domains $\mathrm{dom}(A)$, $\mathrm{dom}(B)$, and $\mathrm{dom}(C)$. A and B are called **conditionally relationally independent** given C, written $A \perp\!\!\!\perp_R B \mid C$, iff

$$\begin{aligned}
&\forall a \in \mathrm{dom}(A) : \forall b \in \mathrm{dom}(B) : \forall c \in \mathrm{dom}(C) : \\
&\qquad R(A = a, C = c \mid B = b) = \min\{R(A = a \mid B = b), R(C = c \mid B = b)\}, \\
\Leftrightarrow \quad &R(A = a, C = c,\ B = b) = \min\{R(A = a,\ B = b), R(C = c,\ B = b)\}.
\end{aligned}$$

- Similar to the corresponding notions of probability theory.

Conditional Independence: Simple Example

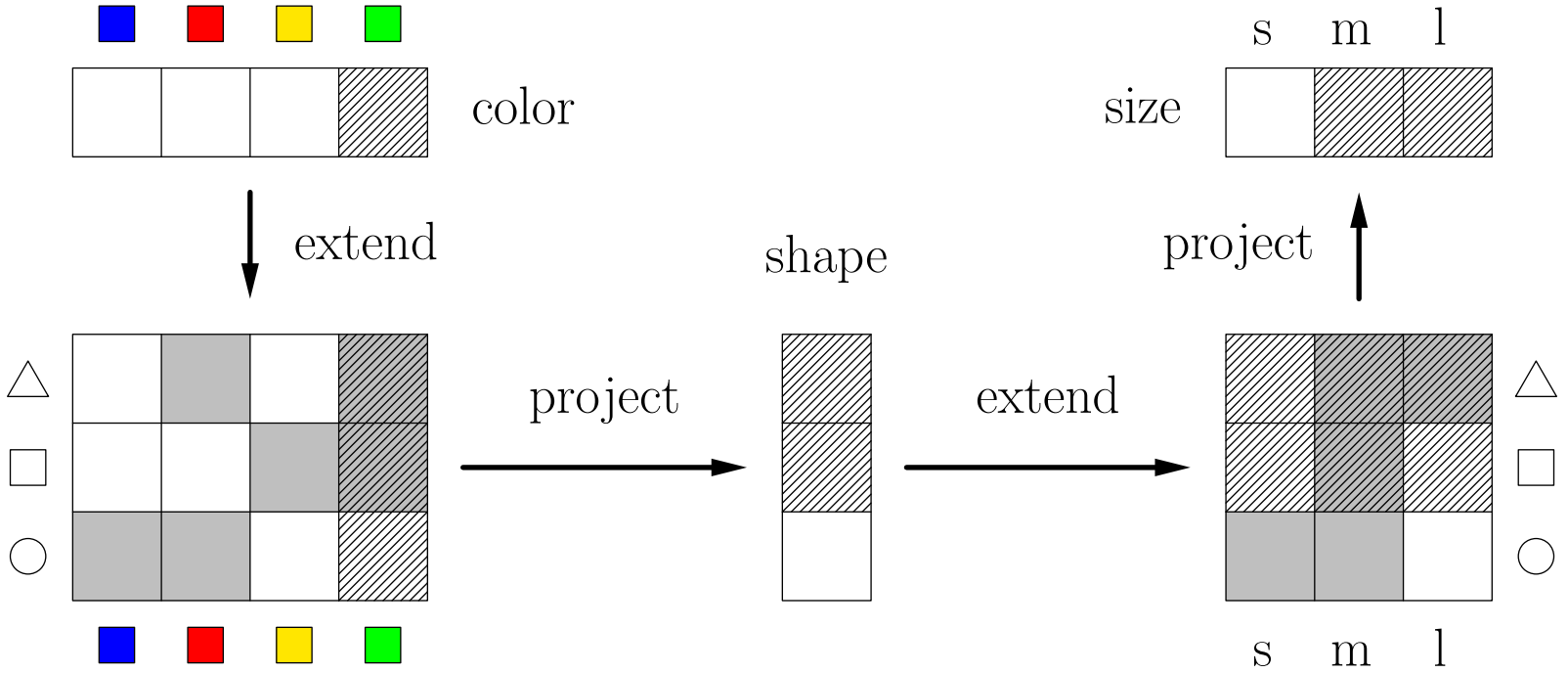


Example relation describing ten simple geometric objects by three attributes: color, shape, and size.

- In this example relation, the color of an object is conditionally relationally independent of its size given its shape.
- Intuitively: if we fix the shape, the colors and sizes that are possible together with this shape can be combined freely.
- Alternative view: once we know the shape, the color does not provide additional information about the size (and vice versa).

Relational Evidence Propagation

Due to the fact that color and size are conditionally independent given the shape, the reasoning result can be obtained using only the projections to the subspaces:



This reasoning scheme can be formally justified with discrete possibility measures.

Relational Evidence Propagation, Step 1

$$
\begin{aligned}
& R(B = b \mid A = a_{\text{obs}}) \\
&= R\Big(\bigvee_{a \in \text{dom}(A)} A = a, B = b, \bigvee_{c \in \text{dom}(C)} C = c \,\Big|\, A = a_{\text{obs}} \Big) \\
&\overset{(1)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{c \in \text{dom}(C)} \{ R(A = a, B = b, C = c \mid A = a_{\text{obs}}) \} \Big\} \\
&\overset{(2)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{c \in \text{dom}(C)} \{ \min\{ R(A = a, B = b, C = c), R(A = a \mid A = a_{\text{obs}}) \} \} \Big\} \\
&\overset{(3)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{c \in \text{dom}(C)} \{ \min\{ R(A = a, B = b), R(B = b, C = c), \\
&\qquad\qquad R(A = a \mid A = a_{\text{obs}}) \} \} \Big\} \\
&= \max_{a \in \text{dom}(A)} \{ \min\{ R(A = a, B = b), R(A = a \mid A = a_{\text{obs}}), \\
&\qquad\qquad \underbrace{\max_{c \in \text{dom}(C)} \{ R(B = b, C = c) \}}_{= R(B=b) \geq R(A=a, B=b)} \} \} \\
&= \max_{a \in \text{dom}(A)} \{ \min\{ R(A = a, B = b), R(A = a \mid A = a_{\text{obs}}) \} \}.
\end{aligned}
$$

Relational Evidence Propagation, Step 1 (continued)

(1) holds because of the second axiom a discrete possibility measure has to satisfy.

(3) holds because of the fact that the relation R_{ABC} can be decomposed w.r.t. the set $\mathcal{M} = \{\{A, B\}, \{B, C\}\}$.

(2) holds, since in the first place

$$R(A = a, B = b, C = c \,|\, A = a_{obs}) = R(A = a, B = b, C = c, A = a_{obs}) = \begin{cases} R(A = a, B = b, C = c), & \text{if } a = a_{\text{obs}}, \\ 0, & \text{otherwise,} \end{cases}$$

and secondly

$$R(A = a \mid A = a_{\text{obs}}) = R(A = a, A = a_{\text{obs}}) = \begin{cases} R(A = a), & \text{if } a = a_{\text{obs}}, \\ 0, & \text{otherwise,} \end{cases}$$

and therefore, since trivially $R(A = a) \geq R(A = a, B = b, C = c)$,

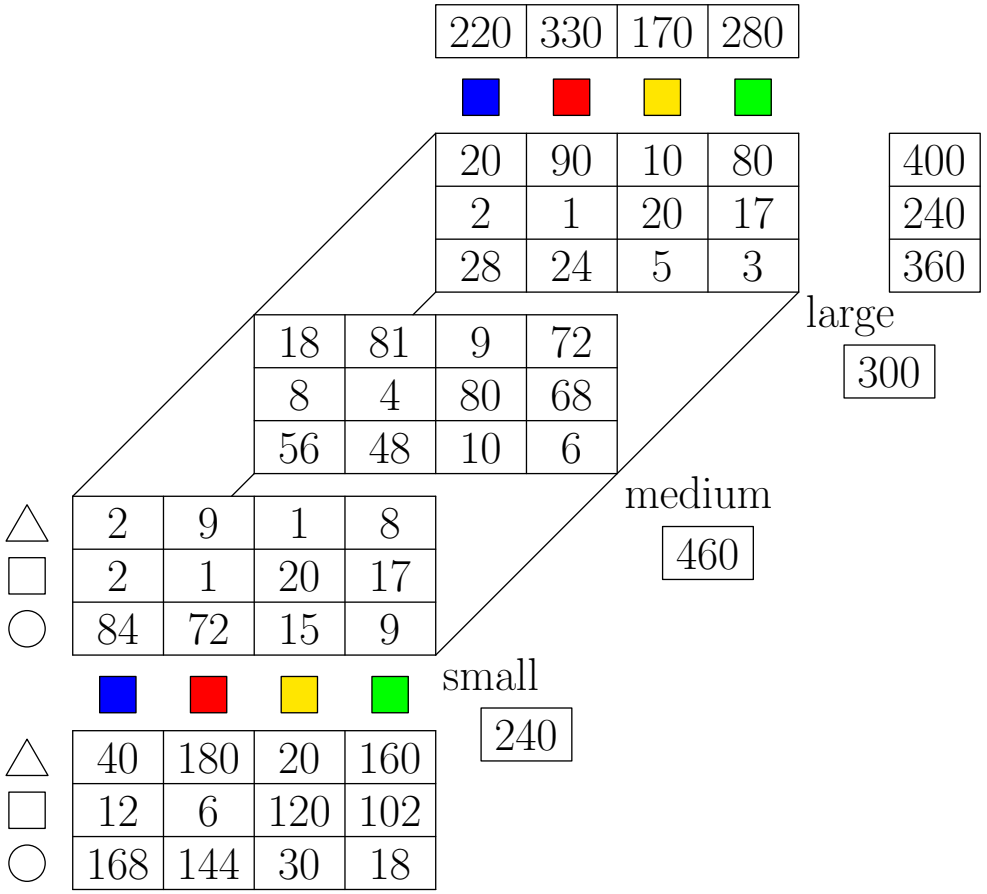
$$R(A = a, B = b, C = c \mid A = a_{obs}) = \min\{R(A = a, B = b, C = c), R(A = a \mid A = a_{\text{obs}})\}.$$

Relational Evidence Propagation, Step 2

$$
\begin{aligned}
& R(C = c \mid A = a_{\text{obs}}) \\
&= R\Big(\bigvee_{a \in \text{dom}(A)} A = a, \bigvee_{b \in \text{dom}(B)} B = b, C = c \,\Big|\, A = a_{\text{obs}} \Big) \\
&\overset{(1)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{b \in \text{dom}(B)} \{ R(A = a, B = b, C = c \mid A = a_{\text{obs}}) \} \Big\} \\
&\overset{(2)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{b \in \text{dom}(B)} \{ \min\{ R(A = a, B = b, C = c), R(A = a \mid A = a_{\text{obs}}) \} \} \Big\} \\
&\overset{(3)}{=} \max_{a \in \text{dom}(A)} \Big\{ \max_{b \in \text{dom}(B)} \{ \min\{ R(A = a, B = b), R(B = b, C = c), \\
&\qquad\qquad R(A = a \mid A = a_{\text{obs}}) \} \} \Big\} \\
&= \max_{b \in \text{dom}(B)} \{ \min\{ R(B = b, C = c), \\
&\qquad \underbrace{\max_{a \in \text{dom}(A)} \{ \min\{ R(A = a, B = b), R(A = a \mid A = a_{\text{obs}}) \} \}}_{= R(B = b \mid A = a_{\text{obs}})} \} \\
&= \max_{b \in \text{dom}(B)} \{ \min\{ R(B = b, C = c), R(B = b \mid A = a_{\text{obs}}) \} \}.
\end{aligned}
$$

A Simple Example:
The Probabilistic Case

A Probability Distribution



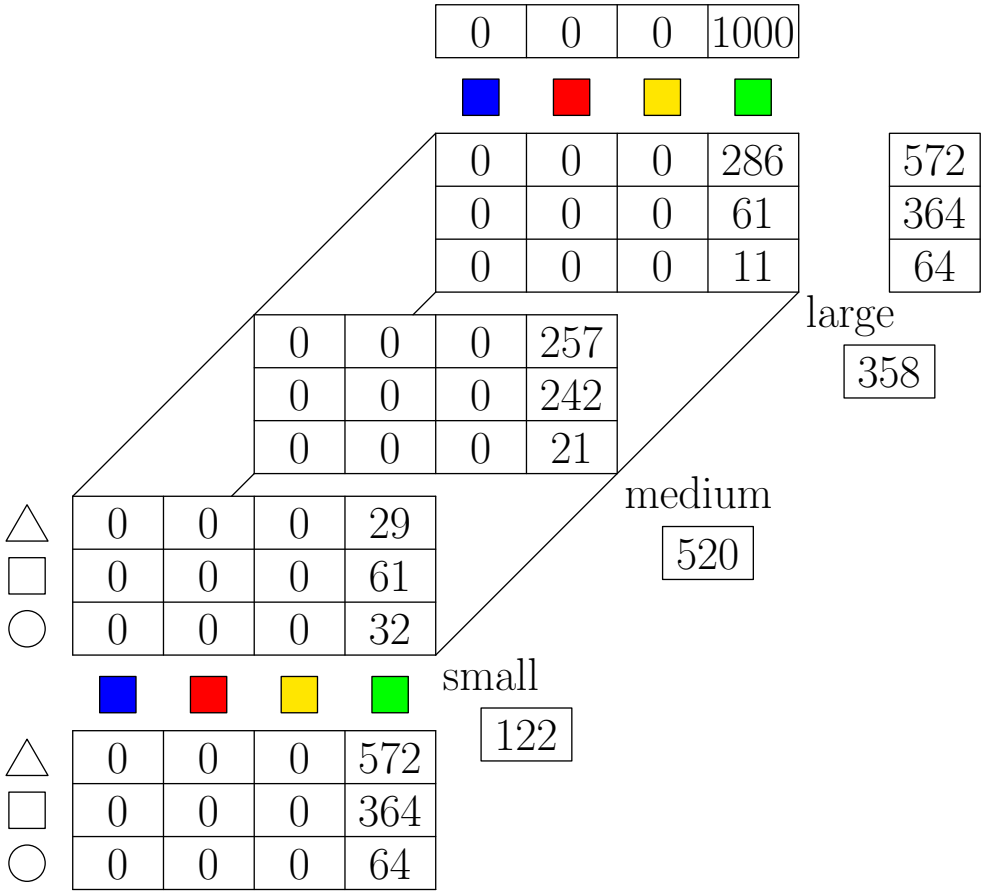
all numbers in
parts per 1000

	s	m	l
△	20	180	200
□	40	160	40
○	180	120	60

large	50	115	35	100
medium	82	133	99	146
small	88	82	36	34

The numbers state the probability of the corresponding value combination.
Compared to the example relation, the possible combinations are now frequent.

Reasoning: Computing Conditional Probabilities



all numbers in parts per 1000

	s	m	l
△	29	257	286
□	61	242	61
○	32	21	11

large	0	0	0	358
medium	0	0	0	531
small	0	0	0	111

Using the information that the given object is green:
The observed color has a posterior probability of 1.

Probabilistic Decomposition: Simple Example

- As for relational graphical models, the three-dimensional probability distribution can be decomposed into projections to subspaces, namely the marginal distribution on the subspace spanned by color and shape and the marginal distribution on the subspace spanned by shape and size.
- The original probability distribution can be reconstructed from the marginal distributions using the following formulae $\forall i, j, k$:

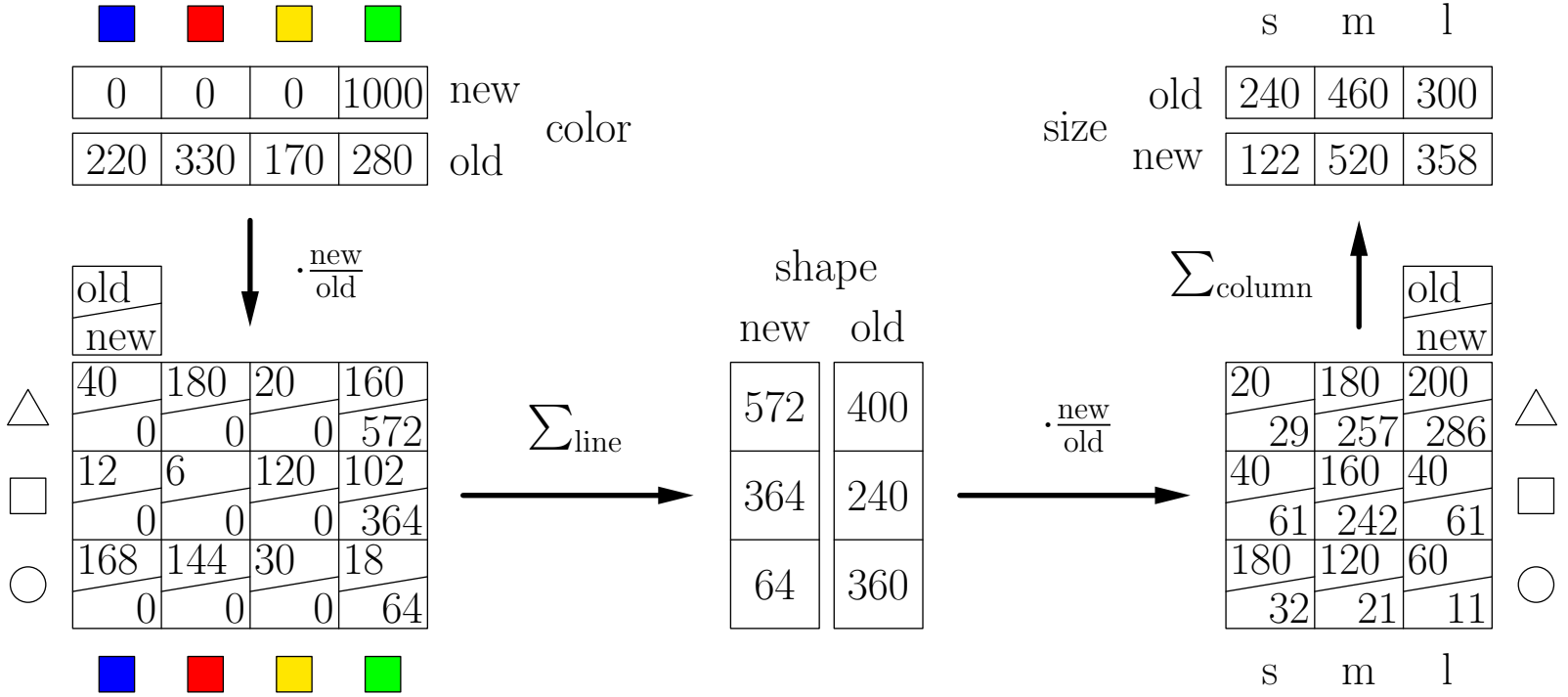
$$\begin{aligned} P\Big(a_i^{(\text{color})}, a_j^{(\text{shape})}, a_k^{(\text{size})}\Big) &= P\Big(a_i^{(\text{color})}, a_j^{(\text{shape})}\Big) \cdot P\Big(a_k^{(\text{size})} \;\Big|\; a_j^{(\text{shape})}\Big) \\ &= \frac{P\Big(a_i^{(\text{color})}, a_j^{(\text{shape})}\Big) \cdot P\Big(a_j^{(\text{shape})}, a_k^{(\text{size})}\Big)}{P\Big(a_j^{(\text{shape})}\Big)} \end{aligned}$$

- These equations express the *conditional independence* of attributes *color* and *size* given the attribute *shape*, since they only hold if $\forall i, j, k$:

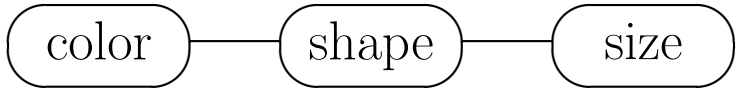
$$P\Big(a_k^{(\text{size})} \;\Big|\; a_j^{(\text{shape})}\Big) = P\Big(a_k^{(\text{size})} \;\Big|\; a_i^{(\text{color})}, a_j^{(\text{shape})}\Big)$$

Reasoning with Projections

Again the same result can be obtained using only projections to subspaces (marginal probability distributions):



This justifies a graph representation:



Probabilistic Graphical Models: Formalization

Probabilistic Decomposition

Definition: Let $U = \{A_1, \ldots, A_n\}$ be a set of attributes and p_U a probability distribution over U. Furthermore, let $\mathcal{M} = \{M_1, \ldots, M_m\} \subseteq 2^U$ be a set of nonempty (but not necessarily disjoint) subsets of U satisfying

$$\bigcup_{M \in \mathcal{M}} M = U.$$

p_U is called **decomposable** or **factorizable** w.r.t. $\mathcal{M}$ iff it can be written as a product of m nonnegative functions $\phi_M : \mathcal{E}_M \to \mathbb{R}_0^+$, $M \in \mathcal{M}$, i.e., iff

$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$p_U\Big(\bigwedge_{A_i \in U} A_i = a_i\Big) = \prod_{M \in \mathcal{M}} \phi_M\Big(\bigwedge_{A_i \in M} A_i = a_i\Big).$$

If p_U is decomposable w.r.t. $\mathcal{M}$ the set of functions

$$\Phi_{\mathcal{M}} = \{\phi_{M_1}, \ldots, \phi_{M_m}\} = \{\phi_M \mid M \in \mathcal{M}\}$$

is called the **decomposition** or the **factorization** of p_U. The functions in $\Phi_{\mathcal{M}}$ are called the **factor potentials** of p_U.

