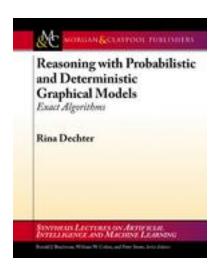
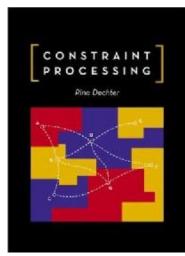
Algorithms for Probabilistic and Deterministic graphical Models

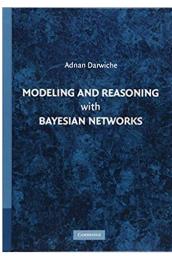
Class 1 Rina Dechter

Dechter-Morgan&claypool book (Dechter 1 book): Chapters 1-2

Text Books







Outline

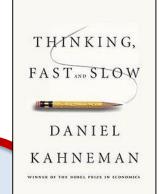
Class page

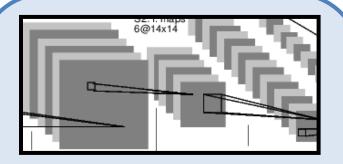
- Introduction: Constraint and probabilistic graphical models.
- Constraint networks: Graphs, modeling, Inference
- Inference in constraints: Adaptive consistency, constraint propagation, arc-conistency
- Graph properties: induced-width, tree-width, chordal graphs, hypertrees, join-trees
- Bayesian and Markov networks: Representing independencies by graphs
- Building Bayesian networks.
- Inference in Probabilistic models: Bucket-elimination (summation and optimization), Tree-decompositions, Join-tree/Junction-tree algorithm
- Search in CSPs: Backtracking, pruning by constraint propagation, backjumping and learning
- Search in Graphical models: AND/OR search Spaces for likelihood, optimization queries
- Approximate Bounded Inference: weighted Mini-bucket, belief-propagation, generalized belief propagation
- Approximation by Sampling: MCMC schemes, Gibbs sampling, Importance sampling
- Causal Inference with causal graphs.

Course Requirements/Textbook

- Homeworks: There will be 5-6 problem sets, graded 50% of the final grades.
- A term project: paper presentation, a programming project (20%).
- Final (30%)
- Books:
 - "Reasoning with probabilistic and deterministic graphical models", R. Dechter, Claypool, 2013
 https://www.morganclaypool.com/doi/abs/10.2200/S00529ED1V01Y201308AIM023
 - "Modeling and Reasoning with Bayesian Networks", A. Darwiche, MIT Press, 2009.
 - 。"Constraint Processing", R. Dechter, Morgan Kauffman, 2003

Al Renaissance

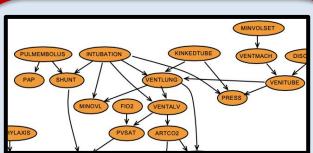




- Deep learning
 - Fast predictions
 - "Instinctive"

Tools:

Tensorflow, PyTorch, ...



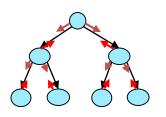
- Probabilistic models
 - Slow reasoning
 - "Logical / deliberative"

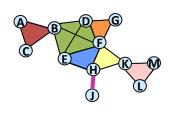
Tools:

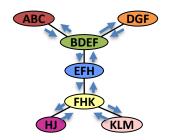
Graphical Models,
Probabilistic programming,
Markov Logic, ...

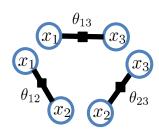
Outline of classes

Part 1: Introduction and Inference

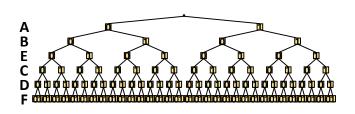


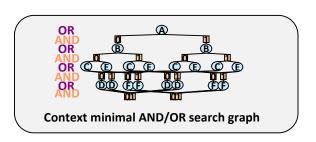




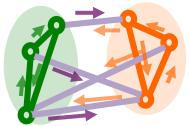


Part 2: Search



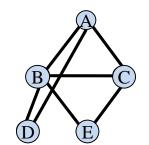


Parr 3: Variational Methods and Monte-Carlo Sampling



RoadMap: Introduction and Inference

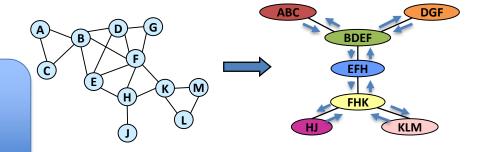
- Basics of graphical models
 - Queries
 - Examples, applications, and tasks
 - Algorithms overview

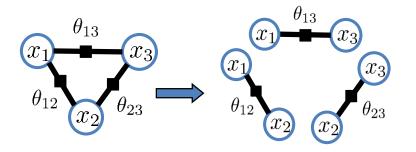


- Inference algorithms, exact
 - Bucket elimination for trees
 - Rucket alimination

For Constraints first

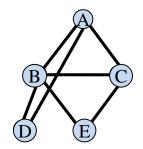
- - Decomposition bounds
 - Mini-bucket & weighted mini-bucket
 - Belief propagation
- Summary and Part 2

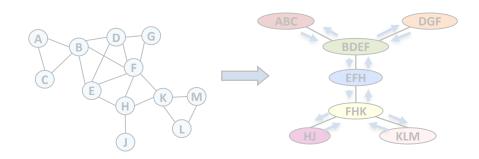




RoadMap: Introduction and Inference

- Basics of graphical models
 - Queries
 - Examples, applications, and tasks
 - Algorithms overview
- Inference algorithms, exact
 - Bucket elimination for trees
 - Bucket elimination
 - Jointree clustering
 - Elimination orders
- Approximate elimination
 - Decomposition bounds
 - Mini-bucket & weighted mini-bucket
 - Belief propagation
- Summary and Class 2







