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Graphical probabilistic models – broadening (time, continuous variables, undirected graphs)

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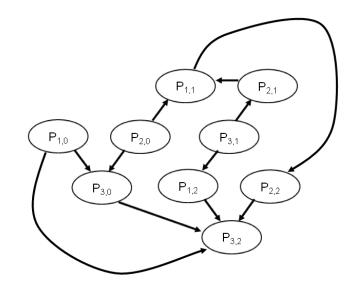
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Outline

- So far we dealt with the "classic" (most simple) BN representation
 - static model,
 - binary variables.
- We will generalize towards
 - dynamic Bayesian networks
 - * capable to capture system development in time,
 - other types of variables
 - * categorical variables, continuous variables and their combinations.
- We will also discuss another type of graphs
 - directed \rightarrow undirected graphs,
 - Markov Random Fields
 - * different properties and application.

Dynamic Bayesian Networks (DBNs)

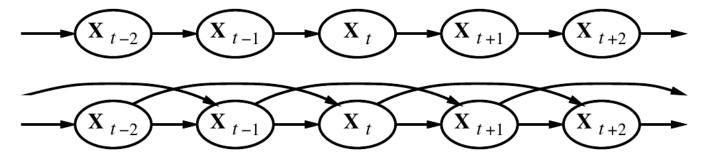
- nodes = variables corresponding to the values of real variables in concrete time,
- real variables re-appear (see $P_{1,t}$, $P_{2,t}$, $P_{3,t}$ in figure),
- edges stand for causal relationship,
- additional constraints must be introduced (otherwise too many possible relationships),



- variable notation (implicit constraints)
 - -t **discrete time** (the choice of step size is problem dependent),
 - $-X_t$ the set of unobservable **state** variables at time t,
 - * $Position_t$, $Velocity_t$, $Acceleration_t$, $Battery_t$, ...
 - $-E_t$ the set of observable **evidence** variables at time t,
 - $* Odometry_t, \dots$
 - $-X_{a:b}-X_a, X_{a+1}, \ldots, X_{b-1}, X_b.$

Dynamic Bayesian Networks (DBNs)

- Constraint #1: *n*th order Markov assumption
 - transition model: $Pr(X_t|X_{0:t-1}) = Pr(X_t|X_{t-n:t-1})$



- sensor model: $Pr(E_t|X_{0:t}, E_{0:t-1}) = Pr(E_t|X_t)$
- Constraint #2: **stationary** process
 - neither transition nor sensor model changes in time

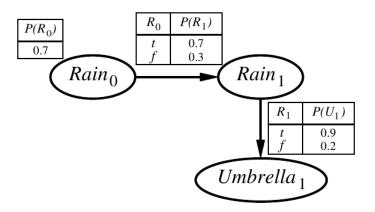
$$\forall t : Pr(X_t | X_{t-n:t-1}) = Pr(X_{t+1} | X_{t-n+1:t})$$

$$\forall t : Pr(E_t|X_t) = Pr(E_{t+1}|X_{t+1})$$

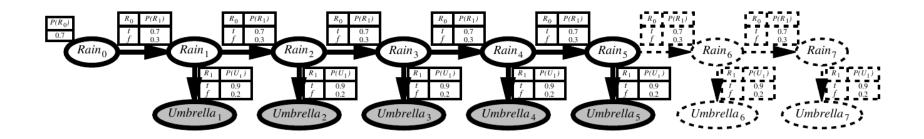
- Under the first-order Markov assumption, DBN can be defined by
 - initial conditions: $Pr(X_0)$,
 - transition and sensor model (for single t only).

DBN example (Russell, Norvig: AIMA)

• the network is defined by the initial conditions and single slice (transition and sensor model)



• the network can be unrolled up to an arbitrary time step.