Conditional Independence

Definition: Let Ω be a (finite) sample space, P a probability measure on Ω, and A, B, and C attributes with respective domains $\mathrm{dom}(A)$, $\mathrm{dom}(B)$, and $\mathrm{dom}(C)$. A and B are called **conditionally probabilistically independent** given C, written $A \perp\!\!\!\perp_P B \mid C$, iff

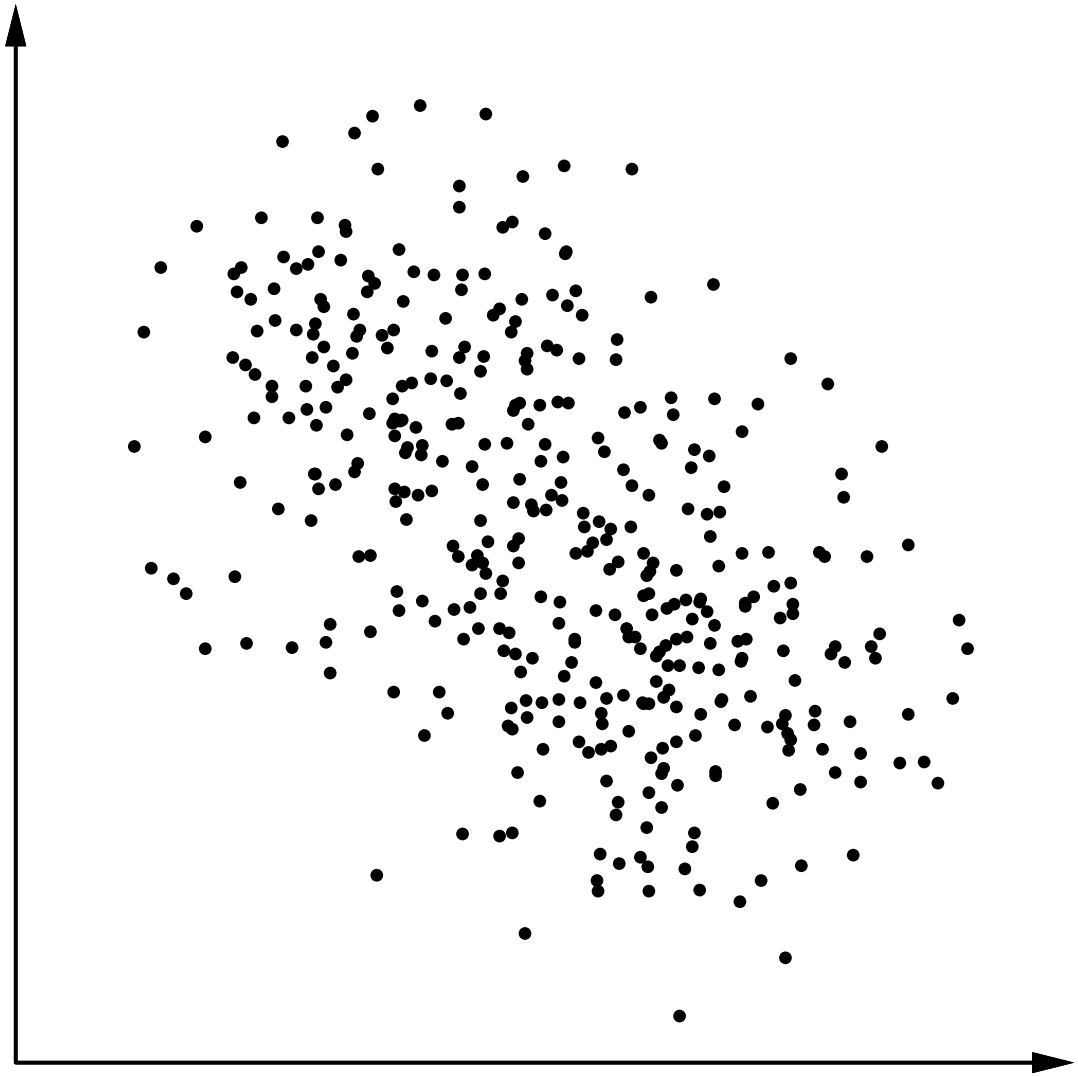
$$\forall a \in \mathrm{dom}(A) : \forall b \in \mathrm{dom}(B) : \forall c \in \mathrm{dom}(C) :$$
$$P(A = a, B = b \mid C = c) = P(A = a \mid C = c) \cdot P(B = b \mid C = c)$$

Equivalent formula:

$$\forall a \in \mathrm{dom}(A) : \forall b \in \mathrm{dom}(B) : \forall c \in \mathrm{dom}(C) :$$
$$P(A = a \mid B = b, C = c) = P(A = a \mid C = c)$$

- Conditional independences make it possible to consider parts of a probability distribution independent of others.
- Therefore it is plausible that a set of conditional independences may enable a decomposition of a joint probability distribution.

Conditional Independence: An Example



Dependence (fictitious) between smoking and life expectancy.

Each dot represents one person.

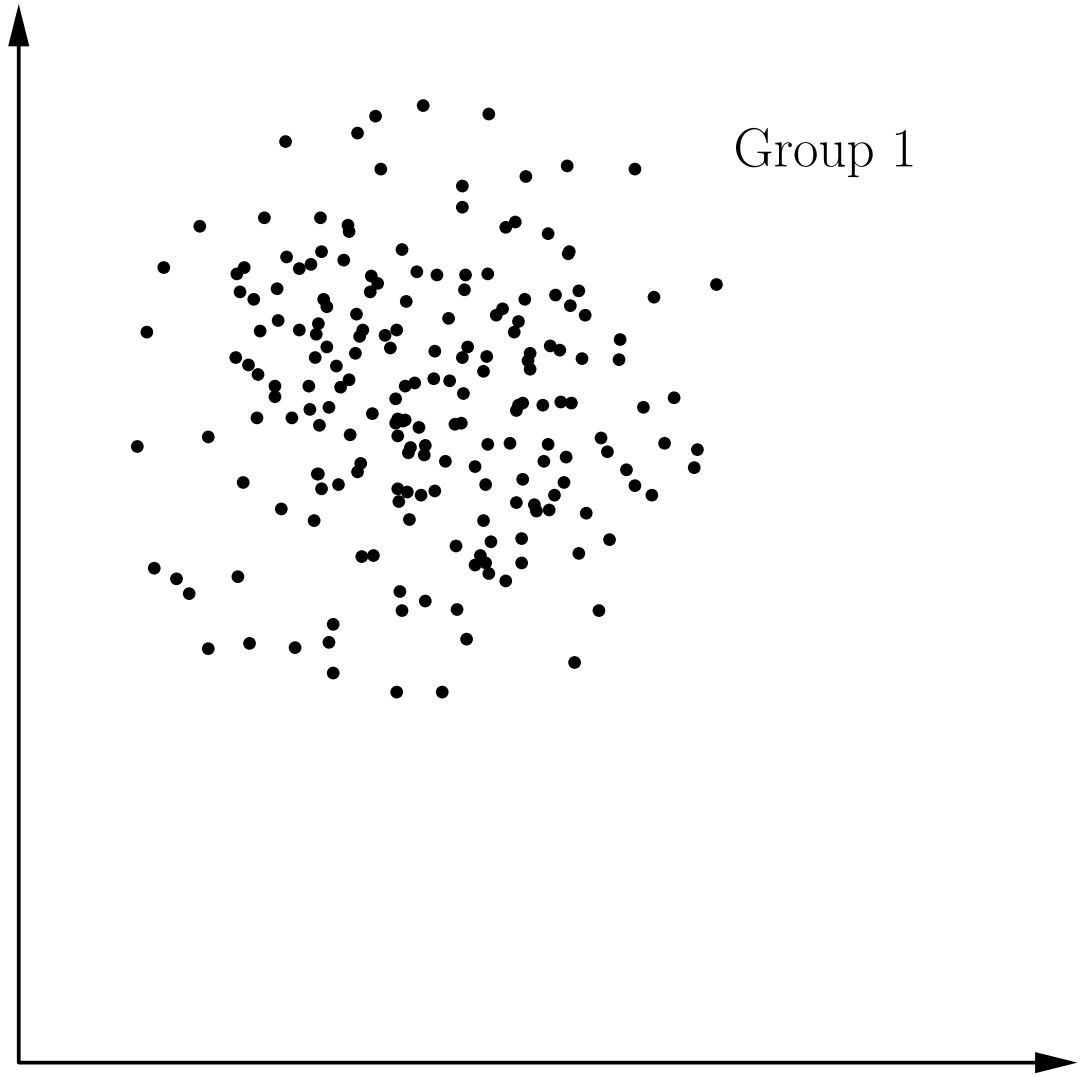
x-axis: age at death
y-axis: average number of cigarettes per day

Weak, but clear dependence:

The more cigarettes are smoked, the lower the life expectancy.

(Note that this data is artificial and thus should not be seen as revealing an actual dependence.)

Conditional Independence: An Example



Conjectured explanation:

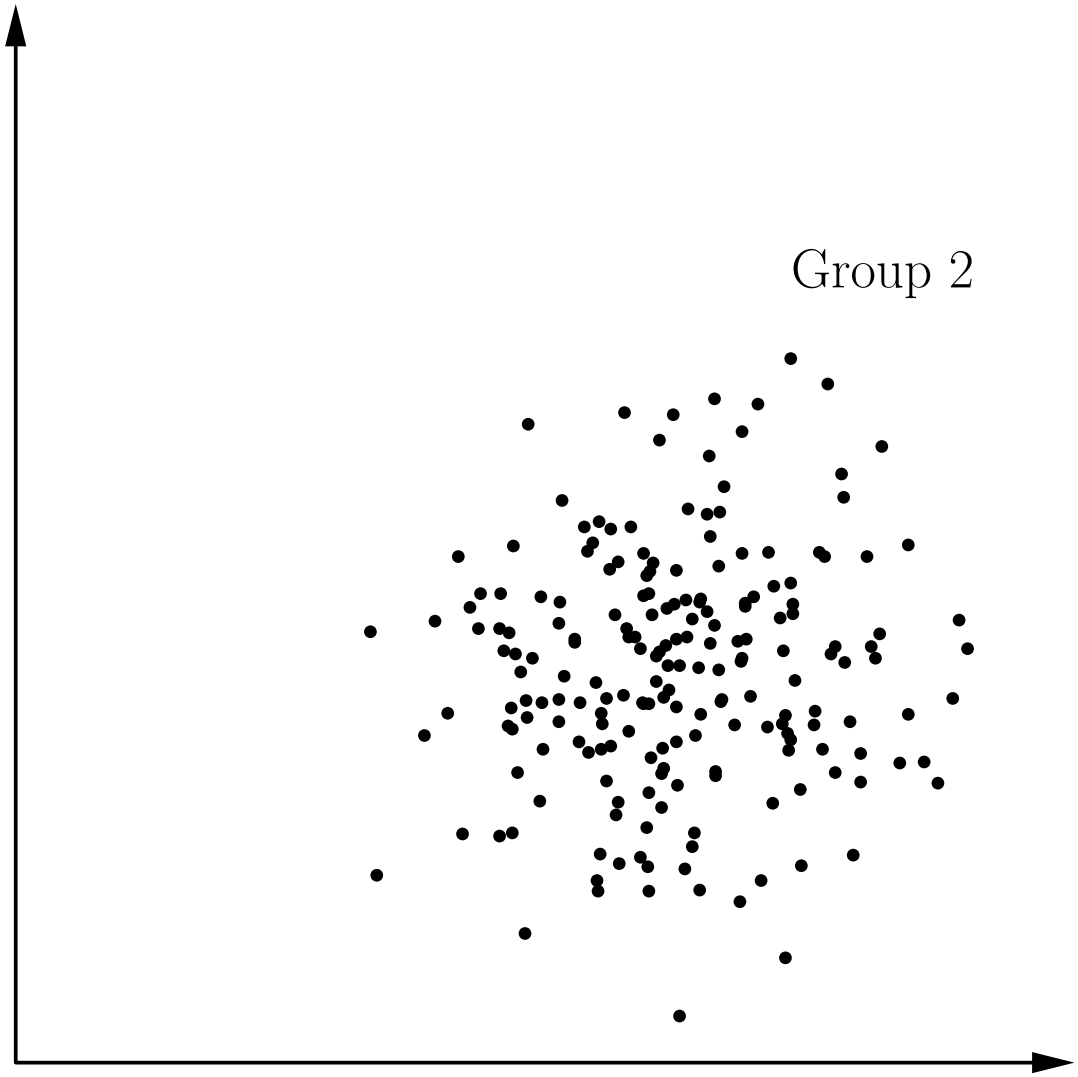
There is a common cause, namely whether the person is exposed to stress at work.

If this were correct, splitting the data should remove the dependence.

Group 1:
exposed to stress at work

(Note that this data is artificial and therefore should not be seen as an argument against health hazards caused by smoking.)

Conditional Independence: An Example



Conjectured explanation:

There is a common cause, namely whether the person is exposed to stress at work.

If this were correct, splitting the data should remove the dependence.

Group 2:
not exposed to stress at work

(Note that this data is artificial and therefore should not be seen as an argument against health hazards caused by smoking.)

Probabilistic Decomposition (continued)

Chain Rule of Probability:

$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$P\Big(\bigwedge_{i=1}^{n} A_i = a_i\Big) = \prod_{i=1}^{n} P\Big(A_i = a_i \,\Big|\, \bigwedge_{j=1}^{i-1} A_j = a_j\Big)$$

- The chain rule of probability is valid in general (or at least for strictly positive distributions).

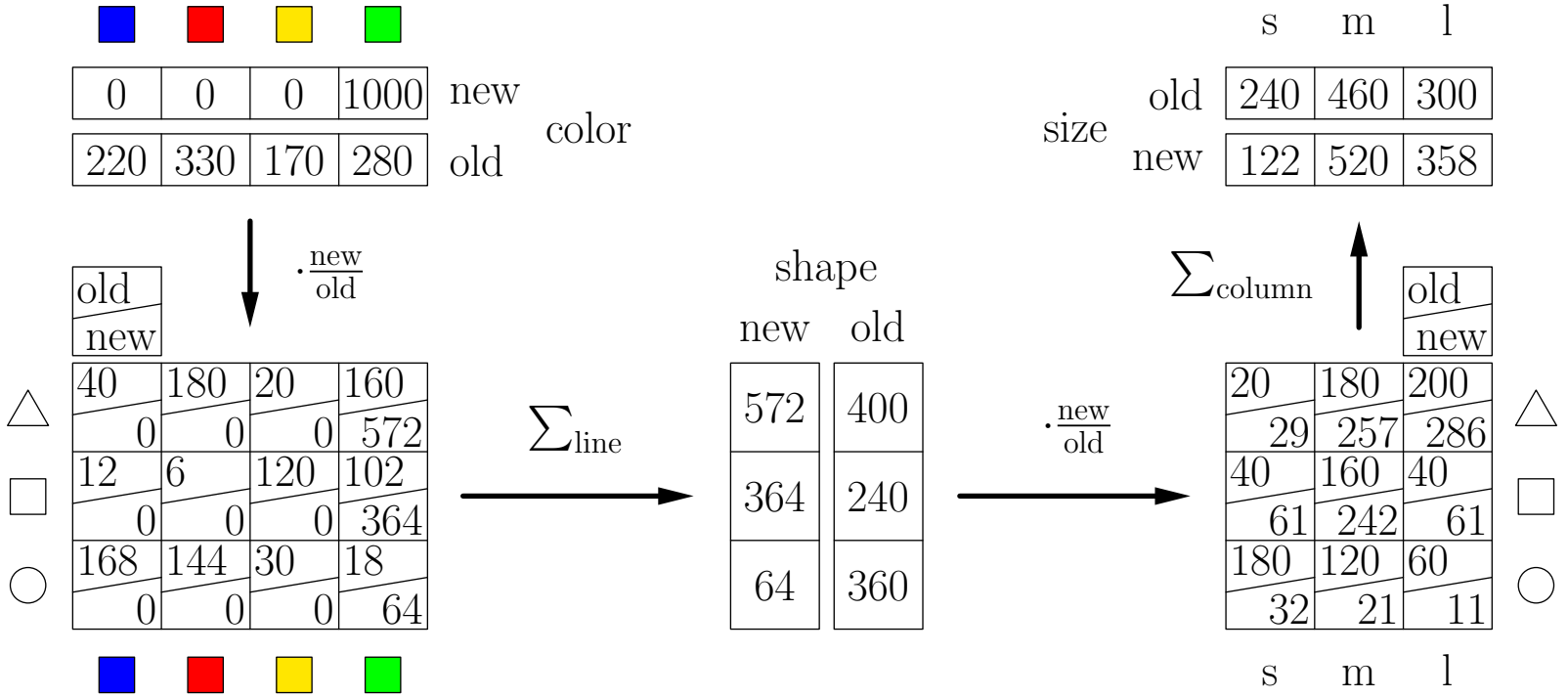
Chain Rule Factorization:

$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$P\Big(\bigwedge_{i=1}^{n} A_i = a_i\Big) = \prod_{i=1}^{n} P\Big(A_i = a_i \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_i)} A_j = a_j\Big)$$

- Conditional independence statements are used to "cancel" conditions.

Reasoning with Projections

Due to the fact that color and size are conditionally independent given the shape, the reasoning result can be obtained using only the projections to the subspaces:



This reasoning scheme can be formally justified with probability measures.

Probabilistic Evidence Propagation, Step 1

$$
\begin{aligned}
&P(B = b \mid A = a_{\text{obs}}) \\
&= P\Big(\bigvee_{a \in \text{dom}(A)} A = a, B = b, \bigvee_{c \in \text{dom}(C)} C = c \,\Big|\, A = a_{\text{obs}} \Big) \\
&\overset{(1)}{=} \sum_{a \in \text{dom}(A)} \sum_{c \in \text{dom}(C)} P(A = a, B = b, C = c \mid A = a_{\text{obs}}) \\
&\overset{(2)}{=} \sum_{a \in \text{dom}(A)} \sum_{c \in \text{dom}(C)} P(A = a, B = b, C = c) \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)} \\
&\overset{(3)}{=} \sum_{a \in \text{dom}(A)} \sum_{c \in \text{dom}(C)} \frac{P(A = a, B = b) P(B = b, C = c)}{P(B = b)} \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)} \\
&= \sum_{a \in \text{dom}(A)} P(A = a, B = b) \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)} \underbrace{\sum_{c \in \text{dom}(C)} P(C = c \mid B = b)}_{=1} \\
&= \sum_{a \in \text{dom}(A)} P(A = a, B = b) \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)}.
\end{aligned}
$$

Probabilistic Evidence Propagation, Step 1 (continued)

(1) holds because of Kolmogorov's axioms.

(3) holds because of the fact that the distribution p_{ABC} can be decomposed w.r.t. the set $\mathcal{M} = \{\{A, B\}, \{B, C\}\}$.