Probabilistic Graphical models

- Describe structure in large problems
 - Large complex system F(X)
 - Made of "smaller", "local" interactions $f_{lpha}(x_{lpha})$
 - Complexity emerges through interdependence

Probabilistic Graphical models

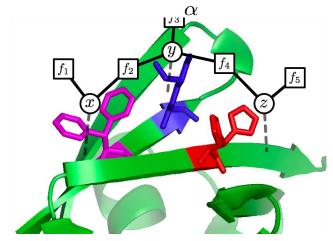
- Describe structure in large problems
 - Large complex system F(X)
 - Protein Structure prediction: predicting the 3d structure from given sequences
 - PDB: Protein design (backbone) algorithms enumerate a combinatorial number of candidate structures to compute the Global Minimum Energy Conformation (GMEC).

$$\mathbf{x}^* = \arg\max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

Phenylalanine

[Yanover & Weiss 2002] [Bruce R. Donald et. Al. 2016]

$$f(\mathbf{x}^*) = \max_{\mathbf{x}} \prod f_{\alpha}(\mathbf{x}_{\alpha})$$



Probabilistic Graphical models

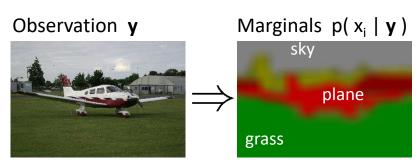
- Describe structure in large problems
 - Large complex system F(X)
 - Made of "smaller", "local" interactions $f_{\alpha}(x_{\alpha})$
 - Complexity emerges through interdependence
- **Examples & Tasks**
 - Summation & marginalization

$$p(x_i) = rac{1}{Z} \sum_{\mathbf{x} \setminus x_i} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$
 and $Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

"partition function"

$$Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

Image segmentation and classification:



Observation **y** Marginals $p(x_i | y)$ cow grass

e.g., [Plath et al. 2009]

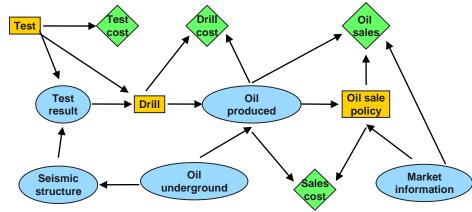
Graphical models

- Describe structure in large problems
 - Large complex system F(X)
 - Made of "smaller", "local" interactions $f_{lpha}(x_{lpha})$
 - Complexity emerges through interdependence
- Examples & Tasks
 - Mixed inference (marginal MAP, MEU, ...)

$$f(\mathbf{x}_{M}^{*}) = \max_{\mathbf{x}_{M}} \sum_{\mathbf{x}_{S}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

Influence diagrams & optimal decision-making

(the "oil wildcatter" problem)



e.g., [Raiffa 1968; Shachter 1986]

In more details...

Constraint Networks

Example: map coloring

Variables - countries (A,B,C,etc.)

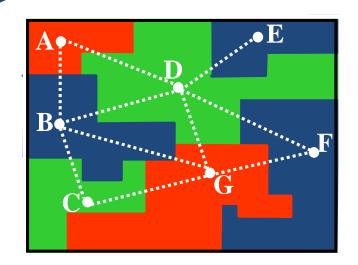
Values - colors (red, green, blue)

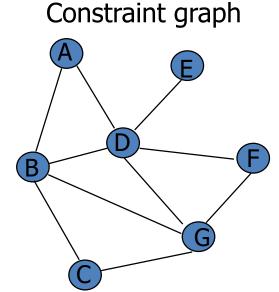
Constraints:

 $A \neq B$, $A \neq D$, $D \neq E$, etc.

A B

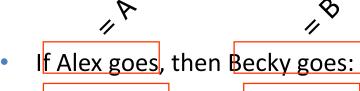
red green
red yellow
green red
green yellow
yellow green
yellow red





Propositional Reasoning

Example: party problem



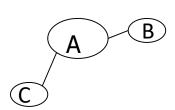
$$A \rightarrow B$$

• If Chris goes, then Alex goes:

$$C \rightarrow A$$



Is it possible that Chris goes to the party but Becky does not?