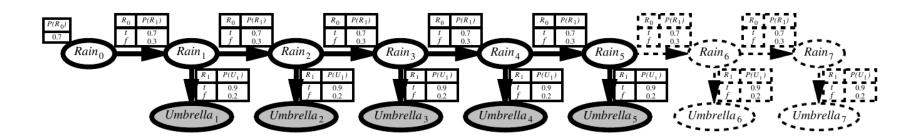


DBN example (Russell, Norvig: AIMA) - continuation

- classical BN inference enumerates prob of arbitrary event given arbitrary evidence,
- naïve approach may ignore the split of variables (state vs evidence), or query the past states,
- what is the difference in prob of rain at day 1 knowing it did not rain at day 4 and umbrellas appeared at day 2?

$$-Pr(r_1) = Pr(r_0, r_1) + Pr(\neg r_0, r_1) = Pr(r_0)Pr(r_1|r_0) + Pr(\neg r_0)Pr(r_1|\neg r_0) = 0.58,$$

- Matlab BNT, jtree_inf_engine: $Pr(r_1|\neg r_4,u_2)=0.68$,
- rain prob at day 1 increased with the evidence,
- the number of time steps can be large/unlimited
 - only specialized tasks can be solved due to computational costs.



DBN inference tasks

- filtering $Pr(X_t|e_{1:t})$
 - get the distribution of current state knowing (all) past evidence variables,
 - the fundamental task in decision making of a rational agent,
- **prediction** $Pr(X_{t+k}|e_{1:t}), k > 0$
 - unlike filtering, a future state is of interest (or filtering without late evidence),
- smoothing $Pr(X_k|e_{1:t})$, $0 \le k < t$
 - improved estimate of past states, essential for learning,
- most likely explanation $\arg\max_{x_{1:t}} Pr(x_{1:t}|e_{1:t})$
 - note it is not repeated smoothing states mutually interact,
 - applied e.g. in speech recognition (speech signal \rightarrow sentence and not the sequence of the most likely characters).

Filtering

- the aim is to devise a recursive state estimation algorithm
 - $-Pr(X_{t+1}|e_{1:t+1}) = f(e_{t+1}, Pr(X_t|e_{1:t})),$
 - filtering at time t and evidence at time $t+1 \rightarrow$ filtering at time t+1,

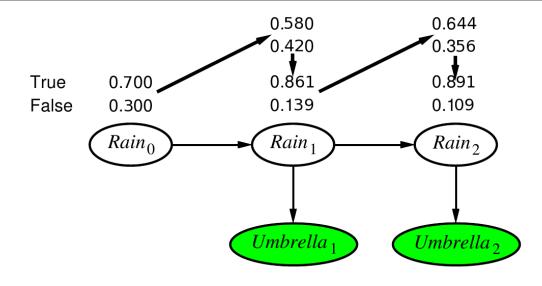
$$\begin{split} Pr(X_{t+1}|e_{1:t+1}) &= Pr(X_{t+1}|e_{1:t},e_{t+1}) = \dots \text{split evidence only} \\ &= \alpha Pr(e_{t+1}|X_{t+1},e_{1:t}) Pr(X_{t+1}|e_{1:t}) = \dots \text{apply Bayes theorem} \\ &= \alpha Pr(e_{t+1}|X_{t+1}) Pr(X_{t+1}|e_{1:t}) \dots \text{follows from Markov property of evidence} \end{split}$$

- filtering was decomposed into
 - prediction $Pr(X_{t+1}|e_{1:t})$ and integration of the last evidence $Pr(e_{t+1}|X_{t+1})$,
- prediction will be solved by summing out X_t

$$-Pr(X_{t+1}|e_{1:t}) = \sum_{x_t} Pr(X_{t+1}|x_t, e_{1:t}) Pr(x_t|e_{1:t}) = \sum_{x_t} Pr(X_{t+1}|x_t) Pr(x_t|e_{1:t}),$$

- ullet the result is a time and space constant (independent of t) recursive function f
 - $-f_{1,t+1} = \mathsf{FORWARD}(f_{1:t},e_{t+1})$, where $f_{1:t} = Pr(X_t|e_{1:t})$