(2) holds, since in the first place

$$P(A = a, B = b, C = c \,|\, A = a_{obs}) = \frac{P(A = a, B = b, C = c, A = a_{obs})}{P(A = a_{\text{obs}})}$$

$$= \begin{cases} \dfrac{P(A = a, B = b, C = c)}{P(A = a_{\text{obs}})}, & \text{if } a = a_{\text{obs}}, \\ 0, & \text{otherwise,} \end{cases}$$

and secondly

$$P(A = a, A = a_{\text{obs}}) = \begin{cases} P(A = a), & \text{if } a = a_{\text{obs}}, \\ 0, & \text{otherwise,} \end{cases}$$

and therefore

$$P(A = a, B = b, C = c \mid A = a_{obs})$$

$$= P(A = a, B = b, C = c) \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)}.$$

Probabilistic Evidence Propagation, Step 2

$$
\begin{aligned}
&P(C = c \mid A = a_{\text{obs}}) \\
&= P\Big(\bigvee_{a \in \text{dom}(A)} A = a, \bigvee_{b \in \text{dom}(B)} B = b, C = c \,\Big|\, A = a_{\text{obs}} \Big) \\
&\overset{(1)}{=} \sum_{a \in \text{dom}(A)} \sum_{b \in \text{dom}(B)} P(A = a, B = b, C = c \mid A = a_{\text{obs}}) \\
&\overset{(2)}{=} \sum_{a \in \text{dom}(A)} \sum_{b \in \text{dom}(B)} P(A = a, B = b, C = c) \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)} \\
&\overset{(3)}{=} \sum_{a \in \text{dom}(A)} \sum_{b \in \text{dom}(B)} \frac{P(A = a, B = b) P(B = b, C = c)}{P(B = b)} \cdot \frac{P(A = a \mid A = a_{\text{obs}})}{P(A = a)} \\
&= \sum_{b \in \text{dom}(B)} \frac{P(B = b, C = c)}{P(B = b)} \underbrace{\sum_{a \in \text{dom}(A)} P(A = a, B = b) \cdot \frac{R(A = a \mid A = a_{\text{obs}})}{P(A = a)}}_{= P(B = b \mid A = a_{\text{obs}})} \\
&= \sum_{b \in \text{dom}(B)} P(B = b, C = c) \cdot \frac{P(B = b \mid A = a_{\text{obs}})}{P(B = b)}.
\end{aligned}
$$

Graphical Models:
The General Theory

(Semi-)Graphoid Axioms

Definition: Let V be a set of (mathematical) objects and $(\cdot \perp\!\!\!\perp \cdot \mid \cdot)$ a three-place relation of subsets of V. Furthermore, let W, X, Y, and Z be four disjoint subsets of V. The four statements

symmetry: $(X \perp\!\!\!\perp Y \mid Z) \Rightarrow (Y \perp\!\!\!\perp X \mid Z)$

decomposition: $(W \cup X \perp\!\!\!\perp Y \mid Z) \Rightarrow (W \perp\!\!\!\perp Y \mid Z) \wedge (X \perp\!\!\!\perp Y \mid Z)$

weak union: $(W \cup X \perp\!\!\!\perp Y \mid Z) \Rightarrow (X \perp\!\!\!\perp Y \mid Z \cup W)$

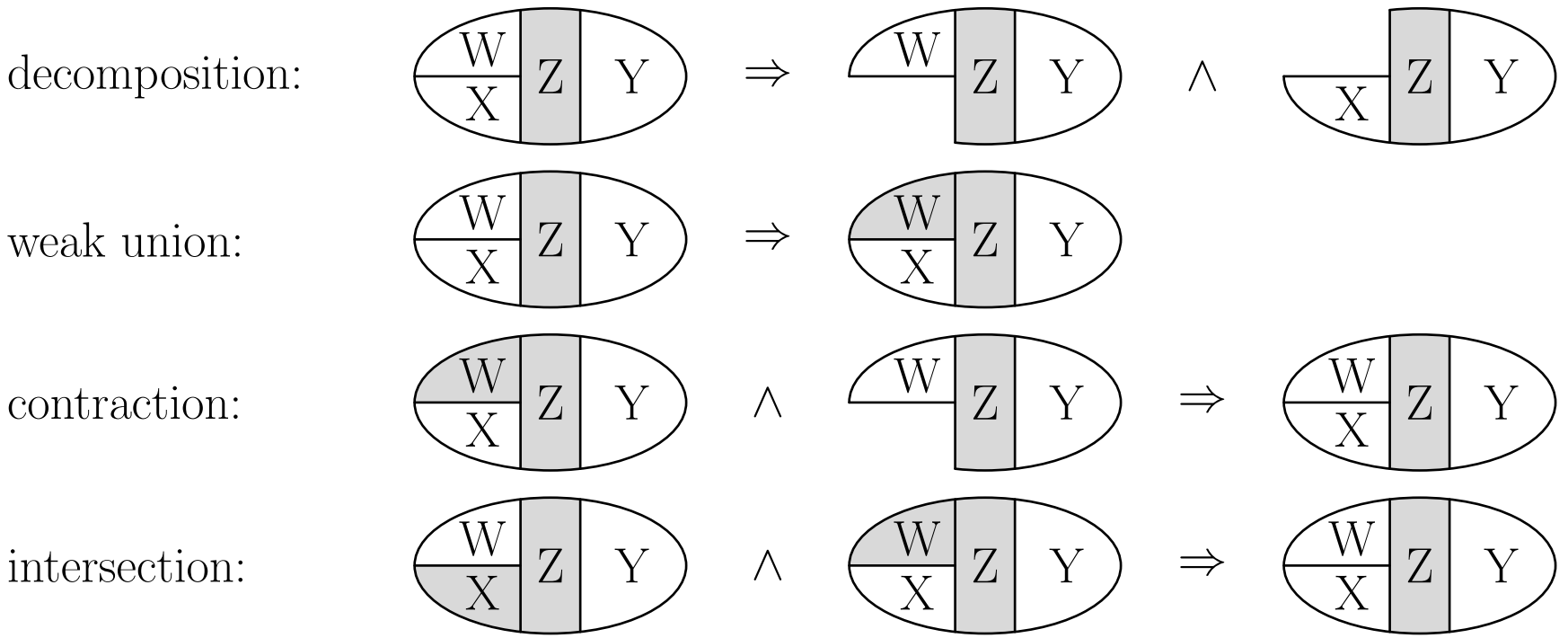
contraction: $(X \perp\!\!\!\perp Y \mid Z \cup W) \wedge (W \perp\!\!\!\perp Y \mid Z) \Rightarrow (W \cup X \perp\!\!\!\perp Y \mid Z)$

are called the **semi-graphoid axioms**. A three-place relation $(\cdot \perp\!\!\!\perp \cdot \mid \cdot)$ that satisfies the semi-graphoid axioms for all W, X, Y, and Z is called a **semi-graphoid**. The above four statements together with

intersection: $(W \perp\!\!\!\perp Y \mid Z \cup X) \wedge (X \perp\!\!\!\perp Y \mid Z \cup W) \Rightarrow (W \cup X \perp\!\!\!\perp Y \mid Z)$

are called the **graphoid axioms**. A three-place relation $(\cdot \perp\!\!\!\perp \cdot \mid \cdot)$ that satisfies the graphoid axioms for all W, X, Y, and Z is called a **graphoid**.

Illustration of the (Semi-)Graphoid Axioms



- Similar to the properties of **separation in graphs**.
- **Idea:** Represent conditional independence by separation in graphs.

Separation in Graphs

Definition: Let $G = (V, E)$ be an undirected graph and X, Y, and Z three disjoint subsets of nodes. Z **u-separates** X and Y in G, written $\langle X \mid Z \mid Y \rangle_G$, iff all paths from a node in X to a node in Y contain a node in Z. A path that contains a node in Z is called **blocked** (by Z), otherwise it is called **active**.

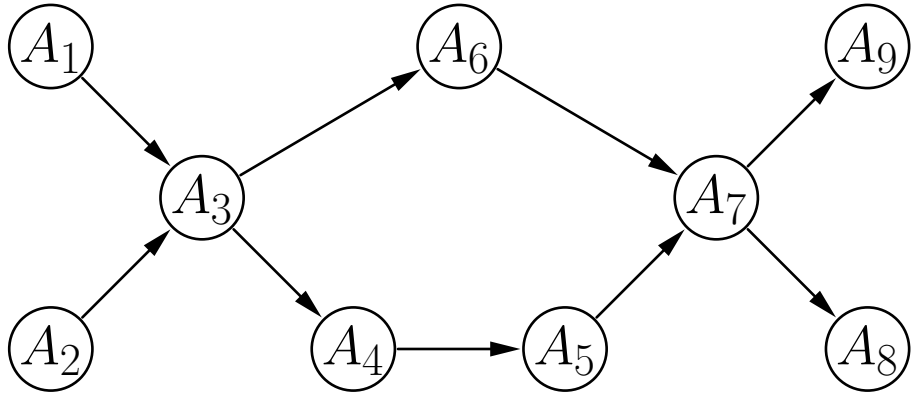
Definition: Let $\vec{G} = (V, \vec{E})$ be a directed acyclic graph and X, Y, and Z three disjoint subsets of nodes. Z **d-separates** X and Y in $\vec{G}$, written $\langle X \mid Z \mid Y \rangle_{\vec{G}}$, iff there is *no* path from a node in X to a node in Y along which the following two conditions hold:

1. every node with converging edges either is in Z or has a descendant in Z,
2. every other node is not in Z.

A path satisfying the two conditions above is said to be **active**,
otherwise it is said to be **blocked** (by Z).

Separation in Directed Acyclic Graphs

Example Graph:



Valid Separations:

$\langle \{A_1\} \mid \{A_3\} \mid \{A_4\} \rangle$

$\langle \{A_3\} \mid \{A_4, A_6\} \mid \{A_7\} \rangle$

$\langle \{A_8\} \mid \{A_7\} \mid \{A_9\} \rangle$

$\langle \{A_1\} \mid \emptyset \mid \{A_2\} \rangle$

Invalid Separations:

$\langle \{A_1\} \mid \{A_4\} \mid \{A_2\} \rangle$

$\langle \{A_4\} \mid \{A_3, A_7\} \mid \{A_6\} \rangle$

$\langle \{A_1\} \mid \{A_6\} \mid \{A_7\} \rangle$

$\langle \{A_1\} \mid \{A_4, A_9\} \mid \{A_5\} \rangle$

Conditional (In)Dependence Graphs

Definition: Let $(\cdot \perp\!\!\!\perp_\delta \cdot \mid \cdot)$ be a three-place relation representing the set of conditional independence statements that hold in a given distribution δ over a set U of attributes. An undirected graph $G = (U, E)$ over U is called a **conditional dependence graph** or a **dependence map** w.r.t. δ, iff for all disjoint subsets $X, Y, Z \subseteq U$ of attributes

$$X \perp\!\!\!\perp_\delta Y \mid Z \;\Rightarrow\; \langle X \mid Z \mid Y \rangle_G,$$

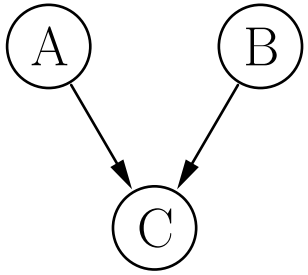
i.e., if G captures by u-separation all (conditional) independences that hold in δ and thus represents only valid (conditional) dependences. Similarly, G is called a **conditional independence graph** or an **independence map** w.r.t. δ, iff for all disjoint subsets $X, Y, Z \subseteq U$ of attributes

$$\langle X \mid Z \mid Y \rangle_G \;\Rightarrow\; X \perp\!\!\!\perp_\delta Y \mid Z,$$

i.e., if G captures by u-separation only (conditional) independences that are valid in δ. G is said to be a **perfect map** of the conditional (in)dependences in δ, if it is both a dependence map and an independence map.

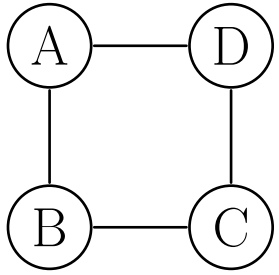
Limitations of Graph Representations

Perfect directed map, no perfect undirected map:



p_{ABC}		$A = a_1$		$A = a_2$	
		$B = b_1$	$B = b_2$	$B = b_1$	$B = b_2$
$C = c_1$		$4/24$	$3/24$	$3/24$	$2/24$
$C = c_2$		$2/24$	$3/24$	$3/24$	$4/24$

Perfect undirected map, no perfect directed map:



p_{ABCD}		$A = a_1$		$A = a_2$	
		$B = b_1$	$B = b_2$	$B = b_1$	$B = b_2$
$C = c_1$	$D = d_1$	$1/47$	$1/47$	$1/47$	$2/47$
	$D = d_2$	$1/47$	$1/47$	$2/47$	$4/47$
$C = c_2$	$D = d_1$	$1/47$	$2/47$	$1/47$	$4/47$
	$D = d_2$	$2/47$	$4/47$	$4/47$	$16/47$

Markov Properties of Undirected Graphs

Definition: An undirected graph $G = (U, E)$ over a set U of attributes is said to have (w.r.t. a distribution δ) the
pairwise Markov property,
iff in δ any pair of attributes which are nonadjacent in the graph are conditionally independent given all remaining attributes, i.e., iff

$$\forall A, B \in U, A \neq B: \quad (A, B) \notin E \;\Rightarrow\; A \perp\!\!\!\perp_\delta B \mid U - \{A, B\},$$

local Markov property,
iff in δ any attribute is conditionally independent of all remaining attributes given its neighbors, i.e., iff

$$\forall A \in U: \quad A \perp\!\!\!\perp_\delta U - \text{closure}(A) \mid \text{boundary}(A),$$

global Markov property,
iff in δ any two sets of attributes which are u-separated by a third are conditionally independent given the attributes in the third set, i.e., iff

$$\forall X, Y, Z \subseteq U: \quad \langle X \mid Z \mid Y \rangle_G \;\Rightarrow\; X \perp\!\!\!\perp_\delta Y \mid Z.$$

Markov Properties of Directed Acyclic Graphs

Definition: A directed acyclic graph $\vec{G} = (U, \vec{E})$ over a set U of attributes is said to have (w.r.t. a distribution δ) the
pairwise Markov property,
iff in δ any attribute is conditionally independent of any non-descendant not among its parents given all remaining non-descendants, i.e., iff

$$\forall A, B \in U: \; B \in \text{nondescs}(A) - \text{parents}(A) \;\Rightarrow\; A \perp\!\!\!\perp_\delta B \mid \text{nondescs}(A) - \{B\},$$

local Markov property,
iff in δ any attribute is conditionally independent of all remaining non-descendants given its parents, i.e., iff

$$\forall A \in U: \quad A \perp\!\!\!\perp_\delta \text{nondescs}(A) - \text{parents}(A) \mid \text{parents}(A),$$

global Markov property,
iff in δ any two sets of attributes which are d-separated by a third are conditionally independent given the attributes in the third set, i.e., iff

$$\forall X, Y, Z \subseteq U: \quad \langle X \mid Z \mid Y \rangle_{\vec{G}} \;\Rightarrow\; X \perp\!\!\!\perp_\delta Y \mid Z.$$

Equivalence of Markov Properties

Theorem: If a three-place relation $(\cdot \perp\!\!\!\perp_\delta \cdot \mid \cdot)$ representing the set of conditional independence statements that hold in a given joint distribution δ over a set U of attributes satisfies the graphoid axioms, then the pairwise, the local, and the global Markov property of an undirected graph $G = (U, E)$ over U are equivalent.

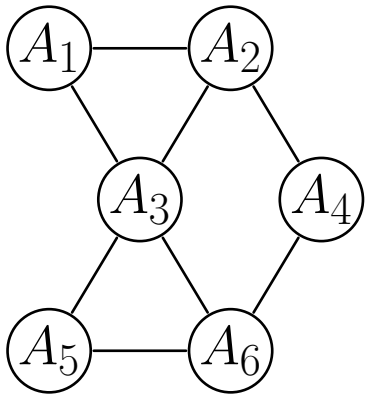
Theorem: If a three-place relation $(\cdot \perp\!\!\!\perp_\delta \cdot \mid \cdot)$ representing the set of conditional independence statements that hold in a given joint distribution δ over a set U of attributes satisfies the semi-graphoid axioms, then the local and the global Markov property of a directed acyclic graph $\vec{G} = (U, \vec{E})$ over U are equivalent.

If $(\cdot \perp\!\!\!\perp_\delta \cdot \mid \cdot)$ satisfies the graphoid axioms, then the pairwise, the local, and the global Markov property are equivalent.

Undirected Graphs and Decompositions

Definition: A probability distribution p_V over a set V of variables is called **decomposable** or **factorizable w.r.t. an undirected graph** $G = (V, E)$ over V iff it can be written as a product of nonnegative functions on the maximal cliques of G. That is, let $\mathcal{M}$ be a family of subsets of variables, such that the subgraphs of G induced by the sets $M \in \mathcal{M}$ are the maximal cliques of G. Then there exist functions $\phi_M : \mathcal{E}_M \to \mathbb{R}_0^+$, $M \in \mathcal{M}$, $\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n)$:

$$p_V\Big(\bigwedge_{A_i \in V} A_i = a_i\Big) = \prod_{M \in \mathcal{M}} \phi_M\Big(\bigwedge_{A_i \in M} A_i = a_i\Big).$$

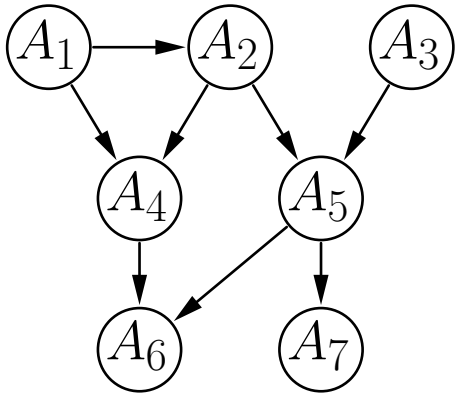


$$\begin{aligned} & p_V(A_1 = a_1, \ldots, A_6 = a_6) \\ = \;& \phi_{A_1A_2A_3}(A_1 = a_1, A_2 = a_2, A_3 = a_3) \\ \cdot \;& \phi_{A_3A_5A_6}(A_3 = a_3, A_5 = a_5, A_6 = a_6) \\ \cdot \;& \phi_{A_2A_4}(A_2 = a_2, A_4 = a_4) \\ \cdot \;& \phi_{A_4A_6}(A_4 = a_4, A_6 = a_6). \end{aligned}$$

Directed Acyclic Graphs and Decompositions

Definition: A probability distribution p_U over a set U of attributes is called **decomposable** or **factorizable w.r.t. a directed acyclic graph** $\vec{G} = (U, \vec{E})$ over U, iff it can be written as a product of the conditional probabilities of the attributes given their parents in $\vec{G}$, i.e., iff

$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$p_U\Big(\bigwedge_{A_i \in U} A_i = a_i\Big) = \prod_{A_i \in U} P\Big(A_i = a_i \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}_{\vec{G}}(A_i)} A_j = a_j\Big).$$



$$\begin{aligned}
&P(A_1 = a_1, \ldots, A_7 = a_7) \\
&= \; P(A_1 = a_1) \cdot P(A_2 = a_2 \mid A_1 = a_1) \cdot P(A_3 = a_3) \\
&\cdot \; P(A_4 = a_4 \mid A_1 = a_1, A_2 = a_2) \\
&\cdot \; P(A_5 = a_5 \mid A_2 = a_2, A_3 = a_3) \\
&\cdot \; P(A_6 = a_6 \mid A_4 = a_4, A_5 = a_5) \\
&\cdot \; P(A_7 = a_7 \mid A_5 = a_5).
\end{aligned}$$

Conditional Independence Graphs and Decompositions

Core Theorem of Graphical Models:
Let p_V be a strictly positive probability distribution on a set V of (discrete) variables. A directed or undirected graph $G = (V, E)$ is a conditional independence graph w.r.t. p_V if and only if p_V is factorizable w.r.t. G.

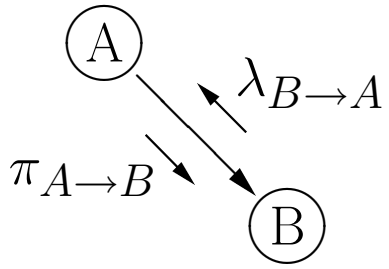
Definition: A **Markov network** is an undirected conditional independence graph of a probability distribution p_V together with the family of positive functions ϕ_M of the factorization induced by the graph.

Definition: A **Bayesian network** is a directed conditional independence graph of a probability distribution p_U together with the family of conditional probabilities of the factorization induced by the graph.

- Sometimes the conditional independence graph is required to be minimal.
- For correct evidence propagation it is not required that the graph is minimal. Evidence propagation may just be less efficient than possible.

Probabilistic Graphical Models: Evidence Propagation in Polytrees

Evidence Propagation in Polytrees



Idea: Node processors communicating by message passing: π-messages are sent from parent to child and λ-messages are sent from child to parent.

Derivation of the Propagation Formulae

Computation of Marginal Distribution:

$$P(A_g = a_g) \;=\; \sum_{\substack{\forall A_i \in U - \{A_g\}: \\ a_i \in \mathrm{dom}(A_i)}} P\Big(\bigwedge_{A_j \in U} A_j = a_j \Big)$$

Chain Rule Factorization w.r.t. the Polytree:

$$P(A_g = a_g) \;=\; \sum_{\substack{\forall A_i \in U - \{A_g\}: \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j \Big)$$

Evidence Propagation in Polytrees (continued)

Decomposition w.r.t. Subgraphs:

$$P(A_g = a_g) = \sum_{\substack{\forall A_i \in U - \{A_g\}: \\ a_i \in \mathrm{dom}(A_i)}} \Big(P\Big(A_g = a_g \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_g)} A_j = a_j\Big) \cdot \prod_{A_k \in U_+(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big) \cdot \prod_{A_k \in U_-(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big).$$

Attribute sets underlying subgraphs:

$$U_B^A(C) = \{C\} \cup \{D \in U \mid D \underset{\vec{G}'}{\approx} C, \vec{G}' = (U, E - \{(A,B)\})\},$$

$$U_+(A) = \bigcup_{C \in \mathrm{parents}(A)} U_A^C(C), \qquad U_+(A,B) = \bigcup_{C \in \mathrm{parents}(A) - \{B\}} U_A^C(C),$$

$$U_-(A) = \bigcup_{C \in \mathrm{children}(A)} U_C^A(C), \qquad U_-(A,B) = \bigcup_{C \in \mathrm{children}(A) - \{B\}} U_A^C(C).$$

Evidence Propagation in Polytrees (continued)

Terms that are independent of a summation variable can be moved out of the corresponding sum. This yields a decomposition into two main factors:

$$
\begin{aligned}
P(A_g = a_g) \;=\; & \Bigg(\sum_{\substack{\forall A_i \in \text{parents}(A_g): \\ a_i \in \text{dom}(A_i)}} P\Big(A_g = a_g \,\Big|\, \bigwedge_{A_j \in \text{parents}(A_g)} A_j = a_j\Big) \\
& \cdot \Big[\sum_{\substack{\forall A_i \in U^*_+(A_g): \\ a_i \in \text{dom}(A_i)}} \prod_{A_k \in U_+(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \text{parents}(A_k)} A_j = a_j\Big)\Big]\Bigg) \\
& \cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_g): \\ a_i \in \text{dom}(A_i)}} \prod_{A_k \in U_-(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \text{parents}(A_k)} A_j = a_j\Big)\Big] \\
=\; & \pi(A_g = a_g) \cdot \lambda(A_g = a_g),
\end{aligned}
$$

where $U^*_+(A_g) = U_+(A_g) - \text{parents}(A_g)$.