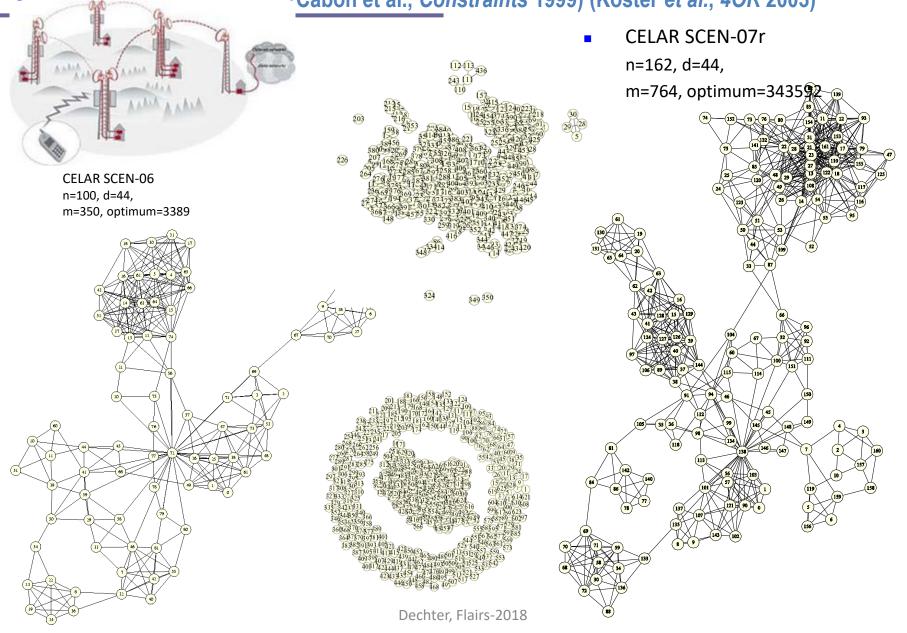


Is the *propositional theory*

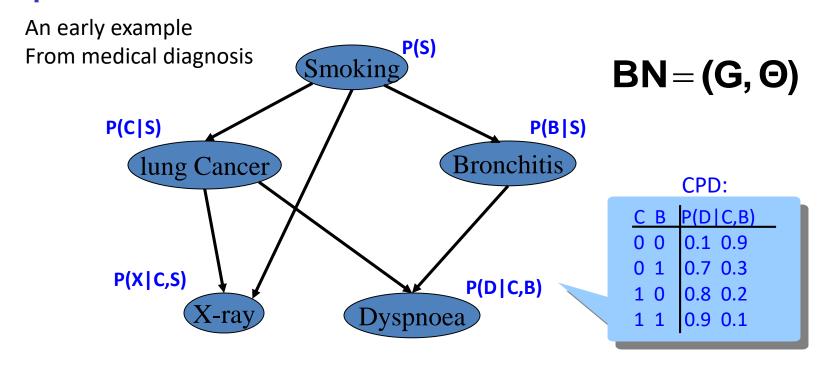
$$\varphi = \{A \rightarrow B, C \rightarrow A, \neg B, C\}$$
 satisfiable?

Radio Link Frequency Assignment Problem

'Cabon et al., Constraints 1999) (Koster et al., 4OR 2003)



Bayesian Networks (Pearl 1988)



P(S, C, B, X, D) = P(S) P(C/S) P(B/S) P(X/C,S) P(D/C,B)

Combination: Product Marginalization: sum/max

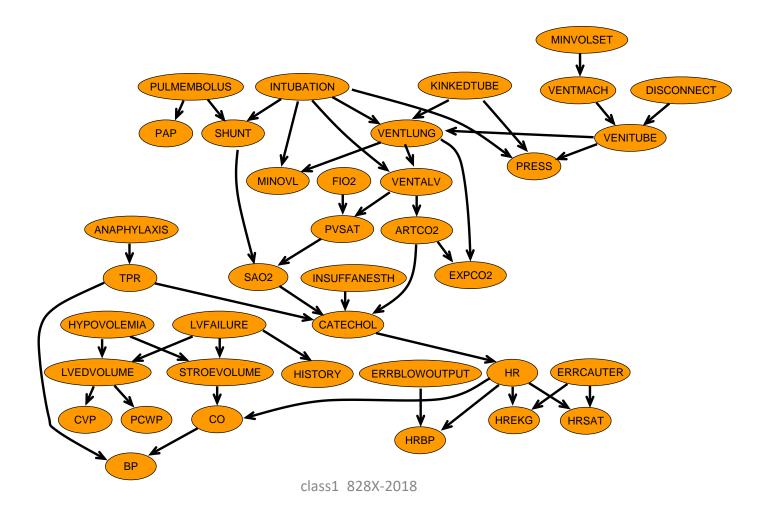
- Posterior marginals, probability of evidence, MPE
- P(D= 0) = $\sum_{S,L,B,X} P(S) \cdot P(C|S) \cdot P(B|S) \cdot P(X|C,S) \cdot P(D|C,B)$ MAP(P)= $\max_{S,L,B,X} P(S) \cdot P(C|S) \cdot P(B|S) \cdot P(X|C,S) \cdot P(D|C,B)$

Alarm network

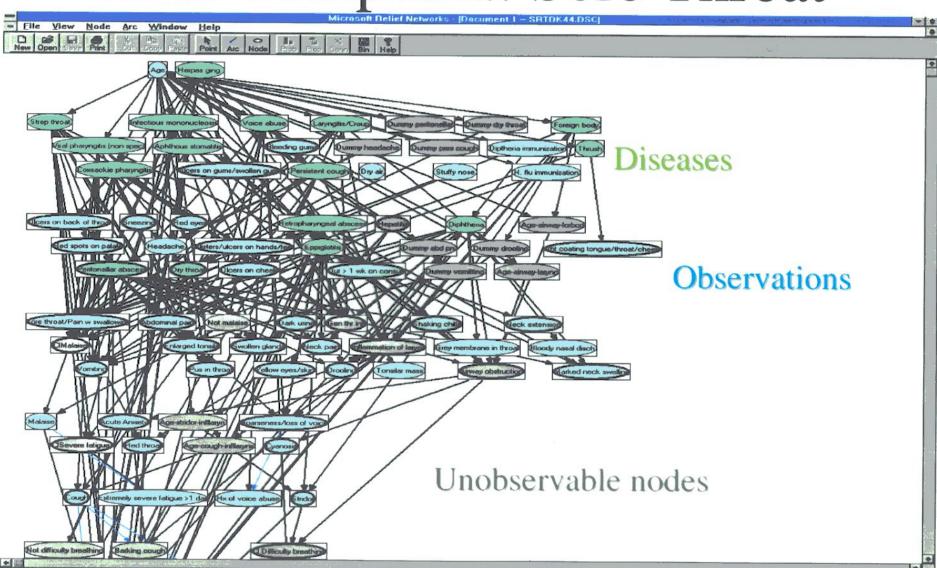
[Beinlich et al., 1989]

Bayes nets: compact representation of large joint distributions

The "alarm" network: 37 variables, 509 parameters (rather than $2^{37} = 10^{11}$!)