Filtering – example



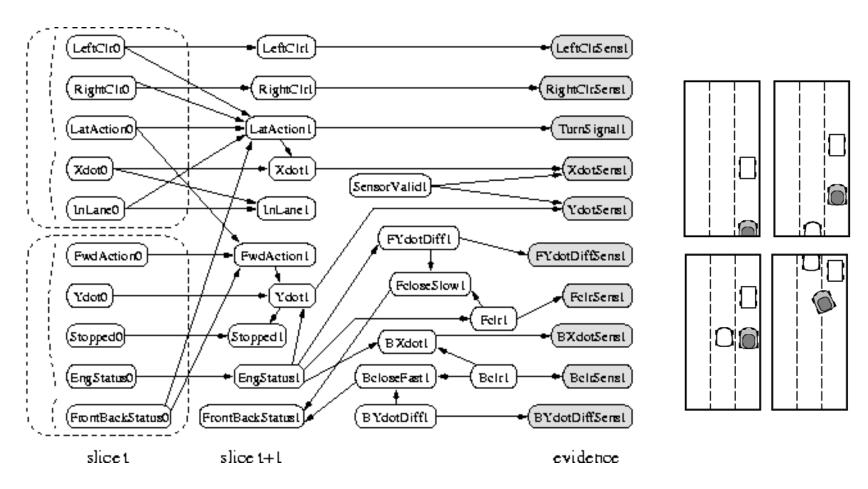
- we observe u_1 and u_2 what is rain prob at day 1 (disregarding u_2) and rain prob at day 2?
 - $-Pr(R_1|u_1) = \alpha_1 Pr(u_1|R_1) \sum_{R_0 \in \{r_0, \neg r_0\}} Pr(R_1|R_0) Pr(R_0),$
 - $-Pr(r_1|u_1) = \alpha_1 \times 0.9 \times (0.7 \times 0.7 + 0.3 \times 0.3) = \alpha_1 \times 0.9 \times 0.58$,
 - $-Pr(\neg r_1|u_1) = \alpha_1 \times 0.2 \times (0.3 \times 0.7 + 0.7 \times 0.3) = \alpha_1 \times 0.2 \times 0.42,$
 - $-\alpha_1 = 1.65 \rightarrow Pr(r_1|u_1) = 0.861, Pr(\neg r_1|u_1) = 0.139$
 - $-Pr(R_2|u_1,u_2)=lpha_2Pr(u_2|R_2)\sum_{R_1\in\{r_1,\neg r_1\}}Pr(R_2|R_1)Pr(R_1|u_1)$,
 - $-Pr(r_2|u_1, u_2) = \alpha_2 \times 0.9 \times (0.7 \times 0.861 + 0.3 \times 0.139) = \alpha_2 \times 0.9 \times 0.644,$
 - $-Pr(\neg r_2|u_1, u_2) = \alpha_2 \times 0.2 \times (0.3 \times 0.861 + 0.7 \times 0.139) = \alpha_2 \times 0.2 \times 0.356,$
 - $-\alpha_2 = 1.54 \rightarrow Pr(r_2|u_1,u_2) = 0.891$, $Pr(\neg r_2|u_1,u_2) = 0.109$

DBN vs HMM

- Hidden Markov Model (HMM)
 - frequent application in speech recognition or biomedicine,
- HMM is a special (and trivial) case of dynamic Bayesian network
 - state is described by the only variable (usually there is a single evidence variable as well),
 - i.e., Rain-Umbrella example represents both DBN and HMM,
- HMM is a statistical model doable by polynomial algorithms in the number of time steps
 - works in simple worlds = the state and sensor variable have a reasonable number of values
 - * a set of discrete (evidence or state) variables can make a single variable (whose values correspond to tuples),
 - simple tasks prevail, HMMs appear more frequently than their DBN generalizations,
 - however, DBNs are more efficient than HMMs in complex tasks with sparse dependencies
 - * DBN decomposes complex systems using independence,
 - * exponentially fewer parameters than HMMs,
 - * ex.: 10 binary state variables, 2 parents each
 - · DBN has $10 \times 2^2 = 400$ parameters, HMM has $2^{10} \times 2^{10} \approx 10^6$ parameters.