Evidence Propagation in Polytrees (continued)

$$\sum_{\substack{\forall A_i \in U^*_+(A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_+(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)$$

$$= \prod_{A_p \in \mathrm{parents}(A_g)} \Bigg(\sum_{\substack{\forall A_i \in \mathrm{parents}(A_p): \\ a_i \in \mathrm{dom}(A_i)}} P\Big(A_p = a_p \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_p)} A_j = a_j\Big)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U^*_+(A_p): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_+(A_p)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big]\Bigg)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_p, A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_p, A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big]$$

$$= \prod_{A_p \in \mathrm{parents}(A_g)} \pi(A_p = a_p)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_p, A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_p, A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big]$$

Evidence Propagation in Polytrees (continued)

$$\sum_{\substack{\forall A_i \in U^*_+(A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_+(A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)$$

$$= \prod_{A_p \in \mathrm{parents}(A_g)} \pi(A_p = a_p)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_p, A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_p, A_g)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big]$$

$$= \prod_{A_p \in \mathrm{parents}(A_g)} \pi_{A_p \to A_g}(A_p = a_p)$$

$$\pi(A_g = a_g) = \sum_{\substack{\forall A_i \in \mathrm{parents}(A_g): \\ a_i \in \mathrm{dom}(A_i)}} P(A_g = a_g \,|\, \bigwedge_{A_j \in \mathrm{parents}(A_g)} A_j = a_j)$$

$$\cdot \prod_{A_p \in \mathrm{parents}(A_g)} \pi_{A_p \to A_g}(A_p = a_p)$$

Evidence Propagation in Polytrees (continued)

$$\lambda(A_g = a_g) = \sum_{\substack{\forall A_i \in U_-(A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_g)} P(A_k = a_k \,|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j)$$

$$= \prod_{A_c \in \mathrm{children}(A_g)} \sum_{a_c \in \mathrm{dom}(A_c)}$$

$$\Big(\sum_{\substack{\forall A_i \in \mathrm{parents}(A_c) - \{A_g\}: \\ a_i \in \mathrm{dom}(A_i)}} P(A_c = a_c \,|\, \bigwedge_{A_j \in \mathrm{parents}(A_c)} A_j = a_j)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U^*_+(A_c, A_g): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_+(A_c, A_g)} P(A_k = a_k \,|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j) \Big] \Big)$$

$$\cdot \underbrace{\Big[\sum_{\substack{\forall A_i \in U_-(A_c): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_c)} P(A_k = a_k \,|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j) \Big]}_{= \lambda(A_c = a_c)}$$

$$= \prod_{A_c \in \mathrm{children}(A_g)} \lambda_{A_c \to A_g}(A_g = a_g)$$

Propagation Formulae without Evidence

$$\pi_{A_p \to A_c}(A_p = a_p)$$

$$= \pi(A_p = a_p) \cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_p, A_c): \\ a_i \in \mathrm{dom}(A_i)}} \prod_{A_k \in U_-(A_p, A_c)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_k)} A_j = a_j\Big)\Big]$$

$$= \frac{P(A_p = a_p)}{\lambda_{A_c \to A_p}(A_p = a_p)}$$

$$\lambda_{A_c \to A_p}(A_p = a_p)$$

$$= \sum_{a_c \in \mathrm{dom}(A_c)} \lambda(A_c = a_c) \sum_{\substack{\forall A_i \in \mathrm{parents}(A_c) - \{A_p\}: \\ a_i \in \mathrm{dom}(A_k)}} P\Big(A_c = a_c \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_c)} A_j = a_j\Big)$$

$$\cdot \prod_{A_k \in \mathrm{parents}(A_c) - \{A_p\}} \pi_{A_k \to A_p}(A_k = a_k)$$

Evidence Propagation in Polytrees (continued)

Evidence: The attributes in a set X_{obs} are observed.

$$P\Big(A_g = a_g \,\Big|\, \bigwedge_{A_k \in X_{\text{obs}}} A_k = a_k^{(\text{obs})}\Big)$$

$$= \sum_{\substack{\forall A_i \in U - \{A_g\}: \\ a_i \in \text{dom}(A_i)}} P\Big(\bigwedge_{A_j \in U} A_j = a_j \,\Big|\, \bigwedge_{A_k \in X_{\text{obs}}} A_k = a_k^{(\text{obs})}\Big)$$

$$= \alpha \sum_{\substack{\forall A_i \in U - \{A_g\}: \\ a_i \in \text{dom}(A_i)}} P\Big(\bigwedge_{A_j \in U} A_j = a_j\Big) \prod_{A_k \in X_{\text{obs}}} P\left(A_k = a_k \,\middle|\, A_k = a_k^{(\text{obs})}\right),$$

where $\alpha = \dfrac{1}{P\left(\bigwedge_{A_k \in X_{\text{obs}}} A_k = a_k^{(\text{obs})}\right)}$

Propagation Formulae with Evidence

$$\pi_{A_p \to A_c}(A_p = a_p)$$

$$= P\left(A_p = a_p \,\middle|\, A_p = a_p^{(\text{obs})}\right) \cdot \pi(A_p = a_p)$$

$$\cdot \Big[\sum_{\substack{\forall A_i \in U_-(A_p, A_c): \\ a_i \in \text{dom}(A_i)}} \prod_{A_k \in U_-(A_p, A_c)} P\Big(A_k = a_k \,\Big|\, \bigwedge_{A_j \in \text{parents}(A_k)} A_j = a_j\Big)\Big]$$

$$= \begin{cases} \beta, & \text{if } a_p = a_p^{(\text{obs})}, \\ 0, & \text{otherwise,} \end{cases}$$

- The value of β is not explicitly determined. Usually a value of 1 is used and the correct value is implicitly determined later by normalizing the resulting probability distribution for A_g.

Propagation Formulae with Evidence

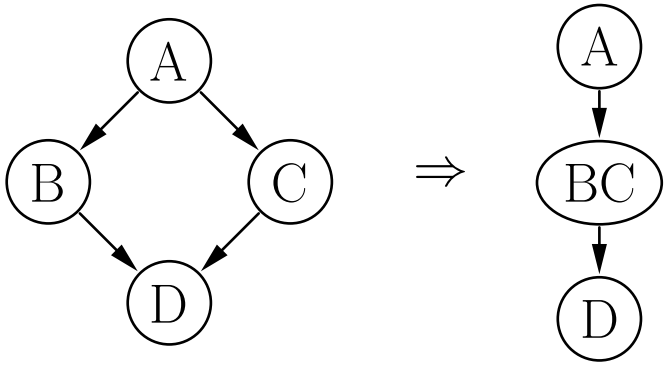
$$
\begin{aligned}
&\lambda_{A_c \to A_p}(A_p = a_p) \\
&= \sum_{a_c \in \mathrm{dom}(A_c)} P\left(A_c = a_c \,\middle|\, A_c = a_c^{(\mathrm{obs})}\right) \cdot \lambda(A_c = a_c) \\
&\quad \cdot \sum_{\substack{\forall A_i \in \mathrm{parents}(A_c) - \{A_p\}: \\ a_i \in \mathrm{dom}(A_k)}} P\Big(A_c = a_c \,\Big|\, \bigwedge_{A_j \in \mathrm{parents}(A_c)} A_j = a_j\Big) \\
&\quad \cdot \prod_{A_k \in \mathrm{parents}(A_c) - \{A_p\}} \pi_{A_k \to A_c}(A_k = a_k)
\end{aligned}
$$

Probabilistic Graphical Models:
Evidence Propagation in Multiply Connected Networks

Propagation in Multiply Connected Networks

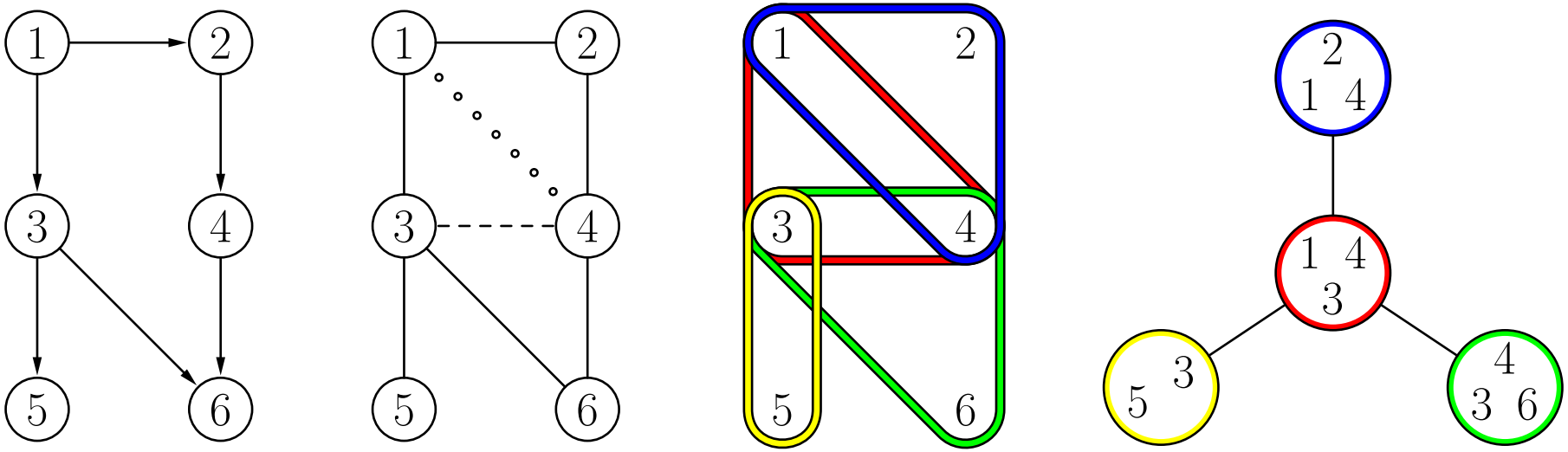
- Multiply connected networks pose a problem:
  - There are several ways on which information can travel from one attribute (node) to another.
  - As a consequence, the same evidence may be used twice to update the probability distribution of an attribute.
  - Since probabilistic update is not idempotent, multiple inclusion of the same evidence usually invalidates the result.
- General idea to solve this problem:

  Transform network into a singly connected structure.



Merging attributes can make the polytree algorithm applicable in multiply connected networks.

Triangulation and Join Tree Construction



original graph | triangulated moral graph | maximal cliques | join tree

- A singly connected structure is obtained by triangulating the graph and then forming a tree of maximal cliques, the so-called **join tree**.
- For evidence propagation a join tree is enhanced by so-called **separators** on the edges, which are intersection of the connected nodes → **junction tree**.

Graph Triangulation

Algorithm: (graph triangulation)

Input: An undirected graph $G = (V, E)$.
Output: A triangulated undirected graph $G' = (V, E')$ with $E' \supseteq E$.

1. Compute an ordering of the nodes of the graph using *maximum cardinality search*, i.e., number the nodes from 1 to $n = |V|$, in increasing order, always assigning the next number to the node having the largest set of previously numbered neighbors (breaking ties arbitrarily).

2. From $i = n$ to $i = 1$ recursively fill in edges between any nonadjacent neighbors of the node numbered i having lower ranks than i (including neighbors linked to the node numbered i in previous steps). If no edges are added, then the original graph is chordal; otherwise the new graph is chordal.

Join Tree Construction

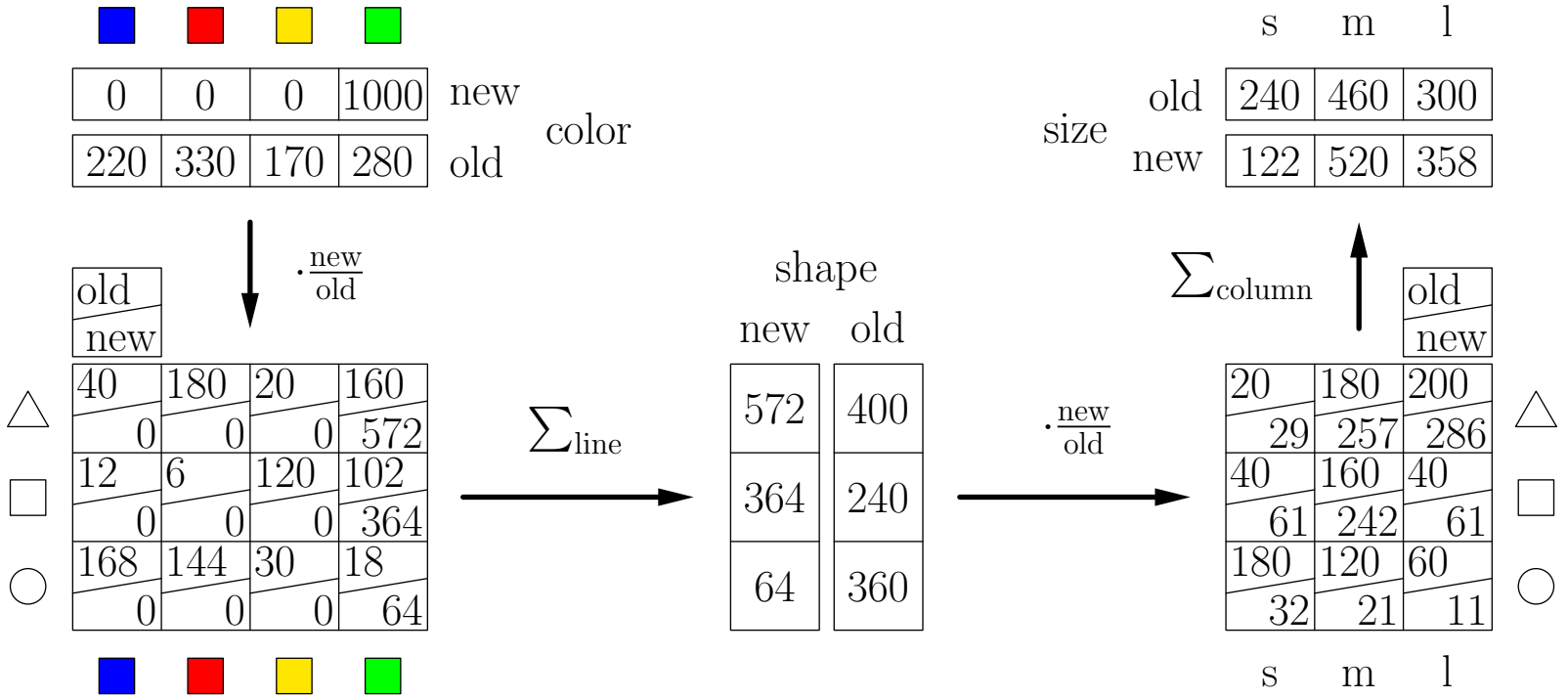
Algorithm: (join tree construction)

Input: A triangulated undirected graph $G = (V, E)$.
Output: A join tree $G' = (V', E')$ for G.

1. Determine a numbering of the nodes of G using maximum cardinality search.
2. Assign to each clique the maximum of the ranks of its nodes.
3. Sort the cliques in ascending order w.r.t. the numbers assigned to them.
4. Traverse the cliques in ascending order and for each clique C_i choose from the cliques $C_1, \ldots, C_{i-1}$ preceding it the clique with which it has the largest number of nodes in common (breaking ties arbitrarily).

Reasoning in Join/Junction Trees

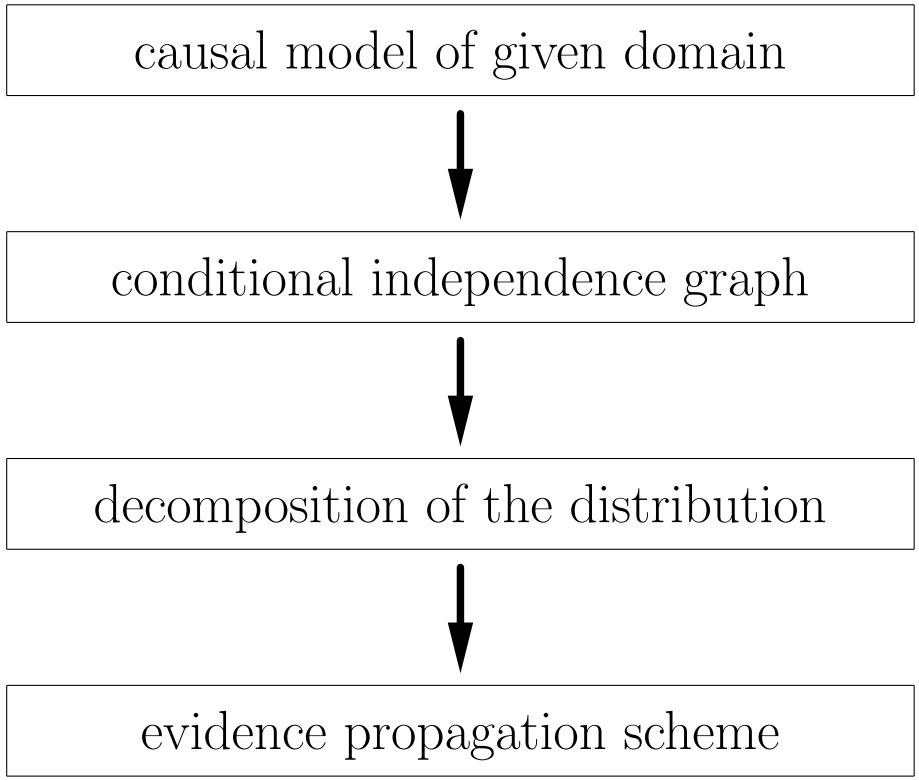
- Reasoning in join trees follows the same lines as shown in the simple example.
- Multiple pieces of evidence from different branches may be incorporated into a distribution before continuing by summing/marginalizing.



Graphical Models:
Manual Model Building

Building Graphical Models: Causal Modeling

Manual creation of a reasoning system based on a graphical model:



heuristics!

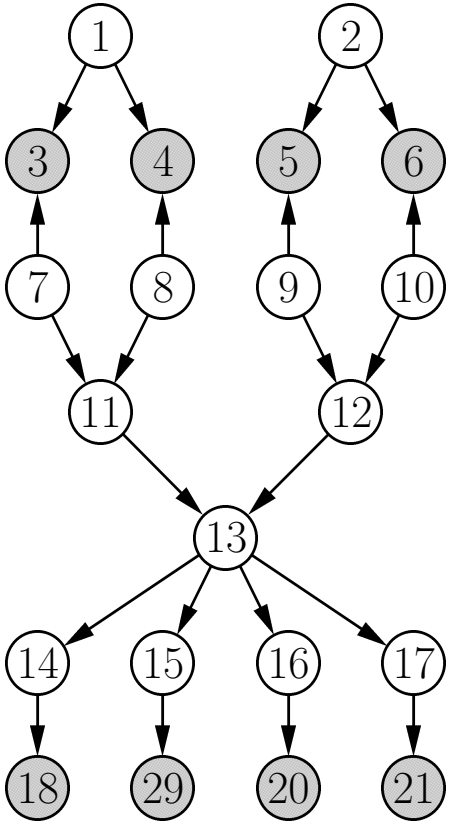
formally provable

formally provable

- Problem: strong assumptions about the statistical effects of causal relations.

Probabilistic Graphical Models: An Example

Danish Jersey Cattle Blood Type Determination



21 attributes:

1 – dam correct?
2 – sire correct?
3 – stated dam ph.gr. 1
4 – stated dam ph.gr. 2
5 – stated sire ph.gr. 1
6 – stated sire ph.gr. 2
7 – true dam ph.gr. 1
8 – true dam ph.gr. 2
9 – true sire ph.gr. 1
10 – true sire ph.gr. 2
11 – offspring ph.gr. 1
12 – offspring ph.gr. 2
13 – offspring genotype
14 – factor 40
15 – factor 41
16 – factor 42
17 – factor 43
18 – lysis 40
19 – lysis 41
20 – lysis 42
21 – lysis 43

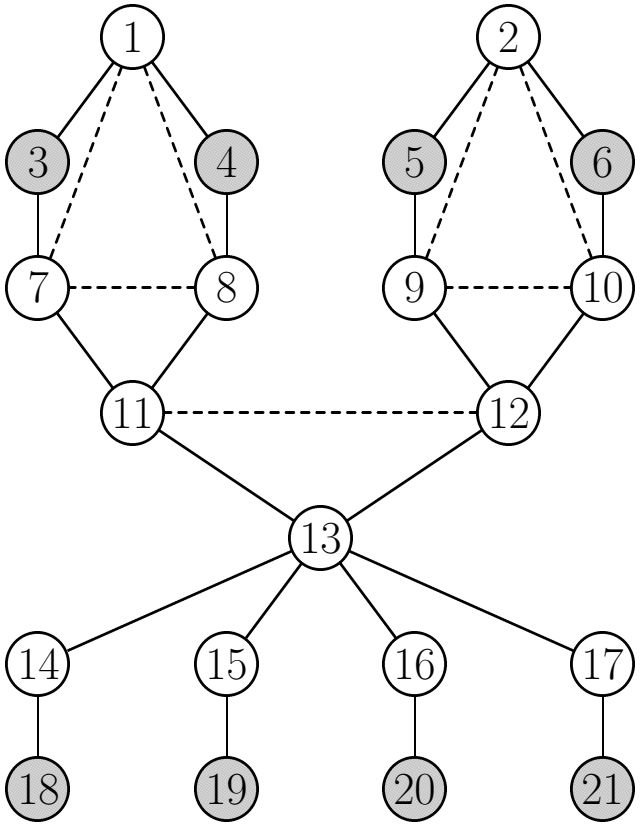
The grey nodes correspond to observable attributes.