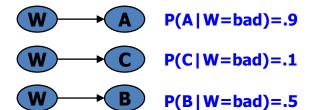
Chief Complaint: Sore Throat



Probabilistic reasoning (directed)

Party example: the weather effect

- Alex is-<u>likely</u>-to-go in bad weather
- Chris <u>rarely</u>-goes in bad weather
- Becky is indifferent but <u>unpredictable</u>



P(W)

Questions:

 Given bad weather, which group of individuals is most likely to show up at the party?

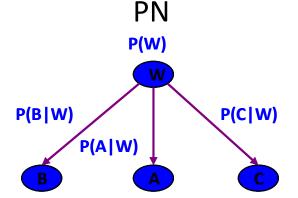
• What is the probability that Chris goes to the party but Becky does not?

	W	Α	P(A W)	
	good	0	.01	
	good	1	.99	
	bad	0	.1	
	bad	1	.9	
-				

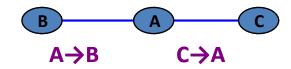
$$P(W,A,C,B) = P(B|W) \cdot P(C|W) \cdot P(A|W) \cdot P(W)$$
 $P(A,C,B|W=bad) = 0.9 \cdot 0.1 \cdot 0.5$
 $P(B|W) \quad P(C|W)$

Mixed Probabilistic and Deterministic networks

Alex is-<u>likely</u>-to-go in bad weather Chris <u>rarely</u>-goes in bad weather Becky is indifferent but <u>unpredictable</u>



CN



Query:

Is it likely that Chris goes to the party if Becky does not but the weather is bad?

$$P(C, \neg B \mid w = bad, A \rightarrow B, C \rightarrow A)$$

Graphical models (cost networks)

A graphical model consists of:

$$X=\{X_1,\ldots,X_n\}$$
 -- variables $D=\{D_1,\ldots,D_n\}$ -- domains (we'll assume discrete)

$$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$$
 -- functions or "factors"

and a combination operator

Example:

$$A \in \{0, 1\}$$
$$B \in \{0, 1\}$$

$$C \subset \{0,1\}$$

$$C \in \{0, 1\}$$

$$f_{AB}(A,B), \quad f_{BC}(B,C)$$

The combination operator defines an overall function from the individual factors,

e.g., "+" :
$$F(A, B, C) = f_{AB}(A, B) + f_{BC}(B, C)$$

Notation:

Discrete Xi values called states

Tuple or configuration: states taken by a set of variables

Scope of f: set of variables that are arguments to a factor f often index factors by their scope, e.g., $f_{\alpha}(X_{\alpha}), \quad X_{\alpha} \subseteq X$

Graphical models (cost networks)

A *graphical model* consists of:

$$X = \{X_1, \dots, X_n\}$$
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 -- functions or "factors"

Example:

$$A \in \{0, 1\}$$

$$B \in \{0, 1\}$$

$$C \in \{0, 1\}$$

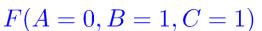
$$f_{AB}(A,B), \quad f_{BC}(B,C)$$

and a combination operator

$$F(A, B, C) = f_{AB}(A, B) + f_{BC}(B, C)$$

For discrete variables, think of functions as "tables" (though we might represent them more efficiently)

A	В	f(A,B)
0	0	6
0	1	0
1	0	0
1	1	6



В	С	f(B,C)
0	0	6
0	1	0
1	0	0
1	1	6



	f(A,B,C)	C	В	A
	12	0	0	0
	6	1	0	0
	0	0	1	0
= 0	6	1	1	0
	6	0	0	1
	0	1	0	1
	6	0	1	1
	12	1	1	1

+6

Graph Visualiization: Primal Graph

A graphical model consists of:

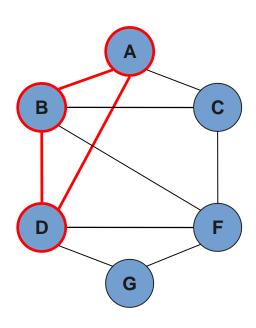
 $X=\{X_1,\ldots,X_n\}$ -- variables $D=\{D_1,\ldots,D_n\}$ -- domains $F=\{f_{\alpha_1},\ldots,f_{\alpha_m}\}$ -- functions or "factors"

and a combination operator

Primal graph:

variables → nodes factors → cliques

$$F(A, B, C, D, F, G) = f_1(A, B, D) + f_2(D, F, G) + f_3(B, C, F) + f_4(A, C)$$



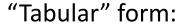
Example: Constraint networks

$$X_i \in \{ red, green, blue \}$$

$$f_{ij}(X_i,X_j)=(X_i
eq X_j)$$
 for adjacent regions i,j

Overall function is "and" of individual constraints:

$$F(X) = f_{01}(X_0, X_1) \wedge f_{12}(X_1, X_2) \wedge f_{02}(X_0, X_2) \wedge \dots$$

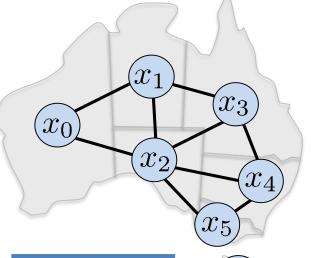


$$f_{ij}(X_i, X_j) = \begin{cases} 1.0 & X_i \neq X_j \\ 0.0 & X_i = X_j \end{cases}$$

$$F(X) = \prod_{ij} f_{ij}(X_i, X_j) = \begin{cases} 1.0 & \text{all valid} \\ 0.0 & \text{any invalid} \end{cases}$$

Tasks: "max": is there a solution?

"sum": how many solutions?