Bayesian Automated Taxi (project, IJCAI paper, 1995)

- the project of autonomous vehicle in regular highway traffic
 - overtaking a slower vehicle and bypassing a stationary vehicle,
 - response to the maneuvers of other drivers or to the change of the number of lanes.



DBNs – overview

- so far, we applied BNs to model constant relationships among different variables
 - time was not concerned,
 - or the model captured a single moment.
- often we need to track time changes
 - the state of the world is described and its dynamics is modeled,
- for the sake of feasibility, constraints must be introduced
 - Markov assumption: the current state depends solely on a limited history of past states,
 - stationarity: transition and evidence probabilities do not change in time, slices stay identical,
 - discrete time: slices (world states at particular time steps) can be distinguished,
 - explicit prior split of variables: hidden/state and observable/evidence variables,
- for each time step a whole slice (state and sensor model) is copied
 - the network is unrolled then,
 - DBN can be understood as an equivalent of static BN,
 - however, this analogy is rarely used due to complexity reasons,
 - new standard tasks: filtering, prediction, smoothing, most likely explanation.

Other types of variables in BN

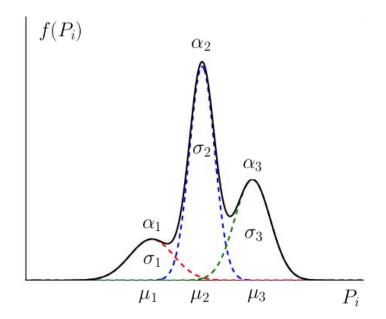
- BN must record $Pr(P_i|parents(P_i))$ by definition
 - CPT is a special case of more general conditional probability distribution (CPD),
- categorical variables
 - (can take on one of a limited, and usually fixed, number of possible values),
 - CPTs again, they just may grow more quickly with the number of parents,
 - $* q_i$... the number of unique instantiations of P_i parents,,
 - * r_i ... the number of distinct P_i values,
 - * r . . . the maximum number of distinct values of one network variable $(r = \max_{i=1}^n r_i)$,
 - * the total number of independent BN parameters

$$K = \sum_{i=1}^{n} q_i(r_i - 1)$$
,

- * for binary variables $r_i = 2$ a $q_i = 2^{|parents(P_i)|}$,
- * for categorical variables $2 \le r_i \le r$ a $q_i \le r^{|parents(P_i)|}$.

Other types of variables in BN

- continuous variables
 - CPT gets infinite, discretization \rightarrow categorical variable
 - * dilemma: large CPTs vs information loss,
 - representation/approximation with canonical probability distributions
 - * finite, often simple parametrization,
 - * the most often option: normal (Gaussian) distribution and its mixtures,
 - * figure: definition of a continuous node without any parent with 9 parameters.

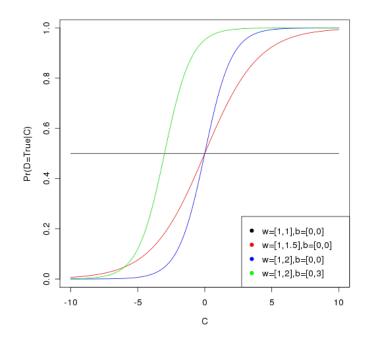


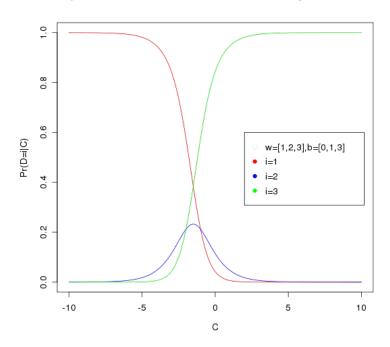
Categorical variable with a continuous parent