Danish Jersey Cattle Blood Type Determination

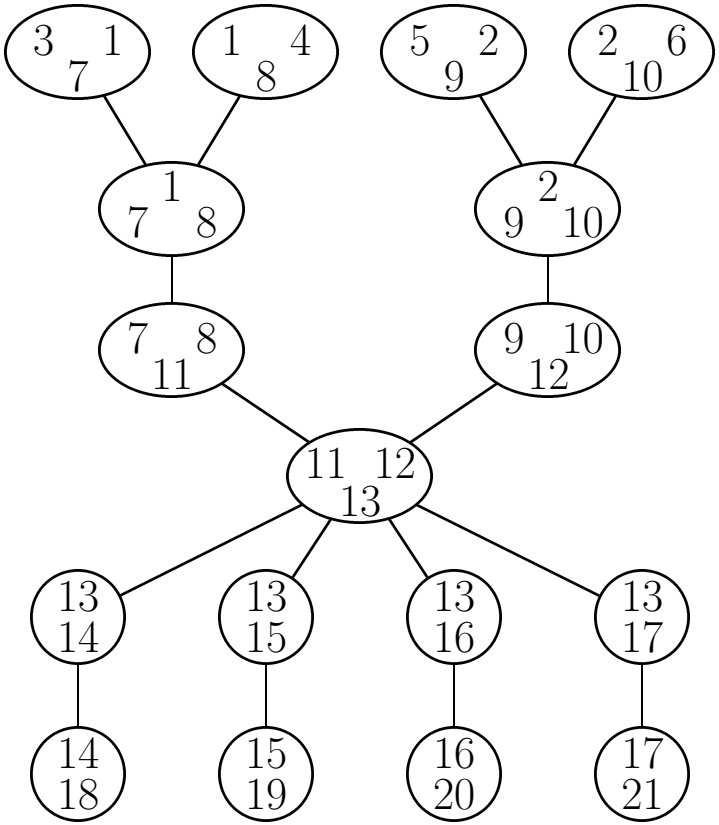
- Full 21-dimensional domain has $2^6 \cdot 3^{10} \cdot 6 \cdot 8^4 = 92\ 876\ 046\ 336$ possible states.
- Bayesian network requires only 306 conditional probabilities.
- Example of a conditional probability table (attributes 2, 9, and 5):

sire correct	true sire phenogroup 1	stated sire phenogroup 1 F1	V1	V2
yes	F1	1	0	0
yes	V1	0	1	0
yes	V2	0	0	1
no	F1	0.58	0.10	0.32
no	V1	0.58	0.10	0.32
no	V2	0.58	0.10	0.32

Danish Jersey Cattle Blood Type Determination



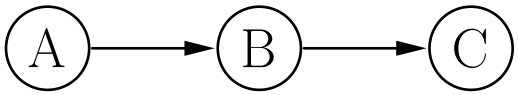
moral graph



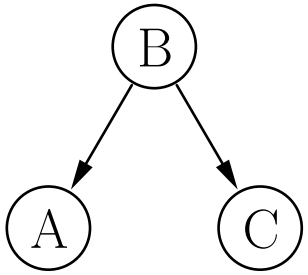
join tree

Graphical Models and Causality

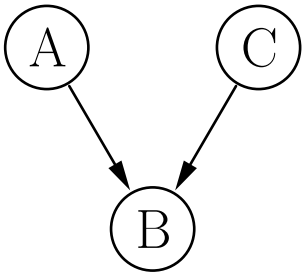
Graphical Models and Causality



causal chain



common cause



common effect

Example:

A – accelerator pedal
B – fuel supply
C – engine speed

$A \not\perp\!\!\!\perp C \mid \emptyset$

$A \perp\!\!\!\perp C \mid B$

Example:

A – ice cream sales
B – temperature
C – bathing accidents

$A \not\perp\!\!\!\perp C \mid \emptyset$

$A \perp\!\!\!\perp C \mid B$

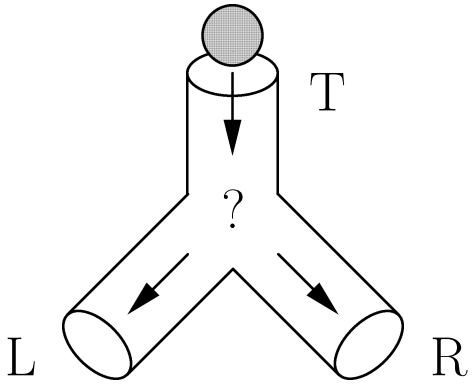
Example:

A – influenza
B – fever
C – measles

$A \perp\!\!\!\perp C \mid \emptyset$

$A \not\perp\!\!\!\perp C \mid B$

Common Cause Assumption (Causal Markov Assumption)



t	r	$\overline{r}$	$\sum$
l	0	$1/2$	$1/2$
$\overline{l}$	$1/2$	0	$1/2$
$\sum$	$1/2$	$1/2$	

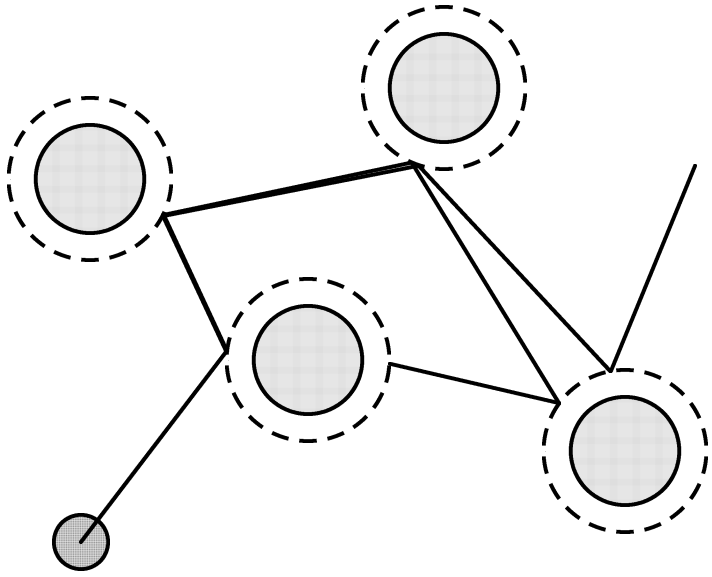
Y-shaped tube arrangement into which a ball is dropped (T). Since the ball can reappear *either* at the left outlet (L) *or* the right outlet (R) the corresponding variables are dependent.

Counter argument: The cause is insufficiently described. If the exact shape, position and velocity of the ball and the tubes are known, the outlet can be determined and the variables become independent.

Counter counter argument: Quantum mechanics states that location and momentum of a particle cannot both at the same time be measured with arbitrary precision.

Sensitive Dependence on the Initial Conditions

- *Sensitive dependence on the initial conditions* means that a small change of the initial conditions (e.g. a change of the initial position or velocity of a particle) causes a deviation that grows *exponentially* with time.
- Many physical systems show, for arbitrary initial conditions, a sensitive dependence on the initial conditions. Due to this quantum mechanical effects sometimes have macroscopic consequences.



Example: Billiard with round (or generally convex) obstacles.

Initial imprecision: $\approx \frac{1}{100}$ degree

after four collisions: ≈ 100 degrees

Learning Graphical Models from Data

Learning Graphical Models from Data

Given: A database of sample cases from a domain of interest.

Desired: A (good) graphical model of the domain of interest.

- **Quantitative or Parameter Learning**
  - The structure of the conditional independence graph is known.
  - Conditional or marginal distributions have to be estimated by standard statistical methods. (*parameter estimation*)
- **Qualitative or Structural Learning**
  - The structure of the conditional independence graph is not known.
  - A good graph has to be selected from the set of all possible graphs. (*model selection*)
  - Tradeoff between model complexity and model accuracy.

Danish Jersey Cattle Blood Type Determination

A fraction of the database of sample cases:

```
y y f1 v2 f1 v2 f1 v2 f1 v2 v2 v2 v2v2 n y n y 0 6 0 6
y y f1 v2 ** ** f1 v2 ** ** ** ** f1v2 y y n y 7 6 0 7
y y f1 v2 f1 f1 f1 v2 f1 f1 f1 f1 f1f1 y y n n 7 7 0 0
y y f1 v2 f1 f1 f1 v2 f1 f1 f1 f1 f1f1 y y n n 7 7 0 0
y y f1 v2 f1 v1 f1 v2 f1 v1 v2 f1 f1v2 y y n y 7 7 0 7
y y f1 f1 ** ** f1 f1 ** ** f1 f1 f1f1 y y n n 6 6 0 0
y y f1 v1 ** ** f1 v1 ** ** v1 v2 v1v2 n y y y 0 5 4 5
y y f1 v2 f1 v1 f1 v2 f1 v1 f1 v1 f1v1 y y y y 7 7 6 7
                  ⋮                             ⋮
```

- 21 attributes
- 500 real world sample cases
- A lot of missing values (indicated by **)

Learning Graphical Models from Data: Learning the Parameters

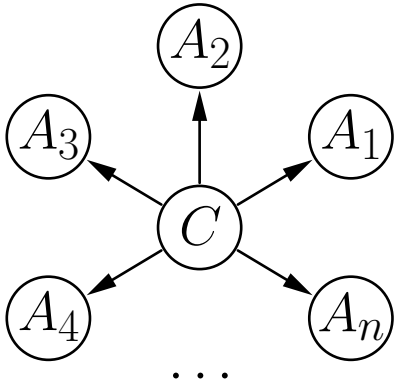
Learning the Parameters of a Graphical Model

Given: A database of sample cases from a domain of interest.
The graph underlying a graphical model for the domain.

Desired: Good values for the numeric parameters of the model.

Example: Naive Bayes Classifiers

- A naive Bayes classifier is a Bayesian network with a star-like structure.
- The class attribute is the only unconditioned attribute.
- All other attributes are conditioned on the class only.



The structure of a naive Bayes classifier is fixed once the attributes have been selected. The only remaining task is to estimate the parameters of the needed probability distributions.

Probabilistic Classification

- A classifier is an algorithm that assigns a class from a predefined set to a case or object, based on the values of descriptive attributes.
- An optimal classifier maximizes the probability of a correct class assignment.
  - Let C be a class attribute with $\mathrm{dom}(C) = \{c_1, \ldots, c_{n_C}\}$, which occur with probabilities p_i, $1 \leq i \leq n_C$.
  - Let q_i be the probability with which a classifier assigns class c_i. ($q_i \in \{0, 1\}$ for a deterministic classifier)
  - The probability of a correct assignment is
$$P(\text{correct assignment}) = \sum_{i=1}^{n_C} p_i q_i.$$
  - Therefore the best choice for the q_i is
$$q_i = \begin{cases} 1, & \text{if } p_i = \max_{k=1}^{n_C} p_k, \\ 0, & \text{otherwise.} \end{cases}$$

Probabilistic Classification (continued)

- Consequence: An optimal classifier should assign the **most probable class**.
- This argument does not change if we take descriptive attributes into account.
  - Let $U = \{A_1, \ldots, A_m\}$ be a set of descriptive attributes with domains $\mathrm{dom}(A_k)$, $1 \leq k \leq m$.
  - Let $A_1 = a_1, \ldots, A_m = a_m$ be an instantiation of the descriptive attributes.
  - An optimal classifier should assign the class c_i for which

$$P(C = c_i \mid A_1 = a_1, \ldots, A_m = a_m) =$$

$$\max_{j=1}^{n_C} \; P(C = c_j \mid A_1 = a_1, \ldots, A_m = a_m)$$

- **Problem:** We cannot store a class (or the class probabilities) for every possible instantiation $A_1 = a_1, \ldots, A_m = a_m$ of the descriptive attributes. (The table size grows exponentially with the number of attributes.)

- Therefore: **Simplifying assumptions are necessary.**

Bayes' Rule and Bayes' Classifiers

- Bayes' rule is a formula that can be used to "invert" conditional probabilities: Let X and Y be events, $P(X) > 0$. Then

$$P(Y \mid X) = \frac{P(X \mid Y) \cdot P(Y)}{P(X)}.$$

- Bayes' rule follows directly from the definition of conditional probability:

$$P(Y \mid X) = \frac{P(X \cap Y)}{P(X)} \qquad \text{and} \qquad P(X \mid Y) = \frac{P(X \cap Y)}{P(Y)}.$$

- Bayes' classifiers: Compute the class probabilities as

$$P(C = c_i \mid A_1 = a_1, \ldots, A_m = a_m) =$$

$$\frac{P(A_1 = a_1, \ldots, A_m = a_m \mid C = c_i) \cdot P(C = c_i)}{P(A_1 = a_1, \ldots, A_m = a_m)}.$$

- Looks unreasonable at first sight: Even more probabilities to store.

Naive Bayes Classifiers

Naive Assumption:
The descriptive attributes are conditionally independent given the class.

Bayes' Rule:

$$P(C = c_i \mid \vec{a}) = \frac{P(A_1 = a_1, \ldots, A_m = a_m \mid C = c_i) \cdot P(C = c_i)}{P(A_1 = a_1, \ldots, A_m = a_m)} \quad \leftarrow p_0 = P(\vec{a})$$

Chain Rule of Probability:

$$P(C = c_i \mid \vec{a}) = \frac{P(C = c_i)}{p_0} \cdot \prod_{k=1}^{m} P(A_k = a_k \mid A_1 = a_1, \ldots, A_{k-1} = a_{k-1}, C = c_i)$$

Conditional Independence Assumption:

$$P(C = c_i \mid \vec{a}) = \frac{P(C = c_i)}{p_0} \cdot \prod_{k=1}^{m} P(A_k = a_k \mid C = c_i)$$

Naive Bayes Classifiers (continued)

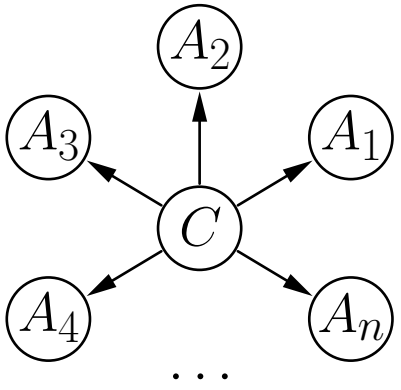
Consequence: Manageable amount of data to store.
Store distributions $P(C = c_i)$ and $\forall 1 \leq j \leq m : P(A_j = a_j \mid C = c_i)$.

Classification: Compute for all classes c_i

$$P(C = c_i \mid A_1 = a_1, \ldots, A_m = a_m) \cdot p_0 \quad = \quad P(C = c_i) \cdot \prod_{j=1}^{n} P(A_j = a_j \mid C = c_i)$$

and predict the class c_i for which this value is largest.

Relation to Bayesian Networks:



Decomposition formula:

$$P(C = c_i, A_1 = a_1, \ldots, A_n = a_n)$$
$$= \quad P(C = c_i) \cdot \prod_{j=1}^{n} P(A_j = a_j \mid C = c_i)$$

Naive Bayes Classifiers: Parameter Estimation

Estimation of Probabilities:

- **Nominal/Categorical Attributes:**

$$\hat{P}(A_j = a_j \mid C = c_i) = \frac{\#(A_j = a_j, C = c_i) + \gamma}{\#(C = c_i) + n_{A_j}\gamma}$$

  $\#(\varphi)$ is the number of example cases that satisfy the condition φ.
  n_{A_j} is the number of values of the attribute A_j.

- γ is called **Laplace correction**.

  $\gamma = 0$: Maximum likelihood estimation.

  Common choices: $\gamma = 1$ or $\gamma = \frac{1}{2}$.

- Laplace correction helps to avoid problems with attribute values that do not occur with some class in the given data.

  It also introduces a bias towards a uniform distribution.

Naive Bayes Classifiers: Parameter Estimation

Estimation of Probabilities:

- **Metric/Numeric Attributes:** Assume a normal distribution.

$$P(A_j = a_j \mid C = c_i) = \frac{1}{\sqrt{2\pi}\sigma_j(c_i)} \exp\left(-\frac{(a_j - \mu_j(c_i))^2}{2\sigma_j^2(c_i)}\right)$$

- Estimate of mean value

$$\hat{\mu}_j(c_i) = \frac{1}{\#(C = c_i)} \sum_{k=1}^{\#(C=c_i)} a_j(k)$$

- Estimate of variance

$$\hat{\sigma}_j^2(c_i) = \frac{1}{\xi} \sum_{j=1}^{\#(C=c_i)} \Big(a_j(k) - \hat{\mu}_j(c_i)\Big)^2$$

$\xi = \#(C = c_i)$: Maximum likelihood estimation
$\xi = \#(C = c_i) - 1$: Unbiased estimation

Naive Bayes Classifiers: Simple Example 1

No	Sex	Age	Blood pr.	Drug
1	male	20	normal	A
2	female	73	normal	B
3	female	37	high	A
4	male	33	low	B
5	female	48	high	A
6	male	29	normal	A
7	female	52	normal	B
8	male	42	low	B
9	male	61	normal	B
10	female	30	normal	A
11	female	26	low	B
12	male	54	high	A

$P(\text{Drug})$	A	B
	0.5	0.5

$P(\text{Sex} \mid \text{Drug})$	A	B
male	0.5	0.5
female	0.5	0.5

$P(\text{Age} \mid \text{Drug})$	A	B
μ	36.3	47.8
σ^2	161.9	311.0

$P(\text{Blood Pr.} \mid \text{Drug})$	A	B
low	0	0.5
normal	0.5	0.5
high	0.5	0

A simple database and estimated (conditional) probability distributions.

Naive Bayes Classifiers: Simple Example 1

$$P(\text{Drug A} \mid \text{male, 61, normal})$$
$$= c_1 \cdot P(\text{Drug A}) \cdot P(\text{male} \mid \text{Drug A}) \cdot P(61 \mid \text{Drug A}) \cdot P(\text{normal} \mid \text{Drug A})$$
$$\approx c_1 \cdot 0.5 \cdot 0.5 \cdot 0.004787 \cdot 0.5 = c_1 \cdot 5.984 \cdot 10^{-4} = 0.219$$

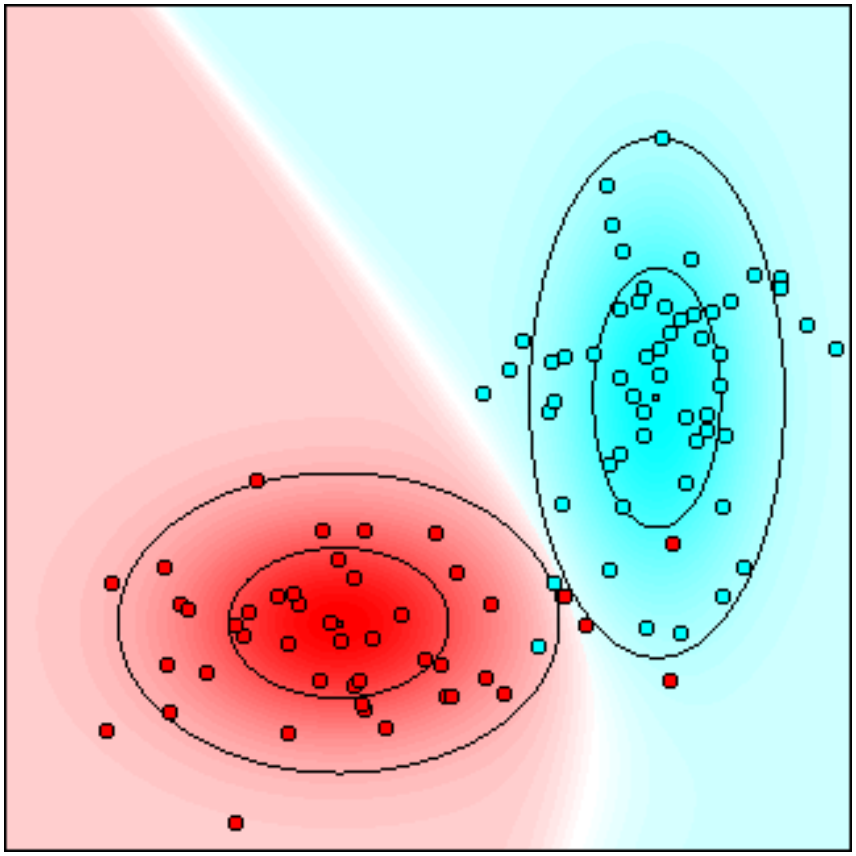
$$P(\text{Drug A} \mid \text{male, 61, normal})$$
$$= c_1 \cdot P(\text{Drug B}) \cdot P(\text{male} \mid \text{Drug B}) \cdot P(61 \mid \text{Drug B}) \cdot P(\text{normal} \mid \text{Drug B})$$
$$\approx c_1 \cdot 0.5 \cdot 0.5 \cdot 0.017120 \cdot 0.5 = c_1 \cdot 2.140 \cdot 10^{-3} = 0.781$$

$$P(\text{Drug A} \mid \text{female, 30, normal})$$
$$= c_2 \cdot P(\text{Drug A}) \cdot P(\text{female} \mid \text{Drug A}) \cdot P(30 \mid \text{Drug A}) \cdot P(\text{normal} \mid \text{Drug A})$$
$$\approx c_2 \cdot 0.5 \cdot 0.5 \cdot 0.027703 \cdot 0.5 = c_2 \cdot 3.471 \cdot 10^{-3} = 0.671$$

$$P(\text{Drug A} \mid \text{female, 30, normal})$$
$$= c_2 \cdot P(\text{Drug B}) \cdot P(\text{female} \mid \text{Drug B}) \cdot P(30 \mid \text{Drug B}) \cdot P(\text{normal} \mid \text{Drug B})$$
$$\approx c_2 \cdot 0.5 \cdot 0.5 \cdot 0.013567 \cdot 0.5 = c_2 \cdot 1.696 \cdot 10^{-3} = 0.329$$