X ₀	X ₁	$f(X_0, X_1)$
0	0	0
0	1	1
0	2	1
1	0	1
1	1	0
1	2	1
2	0	1
2	1	1
2	2	0

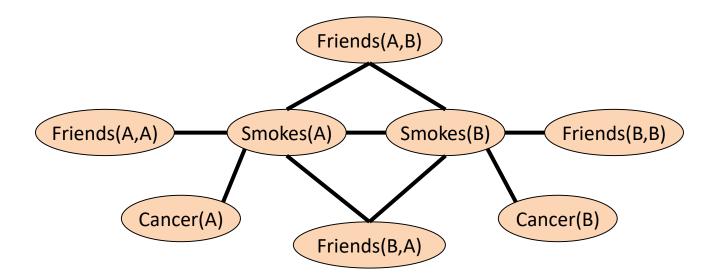
Markov logic, Markov networks

[Richardson & Domingos 2005]

1.5
$$\forall x \ Smokes(x) \Rightarrow Cancer(x)$$

1.1 $\forall x, y \ Friends(x, y) \Rightarrow (Smokes(x) \Leftrightarrow Smokes(y))$

Two constants: **Anna** (A) and **Bob** (B)



SA	CA	$f(S_A, C_A)$
0	0	exp(1.5)
0	1	exp(1.5)
1	0	1.0
1	1	exp(1.5)

F _{AB}	SA	S _B	f(.)
0	0	0	exp(1.1)
0	0	1	exp(1.1)
0	1	0	exp(1.1)
0	1	1	exp(1.1)
1	0	0	exp(1.1)
1	0	1	1.0
1	1	0	1.0
1	1	1	exp(1.1)

Graphical visualization

A graphical model consists of:

$$X = \{X_1, \dots, X_n\}$$
 -- variables $D = \{D_1, \dots, D_n\}$ -- domains

$$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$$
 -- functions or "factors"

and a combination operator

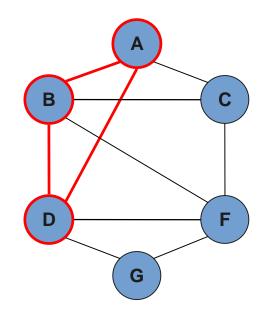


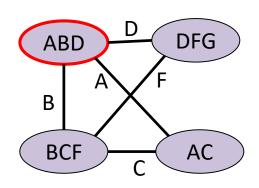
variables
$$\rightarrow$$
 nodes factors \rightarrow cliques

$$F(A, B, C, D, F, G) = f_1(A, B, D) + f_2(D, F, G) + f_3(B, C, F) + f_4(A, C)$$

Dual graph:

factor scopes → nodes edges → intersections (separators)



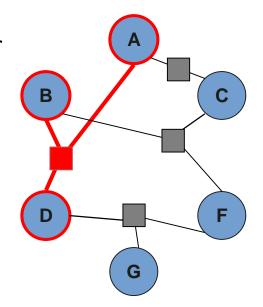


Graphical visualization

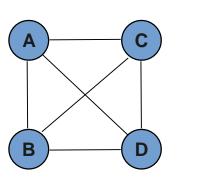
"Factor" graph: explicitly indicate the scope of each factor variables → circles

factors → squares

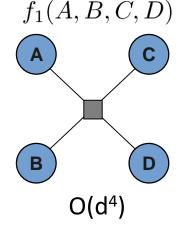
$$F(A, B, C, D, F, G) = f_1(A, B, D) + f_2(D, F, G) + f_3(B, C, F) + f_4(A, C)$$



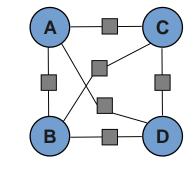
Useful for disambiguating factorization:



?



 $f_1(A,B) + f_2(A,C) + \dots$



VS.

pairwise: O(d²)

Graphical models

A *graphical model* consists of:

$$X = \{X_1, \dots, X_n\}$$
 -- variables

$$D = \{D_1, \ldots, D_n\}$$
 -- domains

$$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$$
 -- functions or "factors"

Operators:

combination operator (sum, product, join, ...)

elimination operator (projection, sum, max, min, ...)

Types of queries:

Marginal: $Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

MPE / MAP: $f(\mathbf{x}^*) = \max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

Marginal MAP: $f(\mathbf{x}_M^*) = \max_{\mathbf{x}_M} \sum_{\mathbf{x}_S} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

Conditional Probability Table (CPT) Relation A C F | P(F|A,C)0.96 green blue 0.40 red blue 0.60 blue 0.35 red green 0.65 0.72 0.68 $f_i := (F = A + C)$ $(A \lor C \lor F)$ В Primal graph (interaction graph) Ε

- All these tasks are NP-hard
 - exploit problem structure
 - identify special cases
 - approximate

Graphical models/reasoning task

Definition 2.1.2 (graphical model) A graphical model \mathcal{M} is a 4-tuple, $\mathcal{M} = \langle X, D, F, \otimes \rangle$, where:

- 1. $X = \{X_1, \ldots, X_n\}$ is a finite set of variables;
- 2. $D = \{D_1, \ldots, D_n\}$ is the set of their respective finite domains of values;
- 3. $\mathbf{F} = \{f_1, \dots, f_r\}$ is a set of positive real-valued discrete functions, defined scopes of $variables S_i \subseteq X$,
- 4. \otimes is a combination operator¹ (e.g., $\otimes \in \{\prod, \sum, \bowtie\}$ (product, sum, join)).

The graphical model represents a global function whose scope is X which is the combination of all its functions: $\bigotimes_{i=1}^r f_i$.