- ullet CPD for a categorical child D with a continuous parent C
 - soft thresholding using softmax function (multinomial logistic function)

$$Pr(D = d_i | C = c) = \frac{e^{w_i \times c + b_i}}{\sum_{j=1}^{|D|} e^{w_j \times c + b_j}}$$

- $ec{w}$ gives softness (slope) of the threshold, $ec{b}$ gives position of the threshold,
- applicable even for multiple continuous parents
 - $-\mathbf{W}$ and \mathbf{B} in a matrix format, contribution of the individual parents gets combined,
- binary D o softmax pprox sigmoid function,
- ternary D probabilities of target values,





Continuous child node, hybrid parents

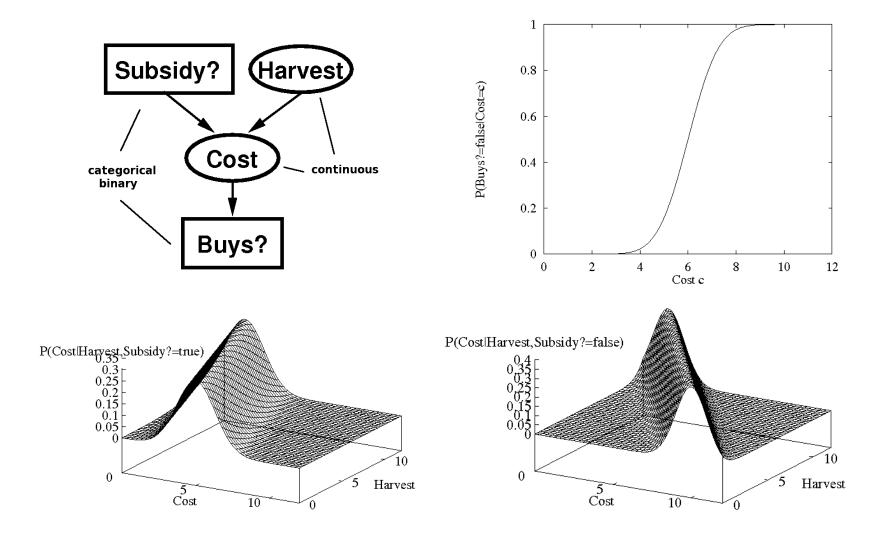
- lacksquare a continuous child C_p having continuous parent C_r and categorical parent D
 - the most common CPD form is the linear Gaussian (LG) model
 - * mean child value varies linearly with the continuous parent, variance is fixed,

$$Pr(C_p = c_p | C_r = c_r, D = d) = N(\mu_d = a_d c_r + b_d, \sigma_d)$$

- * reasonable model provided that the range of continuous parent is likely to be narrow,
- we define a LG child function for each value of categorical parent
 - * for each value d a distinct set of parameters a_d , b_d and σ_d is defined,
- generalization for more parents
 - mean child value corresponds to a linear combination of values of continuous parents,
 - a new LG parametrization must be given for each possible assignment to categorical parents when having more of them.

Continuous nodes – example (Russell, Norvig: AIMA)

• Fruit sales are influenced by price, the price is given by harvest yields and government subsidy.

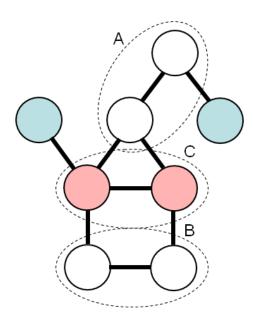


Continuous variables – summary

- parametrization of continuous variables CPDs
 - commonly with normal distribution and its mixtures, linearized by continuous parents,
 - in general not more difficult/demanding than for categorical variables,
 - several combinations for connections wrt node types exist (see BNT for Matlab),
- the global joint probability model
 - having categorical softmax nodes and continuous LG nodes . . .
 - ...joint probability takes a form of multivariate Gaussian
 - (over all continuous variables for each combination of discrete variable values).
- inference in principle does not change
 - nevertheless, more difficult, all the algorithms cannot be applied,
 - they need to be generalized (dealing with atomic events etc.),
- new methods for learning from data appear
 - softmax is in BNT learned by the iteratively reweighted least squares (IRLS) algorithm,
 - for other node and connection models other dedicated algorithms.