Naive Bayes Classifiers: Simple Example 2

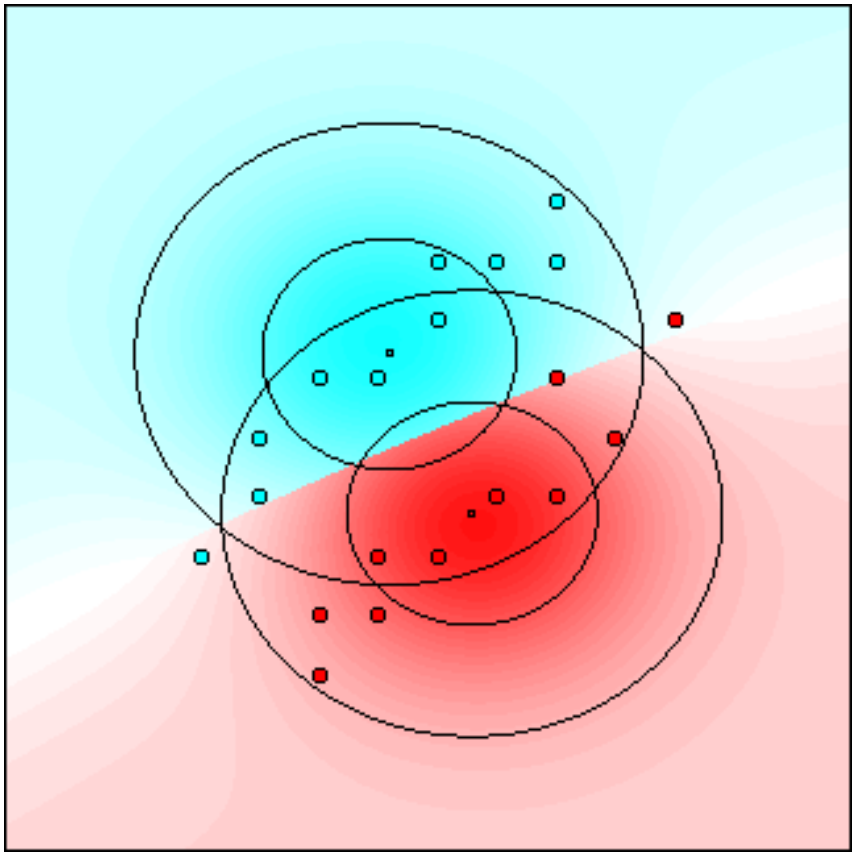
- 100 data points, 2 classes
- Small squares: mean values
- Inner ellipses:
  one standard deviation
- Outer ellipses:
  two standard deviations
- Classes overlap:
  classification is not perfect



Naive Bayes Classifier

Naive Bayes Classifiers: Simple Example 3

- 20 data points, 2 classes
- Small squares: mean values
- Inner ellipses:
  one standard deviation
- Outer ellipses:
  two standard deviations
- Attributes are not conditionally
  independent given the class.



Naive Bayes Classifier

Naive Bayes Classifiers: Iris Data

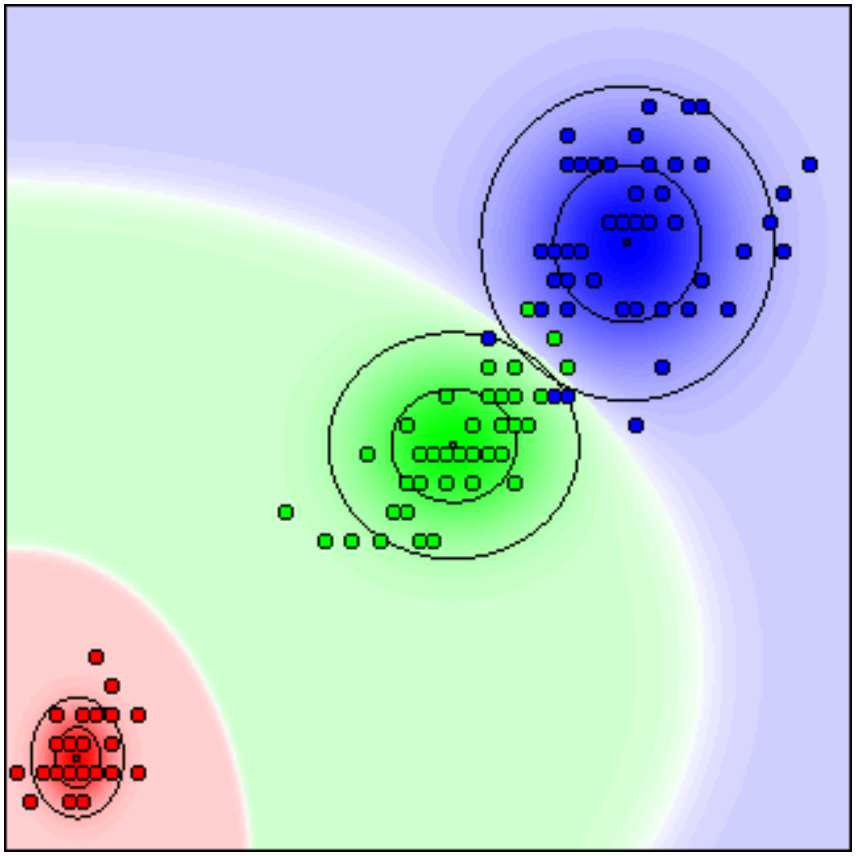
- 150 data points, 3 classes

  Iris setosa (red)
  Iris versicolor (green)
  Iris virginica (blue)

- Shown: 2 out of 4 attributes

  sepal length
  sepal width
  petal length (horizontal)
  petal width (vertical)

- 6 misclassifications
  on the training data
  (with all 4 attributes)



Naive Bayes Classifier

Learning Graphical Models from Data: Learning the Structure

Learning the Structure of Graphical Models from Data

- **Test whether a distribution is decomposable w.r.t. a given graph.**

  This is the most direct approach. It is not bound to a graphical representation, but can also be carried out w.r.t. other representations of the set of subspaces to be used to compute the (candidate) decomposition of the given distribution.

- **Find a suitable graph by measuring the strength of dependences.**

  This is a heuristic, but often highly successful approach, which is based on the frequently valid assumption that in a conditional independence graph an attribute is more strongly dependent on adjacent attributes than on attributes that are not directly connected to them.

- **Find an independence map by conditional independence tests.**

  This approach exploits the theorems that connect conditional independence graphs and graphs that represent decompositions. It has the advantage that a single conditional independence test, if it fails, can exclude several candidate graphs. However, wrong test results can thus have severe consequences.

Evaluation Measures and Search Methods

- All learning algorithms for graphical models consist of
  an **evaluation measure** or **scoring function**, e.g.
  - Hartley information gain (relational networks)
  - Shannon information gain, χ^2, K2 metric (probabilistic networks)

  and a (heuristic) **search method**, e.g.
  - conditional independence search
  - greedy search (spanning tree or K2 algorithm)
  - guided random search (simulated annealing, genetic algorithms)

- An exhaustive search over all graphs is too expensive:
  - $2^{\binom{n}{2}}$ possible undirected graphs for n attributes.
  - $f(n) = \sum_{i=1}^{n} (-1)^{i+1} \binom{n}{i} 2^{i(n-i)} f(n-i)$ possible directed acyclic graphs.

Learning the Structure of a Graphical Model: Testing for Decomposability

Comparing Relations

- In order to evaluate a graph structure, we need a measure that compares the actual relation to the relatio represented by the graph.
- For arbitrary R, E_1, and E_2 it is

$$R(E_1 \cap E_2) \leq \min\{R(E_1), R(E_2)\}.$$

- This relation entails that it is always

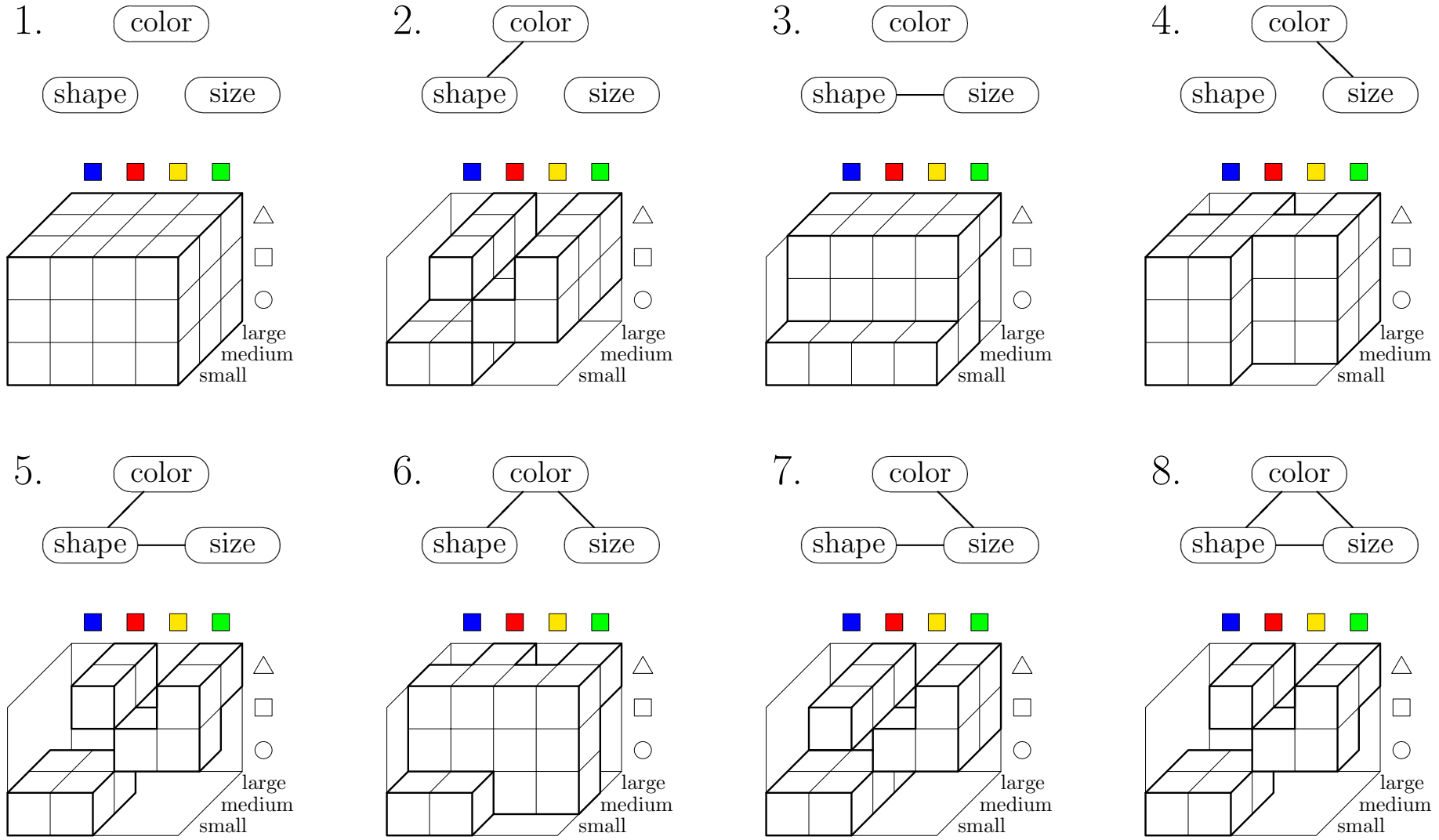
$$\forall a_1 \in \mathrm{dom}(A_1) : \ldots \forall a_n \in \mathrm{dom}(A_n) :$$
$$r_U\Big(\bigwedge_{A_i \in U} A_i = a_i\Big) \leq \min_{M \in \mathcal{M}} \Big\{r_M\Big(\bigwedge_{A_i \in M} A_i = a_i\Big)\Big\}.$$

- Therefore: Measure the quality of a family $\mathcal{M}$ of subset of U as:

$$\sum_{a_1 \in \mathrm{dom}(A_1)} \cdots \sum_{a_n \in \mathrm{dom}(A_n)} \Big(\min_{M \in \mathcal{M}} \Big\{r_M\Big(\bigwedge_{A_i \in M} A_i = a_i\Big)\Big\} - r_U\Big(\bigwedge_{A_i \in U} A_i = a_i\Big)\Big)$$

  Intuitively: Count the number of additional tuples.

Direct Test for Decomposability: Relational



Comparing Probability Distributions

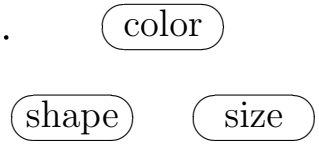
Definition: Let p_1 and p_2 be two strictly positive probability distributions on the same set $\mathcal{E}$ of events. Then

$$I_{\mathrm{KLdiv}}(p_1, p_2) = \sum_{E \in \mathcal{E}} p_1(E) \log_2 \frac{p_1(E)}{p_2(E)}$$

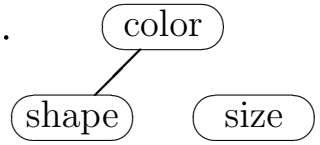
is called the **Kullback-Leibler information divergence** of p_1 and p_2.

- The Kullback-Leibler information divergence is non-negative.
- It is zero if and only if $p_1 \equiv p_2$.
- Therefore it is plausible that this measure can be used to assess the quality of the approximation of a given multi-dimensional distribution p_1 by the distribution p_2 that is represented by a given graph:
  The smaller the value of this measure, the better the approximation.

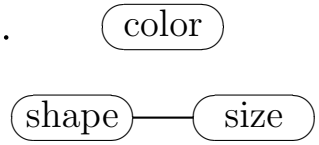
Direct Test for Decomposability: Probabilistic

1. 

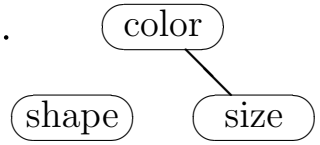
0.640
−5041

2. 

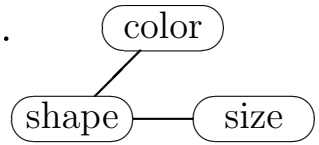
0.211
−4612

3. 

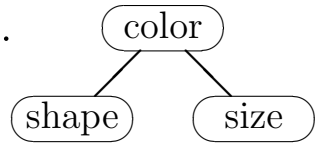
0.429
−4830

4. 

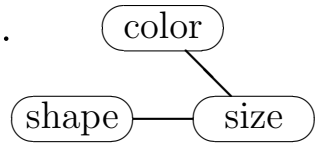
0.590
−4991

5. 

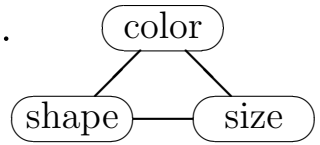
0
−4401

6. 

0.161
−4563

7. 

0.379
−4780

8. 

0
−4401

Upper numbers: The Kullback-Leibler information divergence of the original distribution and its approximation.

Lower numbers: The binary logarithms of the probability of an example database (log-likelihood of data).

Learning the Structure of a Graphical Model: Strength of Marginal Dependences

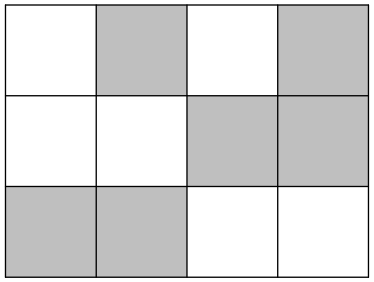
Strength of Marginal Dependences: Relational

- Learning a relational network consists in finding those subspace, for which the intersection of the cylindrical extensions of the projections to these subspaces approximates best the set of possible world states, i.e. contains as few additional tuples as possible.
- Since computing explicitly the intersection of the cylindrical extensions of the projections and comparing it to the original relation is too expensive, local evaluation functions are used, for instance:

subspace	color × shape	shape × size	size × color
possible combinations	12	9	12
occurring combinations	6	5	8
relative number	50%	56%	67%

- The relational network can be obtained by interpreting the relative numbers as edge weights and constructing the minimum weight spanning tree.

Strength of Marginal Dependences: Relational



Hartley information needed to determine

coordinates:	$\log_2 4 + \log_2 3 = \log_2 12$	≈ 3.58
coordinate pair:	$\log_2 6$	≈ 2.58
gain:	$\log_2 12 - \log_2 6 = \log_2 2 = 1$	

Definition: Let A and B be two attributes and R a discrete possibility measure with $\exists a \in \mathrm{dom}(A) : \exists b \in \mathrm{dom}(B) : R(A = a, B = b) = 1$. Then

$$\begin{aligned} I_{\mathrm{gain}}^{(\mathrm{Hartley})}(A, B) &= \log_2 \Big(\textstyle\sum_{a \in \mathrm{dom}(A)} R(A = a) \Big) + \log_2 \Big(\textstyle\sum_{b \in \mathrm{dom}(B)} R(B = b) \Big) \\ &- \log_2 \Big(\textstyle\sum_{a \in \mathrm{dom}(A)} \sum_{b \in \mathrm{dom}(B)} R(A = a, B = b) \Big) \\ &= \log_2 \frac{\Big(\sum_{a \in \mathrm{dom}(A)} R(A = a) \Big) \cdot \Big(\sum_{b \in \mathrm{dom}(B)} R(B = b) \Big)}{\sum_{a \in \mathrm{dom}(A)} \sum_{b \in \mathrm{dom}(B)} R(A = a, B = b)}, \end{aligned}$$

is called the **Hartley information gain** of A and B w.r.t. R.

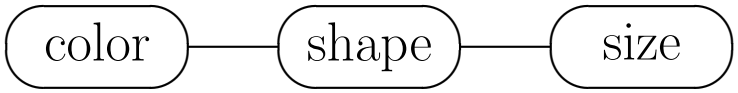
Strength of Marginal Dependences: Simple Example

- **Intuitive interpretation of Hartley information gain:**
  The binary logarithm measures the number of questions to find the obtaining value with a scheme like a binary search. Thus Hartley information gain measures the reduction in the number of necessary questions.

- Results for the simple example:

$$
\begin{aligned}
I_{\text{gain}}^{(\text{Hartley})}(\text{color}, \text{shape}) &= 1.00 \text{ bit} \\
I_{\text{gain}}^{(\text{Hartley})}(\text{shape}, \text{size}) &\approx 0.86 \text{ bit} \\
I_{\text{gain}}^{(\text{Hartley})}(\text{color}, \text{size}) &\approx 0.58 \text{ bit}
\end{aligned}
$$

- Applying the Kruskal algorithm yields as a learning result:



  As we know, this graph describes indeed a decomposition of the relation.

Strength of Marginal Dependences: Probabilistic

Mutual Information / Cross Entropy / Information Gain

Based on Shannon Entropy $H = -\sum_{i=1}^{n} p_i \log_2 p_i$ (Shannon 1948)

$$I_{\text{gain}}(A, B) = \overbrace{H(A)}^{} - \overbrace{H(A \mid B)}^{}$$

$$= \overbrace{-\sum_{i=1}^{n_A} p_{i.} \log_2 p_{i.}}^{H(A)} - \overbrace{\sum_{j=1}^{n_B} p_{.j} \left(-\sum_{i=1}^{n_A} p_{i|j} \log_2 p_{i|j} \right)}^{H(A \mid B)}$$

$H(A)$	Entropy of the distribution on attribute A
$H(A\|B)$	*Expected entropy* of the distribution on attribute A if the value of attribute B becomes known
$H(A) - H(A\|B)$	Expected reduction in entropy or *information gain*

Interpretation of Shannon Entropy

- Let $S = \{s_1, \ldots, s_n\}$ be a finite set of alternatives having positive probabilities $P(s_i)$, $i = 1, \ldots, n$, satisfying $\sum_{i=1}^{n} P(s_i) = 1$.
- **Shannon Entropy:**

$$H(S) = -\sum_{i=1}^{n} P(s_i) \log_2 P(s_i)$$

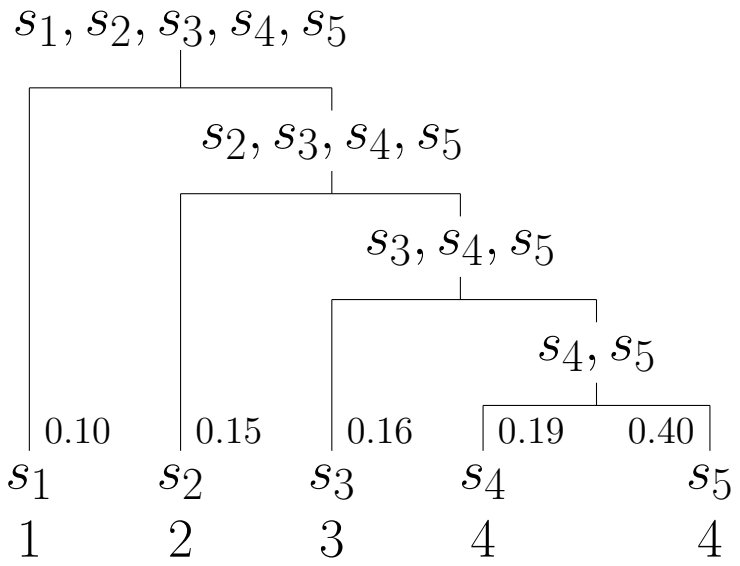
- Intuitively: **Expected number of yes/no questions that have to be asked in order to determine the obtaining alternative.**
  - Suppose there is an oracle, which knows the obtaining alternative, but responds only if the question can be answered with "yes" or "no".
  - A better question scheme than asking for one alternative after the other can easily be found: Divide the set into two subsets of about equal size.
  - Ask for containment in an arbitrarily chosen subset.
  - Apply this scheme recursively $\rightarrow$ number of questions bounded by $\lceil \log_2 n \rceil$.