Definition 2.1.3 (a reasoning problem) A reasoning problem over a graphical model $\mathcal{M} = \langle X, D, F, \otimes \rangle$ and a subset of variable $Y \subset X$ is defined by a marginalization operator $\psi_{\mathbf{Y}}$. If S is the scope of function f then $\psi_{\mathbf{Y}} f \in \{\max_{\mathbf{S}=\mathbf{Y}} f, \min_{\mathbf{S}=\mathbf{Y}} f, \pi_{\mathbf{Y}} f, \sum_{\mathbf{S}=\mathbf{Y}} f\}$ is a marginalization operator. The reasoning problem $\mathcal{P}(\mathcal{M}, \psi_{Y}, \mathbf{Z})$ is the task of computing the function $\mathcal{P}_{\mathcal{M}}(\mathbf{Z}) = \bigcup_{\mathbf{Z}} \otimes_{i=1}^r f_i$, where r is the number of functions in F.

Summary of graphical models types

- Constraint networks
- Cost networks
- Bayesian network
- Markov networks
- Mixed probability and constraint network
- Influence diagrams

Constraint Networks

Map coloring

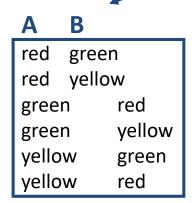
Combination = join
Marginalization = projection

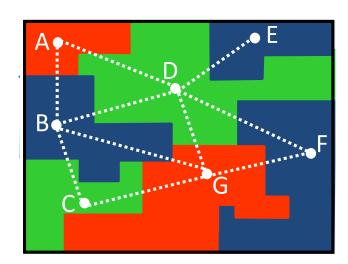
Variables: countries (A B C etc.)

Values: colors (red green blue)

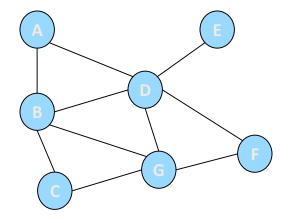
Constraints:

 $A \neq B$, $A \neq D$, $D \neq E$,...





Constraint graph

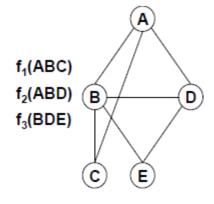


Example of a Cost Network

Α	В	С	f ₁ (ABC)
0	0	0	8
0	0	1	8
0	1	0	8
0	1	1	2
1	0	0	8
1	0	1	2
1	1	0	8
1	1	1	2

Α	В	D	f ₂ (ABD)
0	0	0	1
0	0	1	8
0	1	0	0
0	1	1	2
1	0	0	6
1	0	1	5
1	1	0	6
1	1	1	5

В	D	Е	f ₃ (BDE)
0	0	0	8
0	0	1	3
0	1	0	8
0	1	1	4
1	0	0	8
1	0	1	3
1	1	0	8
1	1	1	4



(a) Cost functions

Figure 2.3: A cost network.

(b) Constraint graph

Combination: sum
Marginalization:min/max

Definition 2.3.2 (WCSP) A Weighted Constraint Satisfaction Problem (WCSP) is a graphical model $\langle X, D, F, \Sigma \rangle$ where each of the functions $f_i \in F$ assigns "0" (no penalty) to allowed tuples and a positive integer penalty cost to the forbidden tuples. Namely, $f_i : D_{X_{i_1}} \times ... \times D_{X_{i_t}} \to \mathbb{N}$, where $S_i = \{X_{i_1}, ..., X_{i_t}\}$ is the scope of the function.

A Bayesian Network

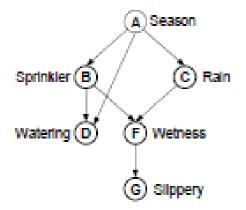
B	C	F	P(F B,C)	B	A=winter	D	P(D A,B)
false	false	true	0.1	false	false	true	0.3
true	false	true	0.9	true	false	true	0.9
false	true	true	0.8	false	true	true	0.1
true	true	true	0.95	true	true	true	1

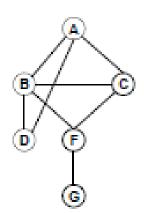
A	C	P(C A)	A	B	P(B A)
Summ	er true	0.1	Summer	true	0.8
Fall	true	0.4	Fall	true	0.4
Winte	er true	0.9	Winter	true	0.1
Sprin	g true	0.3	Spring	true	0.6

F	G	P(G F)
false	true	0.1
true	true	1

Combination: product

Marginalization: sum or min/max





(b) Moral graph

(a) Directed acyclic graph

Belief network P(g, f, c, b, a) = P(g|f)P(f|c, b)P(d|a, b)P(c|1)P(b|a)P(a)

Markov Networks

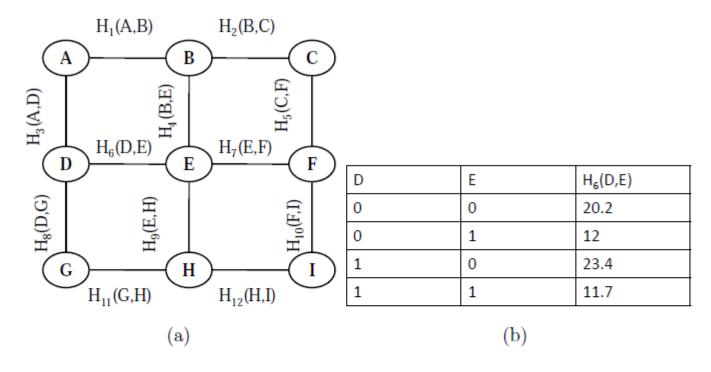


Figure 2.6: (a) An example 3×3 square Grid Markov network (ising model) and (b) An example potential $H_6(D, E)$

network represents a global joint distribution over the variables X given by:

$$P(\boldsymbol{x}) = \frac{1}{Z} \prod_{i=1}^m H_i(\boldsymbol{x}) \quad , \quad Z = \sum_{\boldsymbol{x} \in \boldsymbol{X}} \prod_{i=1}^m H_i(\boldsymbol{x})$$
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Example domains for graphical models