Undirected graphs

- undirected graph model = Markov network = Markov Random Field (MRF),
- the same aim as the directed models
 - to factorize/decompose the joint probability using conditional independence,
- notion of conditional independence in undirected graphs
 - simple graph separation in comparison with directed d-separation it is trivial,
 - $-A \perp\!\!\!\perp B|C$: all the paths from A from B must disappear when all the nodes in C removed.



Undirected graphs

- joint probability factorization is based on the definition of conditional independence
 - for two nodes not connected by an edge it holds

$$Pr(P_i, P_j | P_{\langle i,j \rangle}) = Pr(P_i | P_{\langle i,j \rangle}) Pr(P_j | P_{\langle i,j \rangle})$$

Hammersley-Clifford theorem

$$Pr(P_1,\ldots,P_n) = \frac{1}{Z} \prod_{C \in mcl\{G\}} \psi_C(P_C)$$

Z ... normalization const, $mcl\{G\}$... set of maximal cliques G, ψ_C ... potential function

- possible difficulties
 - factors (usually) do not have interpretation (they are not probabilities),
 - product of factors must be normalized (to express the joint probability),
- potential functions
 - HC theorem assumes their strict positivity,
 - traditionally given as an exponential energy function E $\psi_C(P_C) = \exp^{-E(P_C)}$
 - joint probability corresponds to the sum of energies of all maximal cliques.

MRF: example (Bishop: Graphical models, chapter 8)

• noise filtering in a binary image (2 colors)

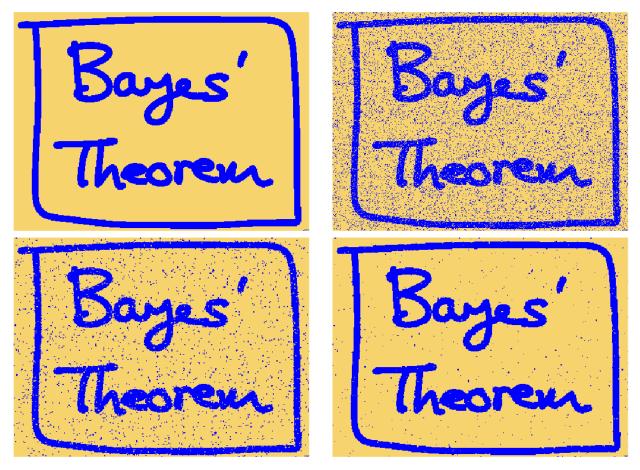
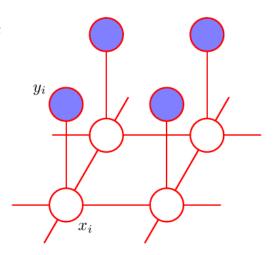


Figure 8.30 Illustration of image de-noising using a Markov random field. The top row shows the original binary image on the left and the corrupted image after randomly changing 10% of the pixels on the right. The bottom row shows the restored images obtained using iterated conditional models (ICM) on the left and using the graph-cut algorithm on the right. ICM produces an image where 96% of the pixels agree with the original image, whereas the corresponding number for graph-cut is 99%.

MRF: example (Bishop: Graphical models, chapter 8)

- structure of the model is proposed a priori
 - color of the adjacent pixels strongly correlated,
 - distant pixels can be ignored (distant=not an immediate neighbor \rightarrow first-order model)
 - * a regular grid of nodes X_i , $X_i \in \{-1, 1\}$
 - noise is modeled by another "layer" of nodes Y_i , $Y_i \in \{-1, 1\}$
 - * low-level noise $(Pr(noise) \ll 0.5)$
 - \rightarrow strong correlation with X_i ,
 - two types of maximal cliques with 2 nodes
 - * adjacent X_i and X_j , connected Y_i and X_i ,
- corresponds to the Ising model.