Question/Coding Schemes

$$P(s_1) = 0.10, \quad P(s_2) = 0.15, \quad P(s_3) = 0.16, \quad P(s_4) = 0.19, \quad P(s_5) = 0.40$$

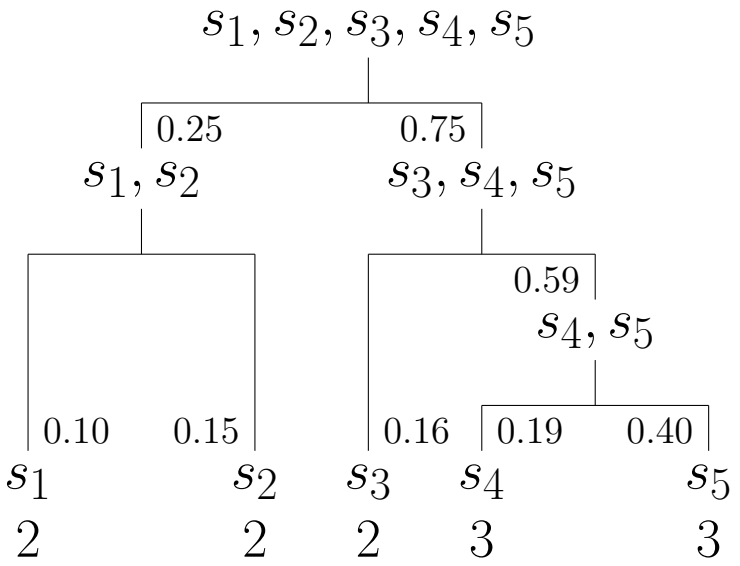
Shannon entropy: $-\sum_i P(s_i) \log_2 P(s_i) = 2.15$ bit/symbol

Linear Traversal



Code length: 3.24 bit/symbol
Code efficiency: 0.664

Equal Size Subsets



Code length: 2.59 bit/symbol
Code efficiency: 0.830

Question/Coding Schemes

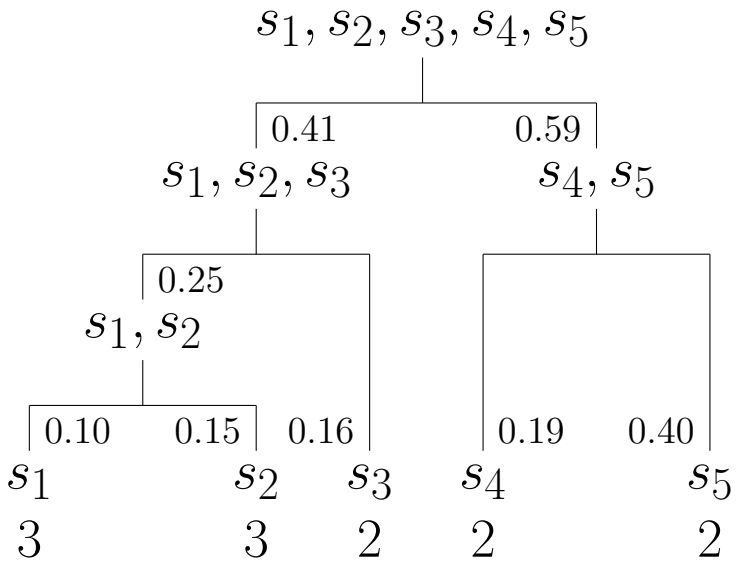
- Splitting into subsets of about equal size can lead to a bad arrangement of the alternatives into subsets $\rightarrow$ high expected number of questions.
- Good question schemes take the probability of the alternatives into account.
- **Shannon-Fano Coding** (1948)
  - Build the question/coding scheme top-down.
  - Sort the alternatives w.r.t. their probabilities.
  - Split the set so that the subsets have about equal *probability* (splits must respect the probability order of the alternatives).
- **Huffman Coding** (1952)
  - Build the question/coding scheme bottom-up.
  - Start with one element sets.
  - Always combine those two sets that have the smallest probabilities.

Question/Coding Schemes

$$P(s_1) = 0.10, \quad P(s_2) = 0.15, \quad P(s_3) = 0.16, \quad P(s_4) = 0.19, \quad P(s_5) = 0.40$$

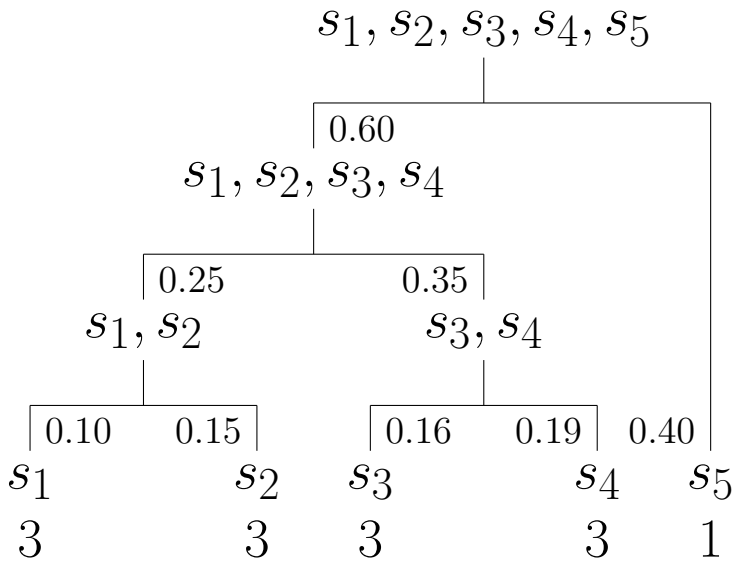
Shannon entropy: $-\sum_i P(s_i) \log_2 P(s_i) = 2.15$ bit/symbol

Shannon–Fano Coding (1948)



Code length: 2.25 bit/symbol
Code efficiency: 0.955

Huffman Coding (1952)



Code length: 2.20 bit/symbol
Code efficiency: 0.977

Question/Coding Schemes

- It can be shown that Huffman coding is optimal if we have to determine the obtaining alternative in a single instance.
  (No question/coding scheme has a smaller expected number of questions.)
- Only if the obtaining alternative has to be determined in a sequence of (independent) situations, this scheme can be improved upon.
- Idea: Process the sequence not instance by instance, but combine two, three or more consecutive instances and ask directly for the obtaining combination of alternatives.
- Although this enlarges the question/coding scheme, the expected number of questions per identification is reduced (because each interrogation identifies the obtaining alternative for several situations).
- However, the expected number of questions per identification cannot be made arbitrarily small. Shannon showed that there is a lower bound, namely the Shannon entropy.

Interpretation of Shannon Entropy

$$P(s_1) = \tfrac{1}{2}, \quad P(s_2) = \tfrac{1}{4}, \quad P(s_3) = \tfrac{1}{8}, \quad P(s_4) = \tfrac{1}{16}, \quad P(s_5) = \tfrac{1}{16}$$

Shannon entropy: $-\sum_i P(s_i) \log_2 P(s_i) = 1.875$ bit/symbol

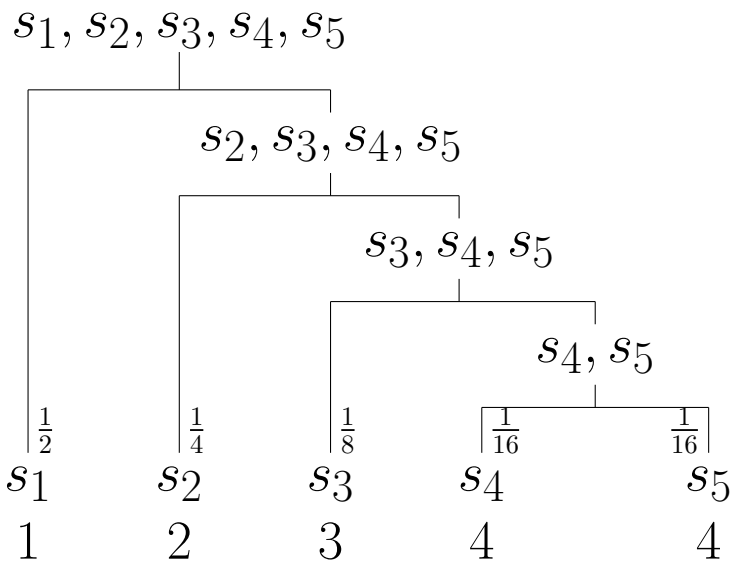
If the probability distribution allows for a perfect Huffman code (code efficiency 1), the Shannon entropy can easily be interpreted as follows:

$$-\sum_i P(s_i) \log_2 P(s_i)$$

$$= \sum_i \underbrace{P(s_i)}_{\text{occurrence probability}} \cdot \underbrace{\log_2 \frac{1}{P(s_i)}}_{\text{path length in tree}} .$$

In other words, it is the expected number of needed yes/no questions.

Perfect Question Scheme



Code length: 1.875 bit/symbol
Code efficiency: 1

Information Gain: Simple Example

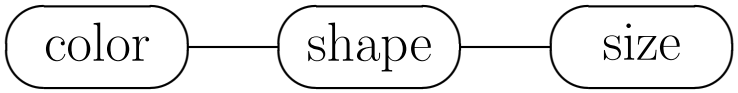
	projection to subspace				product of marginals				information gain
	■	■	■	■	■	■	■	■	
△	40	180	20	160	88	132	68	112	0.429 bit
□	12	6	120	102	53	79	41	67	
○	168	144	30	18	79	119	61	101	
	s	m	l		s	m	l		
△	20	180	200		96	184	120		0.211 bit
□	40	160	40		58	110	72		
○	180	120	60		86	166	108		
	■	■	■	■	■	■	■	■	
large	50	115	35	100	66	99	51	84	0.050 bit
medium	82	133	99	146	101	152	78	129	
small	88	82	36	34	53	79	41	67	

Strength of Marginal Dependences: Simple Example

- Results for the simple example:

$$\begin{aligned} I_{\text{gain}}(\text{color}, \text{shape}) &= 0.429 \text{ bit} \\ I_{\text{gain}}(\text{shape}, \text{size}) &= 0.211 \text{ bit} \\ I_{\text{gain}}(\text{color}, \text{size}) &= 0.050 \text{ bit} \end{aligned}$$

- Applying the Kruskal algorithm yields as a learning result:



- It can be shown that this approach always yields the best possible spanning tree w.r.t. Kullback-Leibler information divergence (Chow and Liu 1968).
- In an extended form this also holds for certain classes of graphs (for example, tree-augmented naive Bayes classifiers).
- For more complex graphs, the best graph need not be found (there are counterexamples, see below).

Strength of Marginal Dependences: General Algorithms

- **Optimum Weight Spanning Tree Construction**
  - Compute an evaluation measure on all possible edges (two-dimensional subspaces).
  - Use the Kruskal algorithm to determine an optimum weight spanning tree.

- **Greedy Parent Selection** (for directed graphs)
  - Define a topological order of the attributes (to restrict the search space).
  - Compute an evaluation measure on all single attribute hyperedges.
  - For each preceding attribute (w.r.t. the topological order): add it as a candidate parent to the hyperedge and compute the evaluation measure again.
  - Greedily select a parent according to the evaluation measure.
  - Repeat the previous two steps until no improvement results from them.

Another Probabilistic Evaluation Measure: K2 Metric

- Idea: Compute the probability of a graph given the data (Bayesian approach)

$$P(\vec{G} \mid D) = \frac{1}{P(D)} \int_{\Theta} P(D \mid \vec{G}, \Theta) f(\Theta \mid \vec{G}) P(\vec{G}) \, \mathrm{d}\Theta$$

  $\vec{G}$ directed acyclic graph underlying the graphical model

  Θ probability parameters of the graphical model

  D database to learn from

- In order to compare two graphs, it is sufficient to compute the **Bayes factor**

$$\frac{P(\vec{G}_1 \mid D)}{P(\vec{G}_2 \mid D)} = \frac{P(\vec{G}_1, D)}{P(\vec{G}_2, D)} = \frac{\int_{\Theta_1} P(D \mid \vec{G}_1, \Theta_1) f(\Theta_1 \mid \vec{G}_1) P(\vec{G}_1) \, \mathrm{d}\Theta_1}{\int_{\Theta_2} P(D \mid \vec{G}_2, \Theta_2) f(\Theta_2 \mid \vec{G}_2) P(\vec{G}_2) \, \mathrm{d}\Theta_2}.$$

  In this way one can avoid computing the probability $P(D)$.
  Assuming equal probability of all graphs simplifies further.

Another Probabilistic Evaluation Measure: K2 Metric

- Assumptions about data and parameter independence yield:

$$P(\vec{G}, D) = \gamma \prod_{k=1}^{r} \prod_{j=1}^{m_k} \int_{\theta_{ijk}} \cdots \int \left(\prod_{i=1}^{n_k} \theta_{ijk}^{N_{ijk}} \right) f(\theta_{1jk}, \ldots, \theta_{n_k jk}) \, \mathrm{d}\theta_{1jk} \ldots \mathrm{d}\theta_{n_k jk}$$

r	number of attributes describing the domain under consideration
n_k	number of values of the k-th attribute A_k, i.e., $n_k = \lvert \mathrm{dom}(A_k) \rvert$
m_k	number of instantiations of the parents of the k-th attribute in $\vec{G}$, i.e., $m_k = \prod_{A_j \in \mathrm{parents}(A_k)} n_j = \prod_{A_j \in \mathrm{parents}(A_k)} \lvert \mathrm{dom}(A_j) \rvert$
θ_{ijk}	probability that the k-th attribute takes its i-th value and its parents in $\vec{G}$ take their j-th instantiation
N_{ijk}	number of sample cases in which the k-th attribute has its i-th value and its parents in $\vec{G}$ have their j-th instantiation
γ	normalization factor

Another Probabilistic Evaluation Measure: K2 Metric

- Choose $f(\theta_{1jk}, \ldots, \theta_{n_k jk}) = \text{const.}$ [Cooper and Herskovits 1992]
- Then the solution can be obtained via Dirichlet's integral:

$$K_2(\vec{G}, D) = \gamma \prod_{k=1}^{r} \prod_{j=1}^{m_k} \frac{(n_k - 1)!}{(N_{\cdot jk} + n_k - 1)!} \prod_{i=1}^{n_k} N_{ijk}!$$

- Since this formula is a product over the attributes, each attribute can be handled more or less separately.
- Core ideas of the K2 algorithm:
  - Fix a topological order of the attributes. (Reduces the search space and ensures that the graph is acyclic.)
  - Select the parents of each attribute greedily based on the K2 metric (or rather its corresponding factor).

A Generalization of the K2 Metric

- Choose a maximum likelihood estimation of the probability parameters:

$$f(\theta_{1jk}, \ldots, \theta_{n_k jk}) = \prod_{i=1}^{n_k} \delta\left(\theta_{ijk} - \frac{N_{ijk}}{N_{.jk}}\right)$$

$$\Rightarrow \qquad g_\infty(\vec{G}, D) = \gamma \prod_{k=1}^{r} \prod_{j=1}^{m_k} \prod_{i=1}^{n_k} \left(\frac{N_{ijk}}{N_{.jk}}\right)^{N_{ijk}} \qquad \text{(equivalent to information gain)}$$

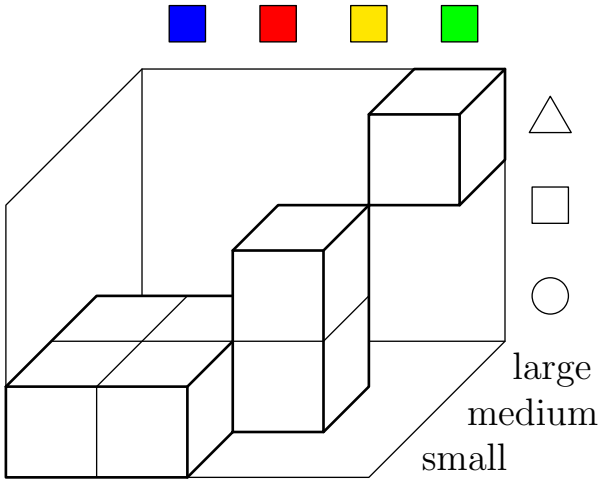
- Choose the likelihood function scaled to maximum 1 and raised to the power α:

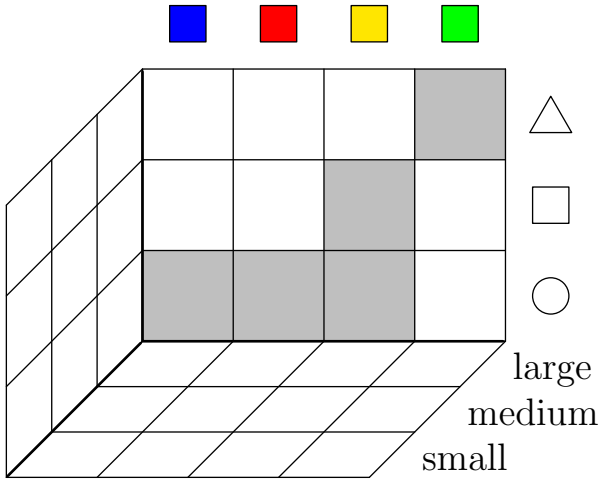
$$f_\alpha(\theta_{1jk}, \ldots, \theta_{n_k jk}) = \beta \cdot \prod_{i=1}^{n_k} \theta_{ijk}^{\alpha N_{ijk}}$$

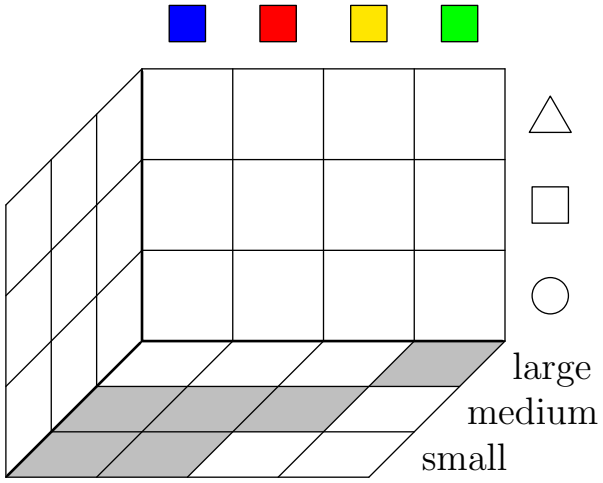
$$\Rightarrow \qquad g_\alpha(\vec{G}, D) = \gamma \prod_{k=1}^{r} \prod_{j=1}^{m_k} \frac{\Gamma(\alpha N_{.jk} + n_k)}{\Gamma((\alpha+1) N_{.jk} + n_k)} \cdot \prod_{i=1}^{n_k} \frac{\Gamma((\alpha+1) N_{ijk} + 1)}{\Gamma(\alpha N_{ijk} + 1)}$$

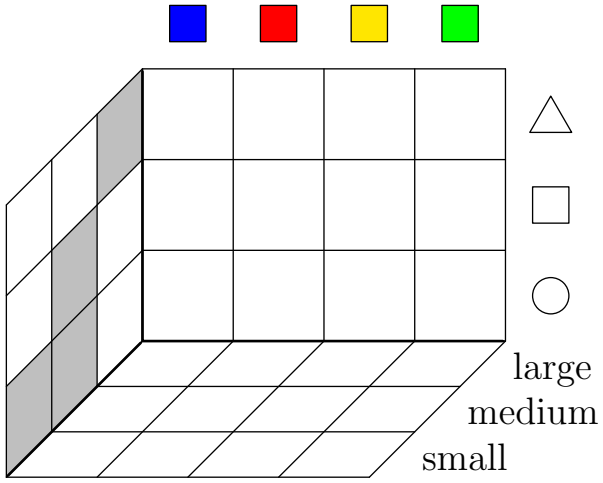
- The parameter α can be interpreted as a sensitivity parameter, which determines the strength of the tendency to select parent attributes.

Strength of Marginal Dependences: Drawbacks

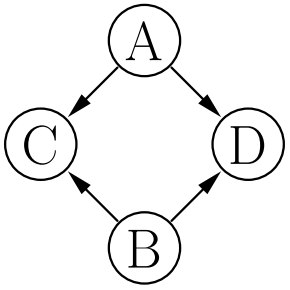








Strength of Marginal Dependences: Drawbacks



p_A	a_1	a_2
	0.5	0.5

p_B	b_1	b_2
	0.5	0.5

$p_{C\|AB}$	a_1b_1	a_1b_2	a_2b_1	a_2b_2
c_1	0.9	0.3	0.3	0.5
c_2	0.1	0.7	0.7	0.5

$p_{D\|AB}$	a_1b_1	a_1b_2	a_2b_1	a_2b_2
d_1	0.9	0.3	0.3	0.5
d_2	0.1	0.7	0.7	0.5

p_{AD}	a_1	a_2
d_1	0.3	0.2
d_2	0.2	0.3

p_{BD}	b_1	b_2
d_1	0.3	0.2
d_2	0.2	0.3

p_{CD}	c_1	c_2
d_1	0.31	0.19
d_2	0.19	0.31

- Greedy parent selection can lead to suboptimal results if there is more than one path connecting two attributes.
- Here: the edge $C \rightarrow D$ is selected first.