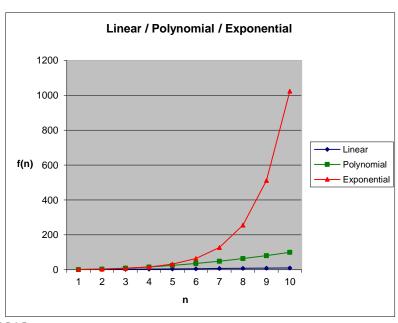
- Natural Language processing
 - Information extraction, semantic parsing, translation, topic models, ...
- Computer vision
 - Object recognition, scene analysis, segmentation, tracking, ...
- Computational biology
 - Pedigree analysis, protein folding and binding, sequence matching, ...
- Networks
 - Webpage link analysis, social networks, communications, citations,
- Robotics
 - Planning & decision making

Complexity of Reasoning Tasks

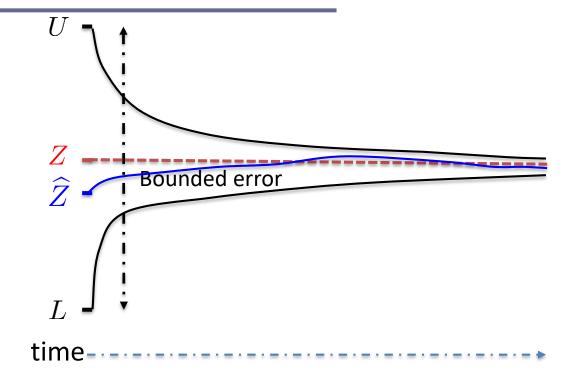
- Constraint satisfaction
- Counting solutions
- Combinatorial optimization
- Belief updating
- Most probable explanation
- Decision-theoretic planning

Reasoning is computationally hard

Complexity is Time and space(memory)



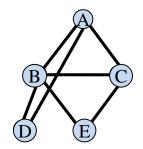
Desired Properties: Guarantee, Anytime, Anyspace

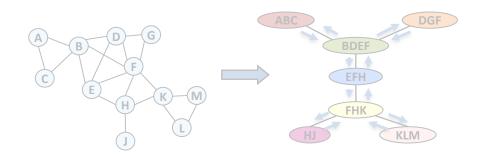


- Anytime
 - valid solution at any point
 - solution quality improves with additional computation
- Anyspace
 - run with limited memory resources

RoadMap: Introduction and Inference

- Basics of graphical models
 - Queries
 - Examples, applications, and tasks
 - Algorithms overview
- Inference algorithms, exact
 - Bucket elimination for trees
 - Bucket elimination
 - Jointree clustering
 - Elimination orders
- Approximate elimination
 - Decomposition bounds
 - Mini-bucket & weighted mini-bucket
 - Belief propagation
- Summary and Class 2







Tree-solving is easy

Belief updating (sum-prod)

P(X) $m_{XY}(X)$ $m_{XZ}(X)$ $m_{ZX}(X)$ $m_{YX}(X)$ P(Z|X) P(Y|X) $m_{YT}(Y)$ $m_{YR}(Y)$ $m_{ZL}(Z)$ $m_{ZM}(Z)$ $m_{RY}(Y)$ $m_{LZ}(Z)$ $m_{MZ}(Z)$ $m_{TY}(Y)$ P(M|Z)(P(R|Y) P(L|Z) P(T|Y

CSP – consistency (projection-join)

MPE (max-prod)

#CSP (sum-prod)

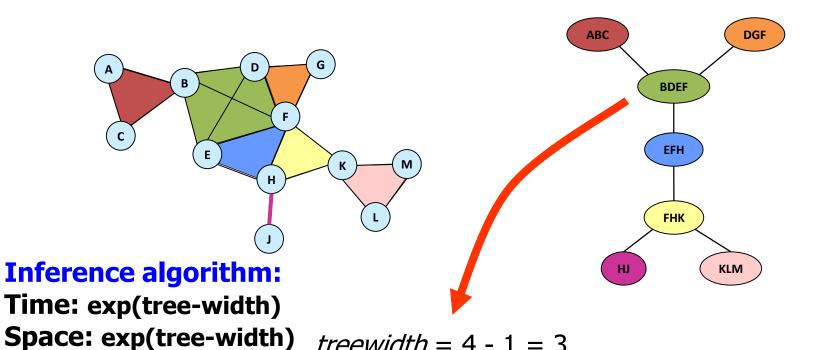
Trees are processed in linear time and memory

Transforming into a Tree

- By Inference (thinking)
 - Transform into a single, equivalent tree of subproblems

- By Conditioning (guessing)
 - Transform into many tree-like sub-problems.