MRF: example (Bishop: Graphical models, chapter 8)

- learning of joint probability Pr(X, Y)
 - clique energy: $-\eta X_i Y_i$ and $-\beta X_i X_j$,
 - * η and β positive parametrization constants,
 - * in case of agreement of node signs the energy is lower and the probability is higher,
 - the energy function

$$E(X, Y) = h \sum_{i} X_i - \beta \sum_{\{i,j\}} X_i X_j - \eta \sum_{i} X_i Y_i$$

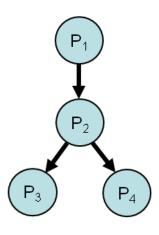
- * first term prefers one of the colors (background color is more frequent a priori),
- the target probability

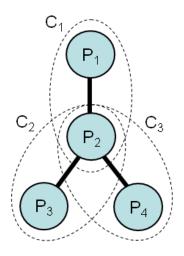
$$Pr(X, Y) = \frac{1}{Z} \prod_{C} \psi_{C}(P_{C}) = \frac{1}{Z} \exp{-E(X, Y)}$$

- de-noising = learning of the model
 - $-Y_i$ is observed (noisy image), we search for X_i such that Pr(X,Y) is maximized,
 - can be done by a gradient-descent algorithm (which concerns pixel coordinates)
 - 1. initialization \mathbb{X} ($\forall i \ X_i = Y_i$),
 - 2. $\forall i$ gradually and repeatedly (in a random order or in a systematic order)
 - (a) determine the total energy for $X_i = +1$ and $X_i = -1$,
 - (b) take the setting with the lower energy,
 - 3. stop if energy did not decrease (after all the cycle $\forall i$).

Transformation from directed to undirected model

- an important part of the junction tree inference algorithm,
- clique potentials must concern the conditional probabilities in directed graph,
- this is easy to meet in directed graphs where nodes have at most one parent.





$$Pr(P_1, ..., P_4) = \psi_{C_1}(P_{C_1}) = \psi_{1,2}(P_1, P_2) = Pr(P_1)Pr$$

= $Pr(P_1)Pr(P_2|P_1)Pr(P_3|P_2)Pr(P_4|P_2) \quad \psi_{C_2}(P_{C_2}) = \psi_{2,3}(P_2, P_3) = Pr(P_3|P_2)$

$$Pr(P_1, \dots, P_4) = \frac{1}{Z} \prod_i \psi_{C_i}(P_{C_i})$$

$$\psi_{C_1}(P_{C_1}) = \psi_{1,2}(P_1, P_2) = Pr(P_1)Pr(P_2|P_1)$$

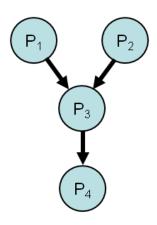
$$\psi_{C_2}(P_{C_2}) = \psi_{2,3}(P_2, P_3) = Pr(P_3|P_2)$$

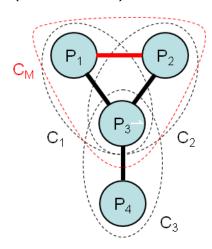
$$\psi_{C_3}(P_{C_3}) = \psi_{2,4}(P_2, P_4) = Pr(P_4|P_2)$$

$$Z = 1$$

Transformation from directed to undirected model

- the networks with converging nodes must be moralized (see junction tree algorithm),
 - otherwise, there are some conditional probs that cannot be applied within any of the cliques!
 - undirected graph would encode a different set of (conditional) independence relationships.





$$Pr(P_1, ..., P_4) =$$

= $Pr(P_1)Pr(P_2)Pr(P_3|P_1, P_2)Pr(P_4|P_3)$

$$Pr(P_1, \dots, P_4) = \frac{1}{Z} \prod_i \psi_{C_i}(P_{C_i}) \quad (Z = 1)$$

$$\psi_{C_M}(P_{C_M}) = \psi_{1,2,3}(P_1, P_2, P_3) =$$

$$= Pr(P_1)Pr(P_2)Pr(P_3|P_1, P_2)$$

$$\psi_{C_3}(P_{C_3}) = \psi_{3,4}(P_3, P_4) = Pr(P_4|P_3)$$

• transformation from undirected to directed model more difficult and less frequent.