Learning the Structure of a Graphical Model: Conditional Independence Tests

Structure Learning with Conditional Independence Tests

General Idea: Exploit the theorems that connect conditional independence graphs and graphs that represent decompositions.

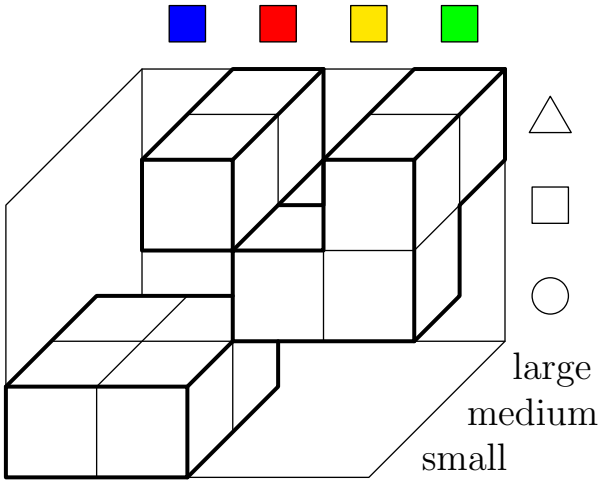
In other words: we want a graph describing a decomposition,
but we search for a conditional independence graph.

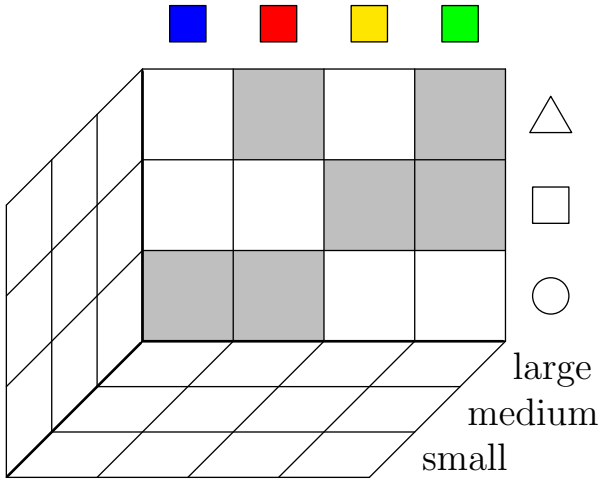
This approach has the advantage that a single conditional independence test, if it fails, can exclude several candidate graphs.

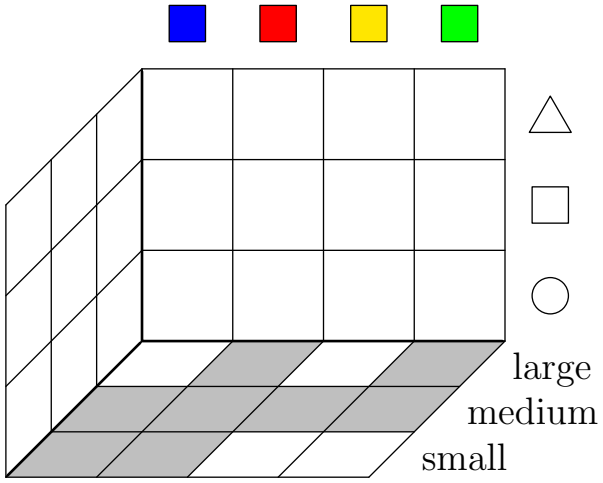
Assumptions:

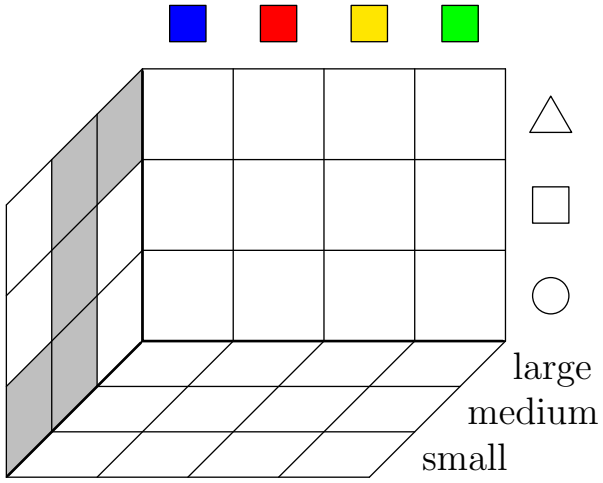
- *Faithfulness:* The domain under consideration can be accurately described with a graphical model (more precisely: there exists a perfect map).
- *Reliability of Tests:* The result of all conditional independence tests coincides with the actual situation in the underlying distribution.
- Other assumptions that are specific to individual algorithms.

Conditional Independence Tests: Relational









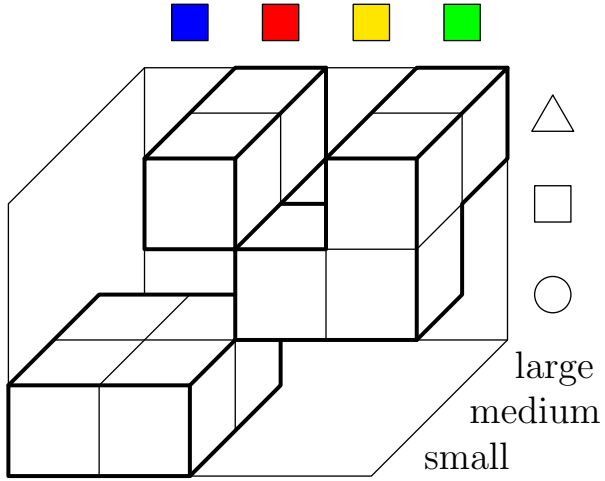
Conditional Independence Tests: Relational

- The Hartley information gain can be used directly to test for (approximate) **marginal independence**.

attributes	relative number of possible value combinations	Hartley information gain
color, shape	$\frac{6}{3 \cdot 4} = \frac{1}{2} = 50\%$	$\log_2 3 + \log_2 4 - \log_2 6 = 1$
color, size	$\frac{8}{3 \cdot 4} = \frac{2}{3} \approx 67\%$	$\log_2 3 + \log_2 4 - \log_2 8 \approx 0.58$
shape, size	$\frac{5}{3 \cdot 3} = \frac{5}{9} \approx 56\%$	$\log_2 3 + \log_2 3 - \log_2 5 \approx 0.85$

- In order to test for (approximate) **conditional independence**:
  - Compute the Hartley information gain for each possible instantiation of the conditioning attributes.
  - Aggregate the result over all possible instantiations, for instance, by simply averaging them.

Conditional Independence Tests: Simple Example



color	Hartley information gain
■	$\log_2 1 + \log_2 2 - \log_2 2 = 0$
■	$\log_2 2 + \log_2 3 - \log_2 4 \approx 0.58$
■	$\log_2 1 + \log_2 1 - \log_2 1 = 0$
■	$\log_2 2 + \log_2 2 - \log_2 2 = 1$
	average: ≈ 0.40

shape	Hartley information gain
△	$\log_2 2 + \log_2 2 - \log_2 4 = 0$
□	$\log_2 2 + \log_2 1 - \log_2 2 = 0$
○	$\log_2 2 + \log_2 2 - \log_2 4 = 0$
	average: $= 0$

size	Hartley information gain
large	$\log_2 2 + \log_2 1 - \log_2 2 = 0$
medium	$\log_2 4 + \log_2 3 - \log_2 6 = 1$
small	$\log_2 2 + \log_2 1 - \log_2 2 = 0$
	average: ≈ 0.33

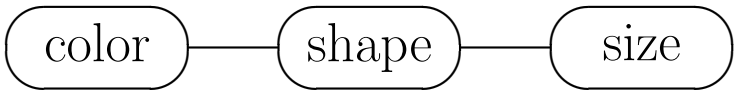
Conditional Independence Tests: Simple Example

- The Shannon information gain can be used directly to test for (approximate) **marginal independence**.
- Conditional independence tests may be carried out by summing the information gain for all instantiations of the conditioning variables:

$$I_{\text{gain}}(A, B \mid C)$$
$$= \sum_{c \in \text{dom}(C)} P(c) \sum_{a \in \text{dom}(A)} \sum_{b \in \text{dom}(B)} P(a, b \mid c) \log_2 \frac{P(a, b \mid c)}{P(a \mid c)\, P(b \mid c)},$$

  where $P(c)$ is an abbreviation of $P(C = c)$ etc.

- Since $I_{\text{gain}}(\text{color}, \text{size} \mid \text{shape}) = 0$ indicates the only conditional independence, we get the following learning result:



Conditional Independence Tests: General Algorithm

Algorithm: (conditional independence graph construction)

1. For each pair of attributes A and B, search for a set $S_{AB} \subseteq U \backslash \{A, B\}$ such that $A \perp\!\!\!\perp B \mid S_{AB}$ holds in $\widehat{P}$, i.e., A and B are independent in $\widehat{P}$ conditioned on S_{AB}. If there is no such S_{AB}, connect the attributes by an undirected edge.

2. For each pair of non-adjacent variables A and B with a common neighbour C (i.e., C is adjacent to A as well as to B), check whether $C \in S_{AB}$.
   - If it is, continue.
   - If it is not, add arrow heads pointing to C, i.e., $A \rightarrow C \leftarrow B$.

3. Recursively direct all undirected edges according to the rules:
   - If for two adjacent variables A and B there is a strictly directed path from A to B not including $A \rightarrow B$, then direct the edge towards B.
   - If there are three variables A, B, and C with A and B not adjacent, $B - C$, and $A \rightarrow C$, then direct the edge $C \rightarrow B$.

Conditional Independence Tests: Simple Example

Suppose that the following conditional independence statements hold:

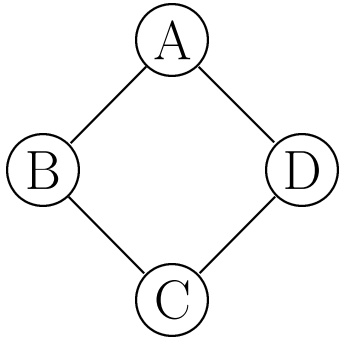
$$A \perp\!\!\!\perp_{\hat{P}} B \mid \emptyset \qquad B \perp\!\!\!\perp_{\hat{P}} A \mid \emptyset$$
$$A \perp\!\!\!\perp_{\hat{P}} D \mid C \qquad D \perp\!\!\!\perp_{\hat{P}} A \mid C$$
$$B \perp\!\!\!\perp_{\hat{P}} D \mid C \qquad D \perp\!\!\!\perp_{\hat{P}} B \mid C$$

All other possible conditional independence statements that can be formed with the attributes A, B, C, and D (with single attributes on the left) do not hold.

- **Step 1:** Since there is no set rendering A and C, B and C and C and D independent, the edges $A - C$, $B - C$, and $C - D$ are inserted.
- **Step 2:** Since C is a common neighbor of A and B and we have $A \perp\!\!\!\perp_{\hat{P}} B \mid \emptyset$, but $A \not\perp\!\!\!\perp_{\hat{P}} B \mid C$, the first two edges must be directed $A \rightarrow C \leftarrow B$.
- **Step 3:** Since A and D are not adjacent, $C - D$ and $A \rightarrow C$, the edge $C - D$ must be directed $C \rightarrow D$.
  (Otherwise step 2 would have already fixed the orientation $C \leftarrow D$.)

Conditional Independence Tests: Drawbacks

- The conditional independence graph construction algorithm presupposes that there is a **perfect map**. If there is no perfect map, the result may be invalid.



p_{ABCD}		$A = a_1$		$A = a_2$	
		$B = b_1$	$B = b_2$	$B = b_1$	$B = b_2$
$C = c_1$	$D = d_1$	$1/47$	$1/47$	$1/47$	$2/47$
	$D = d_2$	$1/47$	$1/47$	$2/47$	$4/47$
$C = c_2$	$D = d_1$	$1/47$	$2/47$	$1/47$	$4/47$
	$D = d_2$	$2/47$	$4/47$	$4/47$	$16/47$

- **Independence tests of high order**, i.e., with a large number of conditions, may be necessary.
- There are approaches to mitigate these drawbacks.
  (For example, the order is restricted and all tests of higher order are assumed to fail, if all tests of lower order failed.)

The Cheng–Bell–Liu Algorithm

- **Drafting:** Build a so-called Chow–Liu tree as an initial graphical model.
  - Evaluate all attribute pairs (candidate edges) with information gain.
  - Discard edges with evaluation below independence threshold ($\sim$0.1 bits).
  - Build optimum (maximum) weight spanning tree.
- **Thickening:** Add necessary edges.
  - Traverse remaining candidate edges in the order of decreasing evaluation.
  - Test for conditional independence in order to determine whether an edge is needed in the graphical model.
  - Use local Markov property to select a condition set: an attribute is conditionally independent of all non-descendants given its parents.
  - Since the graph is undirected in this step, the set of adjacent nodes is reduced iteratively and greedily in order to remove possible children.

The Cheng–Bell–Liu Algorithm (continued)

- **Thinning:** Remove superfluous edges.
  - In the thickening phase a conditional independence test may have failed, because the graph was still too sparse.
  - Traverse all edges that have been added to the current graphical model and test for conditional independence.
  - Remove unnecessary edges.
    (two phases/approaches: heuristic test/strict test)
- **Orienting:** Direct the edges of the graphical model.
  - Identify the v-structures (converging directed edges).
    (Markov equivalence: same skeleton and same set of v-structures.)
  - Traverse all pairs of attributes with common neighbors and check which common neighbors are in the (maximally) reduced set of conditions.
  - Direct remaining edges by extending chains and avoiding cycles.

Learning Undirected Graphical Models Directly

- **Drafting:** Build a Chow–Liu tree as an initial graphical model
  - Evaluate all attribute pairs (candidate edges) with specificity gain.
  - Discard edges with evaluation below independence threshold ($\sim$0.015).
  - Build optimum (maximum) weight spanning tree.
- **Thickening:** Add necessary edges.
  - Traverse remaining candidate edges in the order of decreasing evaluation.
  - Test for conditional independence in order to determine whether an edge is needed in the graphical model.
  - Use local Markov property to select a condition set: an attribute is conditionally independent of any non-neighbor given its neighbors.
  - Since the graphical model to be learned is undirected, *no (iterative) reduction of the condition set is needed* (decisive difference to Cheng–Bell–Liu Algorithm).

Learning Undirected Graphical Models Directly

- **Moralizing:** Take care of possible v-structures.
  - If one assumes a perfect undirected map, this step is unnecessary. However, v-structures are too common and cannot be represented without loss in an undirected graphical model.
  - Possible v-structures can be taken care of by connecting the parents.
  - Traverse all edges with an evaluation below the independence threshold that have a common neighbor in the graph.
  - Add edge if conditional independence given the neighbors does not hold.
- **Thinning:** Remove superfluous edges.
  - In the thickening phase a conditional independence test may have failed, because the graph was still too sparse.
  - Traverse all edges that have been added to the current graphical model and test for conditional independence.

Learning the Structure of a Graphical Model: Experiments and Applications

Danish Jersey Cattle Blood Type Determination

network	edges	params.	train	test
indep.	0	59	−19921.2	−20087.2
orig.	22	219	−11391.0	−11506.1

Optimum Weight Spanning Tree Construction

measure	edges	params.	train	test
I_{gain}	20.0	285.9	−12122.6	−12339.6
χ^2	20.0	282.9	−12122.6	−12336.2

Greedy Parent Selection w.r.t. a Topological Order

measure	edges	add.	miss.	params.	train	test
I_{gain}	35.0	17.1	4.1	1342.2	−11229.3	−11817.6
χ^2	35.0	17.3	4.3	1300.8	−11234.9	−11805.2
K2	23.3	1.4	0.1	229.9	−11385.4	−11511.5
$L_{\text{red}}^{(\text{rel})}$	22.5	0.6	0.1	219.9	−11389.5	−11508.2

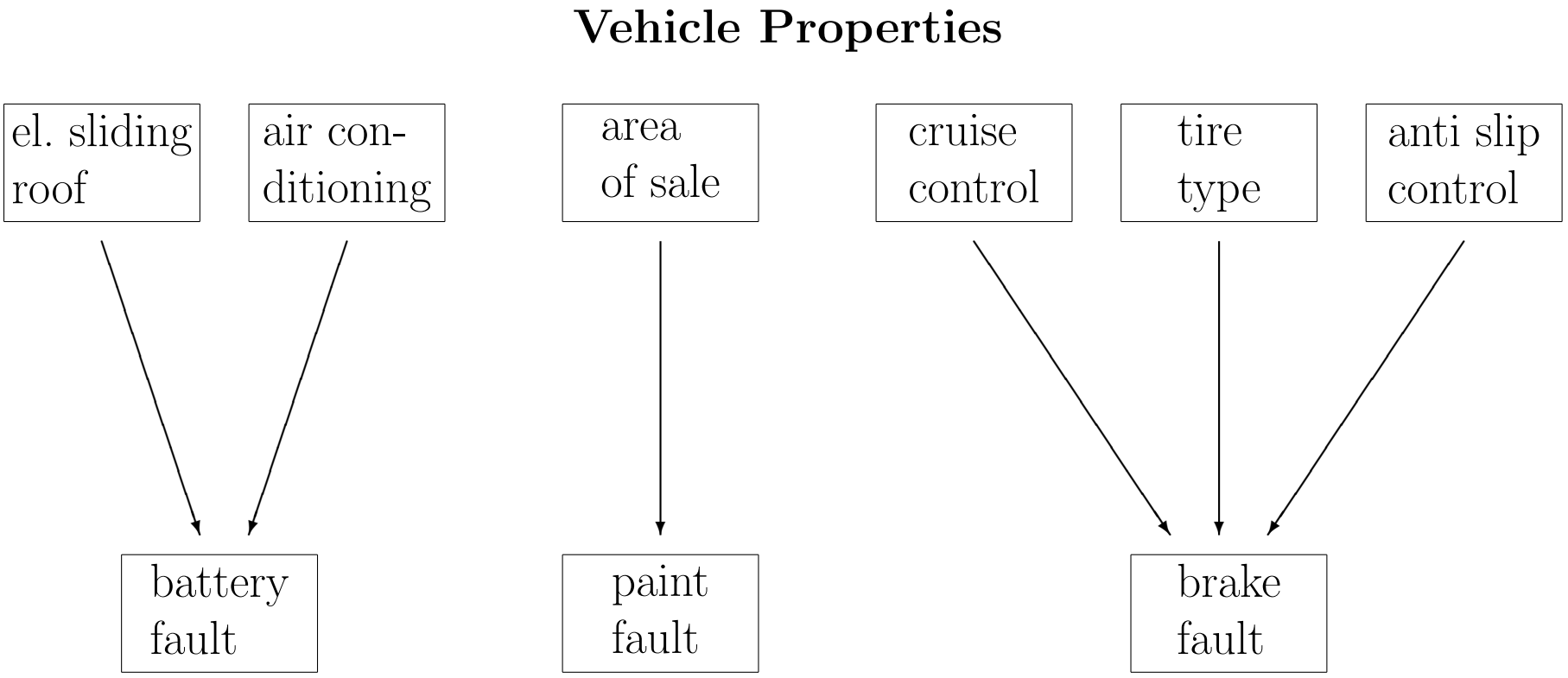
Fields of Application (DaimlerChrysler AG)

- **Improvement of Product Quality by Finding Weaknesses**
  - Learn decision trees or inference network for vehicle properties and faults.
  - Look for unusual conditional fault frequencies.
  - Find causes for these unusual frequencies.
  - Improve construction of vehicle.

- **Improvement of Error Diagnosis in Garages**
  - Learn decision trees or inference network for vehicle properties and faults.
  - Record properties of new faulty vehicle.
  - Test for the most probable faults.

A Simple Approach to Fault Analysis

- Check subnets consisting of an attribute and its parent attributes.
- Select subnets with highest deviation from independent distribution.



Example Subnet

Influence of special equipment on battery faults:

(fictitious) frequency of battery faults		air conditioning with	air conditioning without
electrical sliding roof	with	8 %	3 %
	without	3 %	2 %

- Significant deviation from independent distribution.
- Hints to possible causes and improvements.
- Here: Larger battery may be required, if an air conditioning system. *and* an electrical sliding roof are built in.

(The dependencies and frequencies of this example are fictitious, true numbers are confidential.)

Summary

- **Decomposition:** Under certain conditions a distribution δ (e.g. a probability distribution) on a multi-dimensional domain, which encodes *prior* or *generic knowledge* about this domain, can be decomposed into a set $\{\delta_1, \ldots, \delta_s\}$ of (overlapping) distributions on lower-dimensional subspaces.
- **Simplified Reasoning:** If such a decomposition is possible, it is sufficient to know the distributions on the subspaces to draw all inferences in the domain under consideration that can be drawn using the original distribution δ.
- **Graphical Model:** The decomposition is represented by a graph (in the sense of graph theory). The edges of the graph indicate the paths along which evidence has to be propagated. Efficient and correct evidence propagation algorithms can be derived, which exploit the graph structure.
- **Learning from Data:** There are several highly successful approaches to learn graphical models from data, although all of them are based on heuristics. Exact learning methods are usually too costly.