Inference and Treewidth

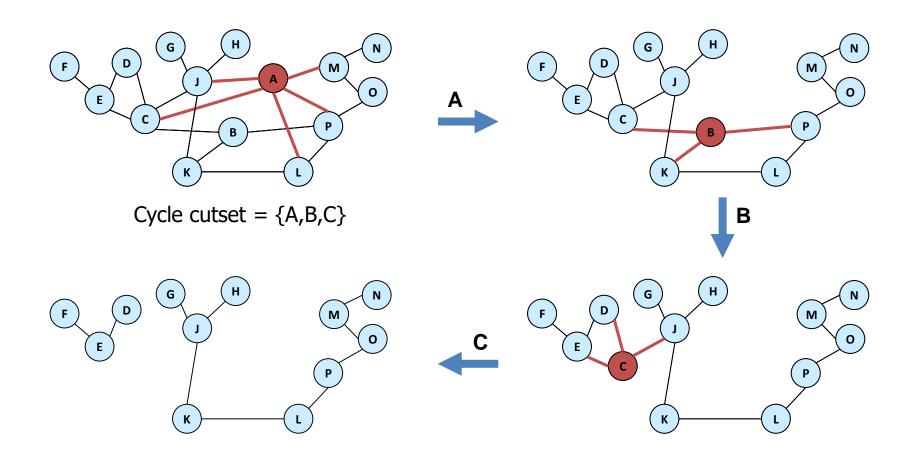


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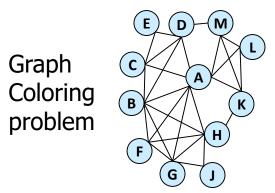
treewidth = 4 - 1 = 3

treewidth = (maximum cluster size) - 1

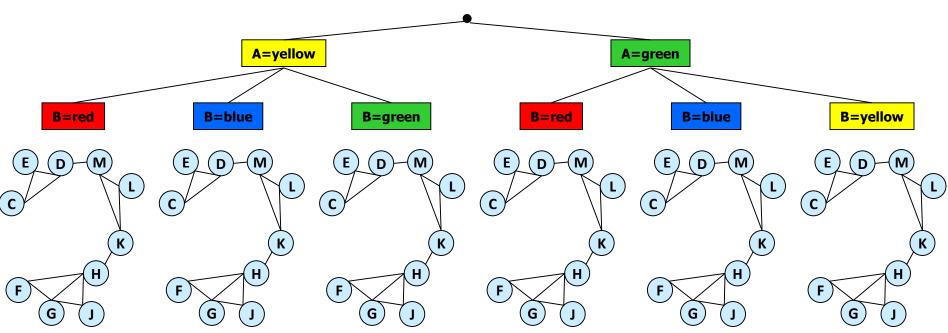
Conditioning and Cycle cutset



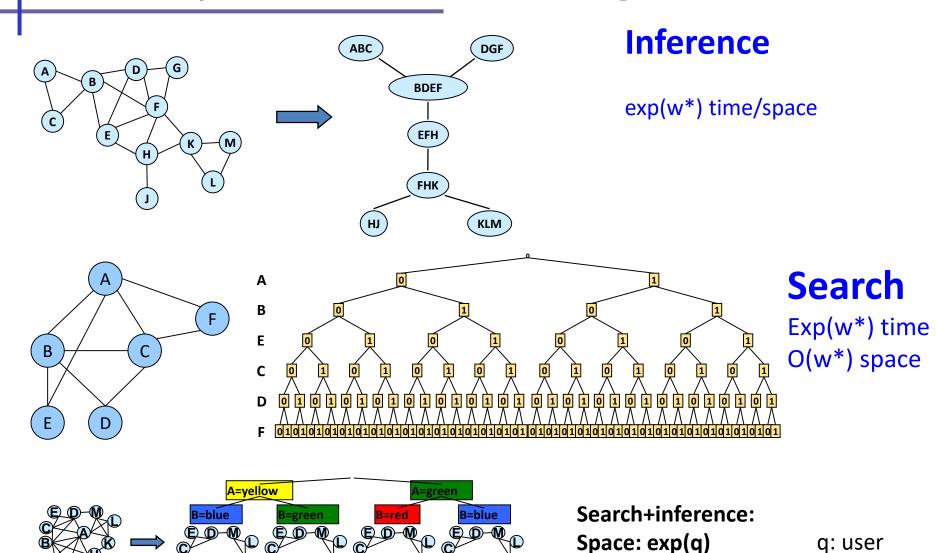
Search over the Cutset



- Inference may require too much memory
- Condition on some of the variables



Bird's-eye View of Exact Algorithms



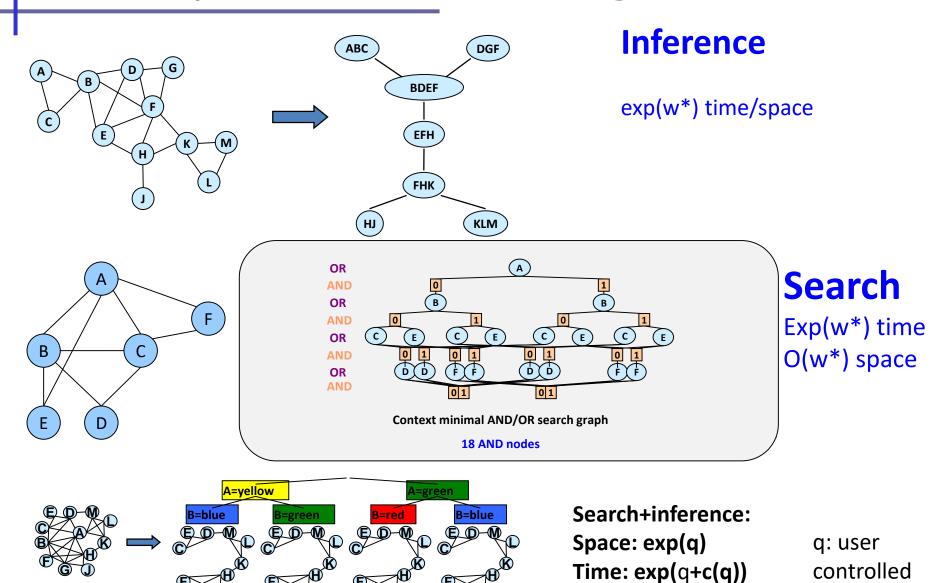
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q: user

Time: exp(q+c(q))

controlled

Bird's-eye View of Exact Algorithms



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Bird's-eye View of Approximate Algorithms