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Summary

- BNs belong to a large class of graphical stochastic models,
- BN frequently used in
 - knowledge-based systems, causal diagrams,
- changes in the formalism or additional constraints lead to models applicable in other domains
 - BN vs DBN/HMM
 - * speech recognition, signal processing, time series,
 - BN vs MRF
 - * gases and fluids, society, images,
- variables can be both discrete and continuous
 - for simplicity and educational reasons this course focused on binary variables.

Applications of Bayesian networks

- PATHFINDER (Stanford, 1980')
 - diagnosis of the lymph nodes diseases,
 - tested on 53 patients, diagnostics outperformed the best pathologists,
 - followed by a series of medical diagnostic systems,
- other diagnostic systems/applications
 - interpretation of electromyography (EMG),
 - gas turbines,
 - corn yields,
- gene expression modeling
 - mutual interactions among genes (gene regulatory networks),
 - G1 encodes an enzyme that stimulates expression of another gene G2,
 - G1 "causes" G2.
- interactive problem solving in MS Windows systems
 - troubleshoots both HW and SW problems,
 - similarly car diagnostics, jet engines etc,
- modeling in geology, hydrology, sociology,
- among others BN Weka classifier.

BN – summary

- probability is a rigorous tool for uncertainty modeling,
- each atomic event has its joint probability,
- queries answered by aggregation (adding with subsequent division) of atomic events,
- needs to be simplified in non-trivial domains,
- the tool is independence and conditional independence
 - Bayesian network = graph (ind. relationships) + conditional probability distributions (quantities),
 - inference is still NP-hard wrt to the number of variables,
 - solution can be in special network types (singly connected, sparse networks), ex.: trees –
 at most one parent,
 - or approximate inference,
- BNs can be learned from data, two tasks exist
 - parameter learning, less difficult, can be seen as a subtask of . . .
 - structure learning.

Advantages of Bayesian networks

- the problem structure given as a graph is clear and its semantics understandable for user
 - it can naturally be interpreted in the cause-effect way, one can also manually generate it,
 - it implements both causal and diagnostic inference,
 - evidence can be propagated in an arbitrary way a universal model,
 - for comparison, a neural network as a "black box",
- ability to merge prior knowledge with data
 - existing network (typically outlined by an expert) can be modified to explain the data,
 - learning purely from data is a special case (empty/random init model),
- theoretically sound, robust, widely applicable
 - small modifications in model result in small perturbations in results, does not overfit,
 - application in exploration analysis, classification or regression,
- ability to deal with missing values and hidden variables
 - model can estimate a missing value given its relations to other values/variables,
 - hidden variable may explain "suspicious" dependency between two observed variables,
- what stands against?
 - learning is difficult,
 - there is no general and widely-applicable algorithm applicable without its understanding.

Recommended reading, lecture resources

- Russel, Norvig: AI: A Modern Approach, Uncertain Knowledge and Reasoning (Part IV)
 - representation of CPDs with continuous variables,
 - temporal probability models (chap. 15, not in the first edition),
 - Google books (isbn:0136042597),
- Murphy: A Brief Introduction to Graphical Models and Bayesian Networks.
 - BN Toolbox and continuous variables?
 - http://www.cs.ubc.ca/~murphyk/Bayes/bayes.html,
- Bishop: Pattern Recognition & Machine Learning, Graphical Models (Chapter 8)
 - a general chapter, in this lecture it inspired the part on undirected graphs,
 - http://research.microsoft.com/en-us/um/people/cmbishop/prml/Bishop-PRML-sample.pdf.
- Forbes et al.: The BATmobile: Towards a Bayesian Automated Taxi, IJCAI 1995
 - TAXI case study,
 - http://www.cs.berkeley.edu/~russell/papers/ijcai95.



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