# Advances in Combinatorial Optimization for Graphical Models 

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## Outline

- Introduction
- Graphical models
- Optimization tasks for graphical models
- Inference
- Variable Elimination, Bucket Elimination
- Bounds and heuristics
- Basics of search
- Bounded variable elimination and iterative cost shifting
- ANDIOR Search
- AND/OR search spaces
- Depth-First Branch and Bound, Best-First search
- Exploiting parallelism
- Distributed and parallel search
- Software


## Combinatorial Optimization

Earth observing satellites


Find an optimal schedule for the satellite that maximizes the number of photographs taken, subject to on-board recording capacity

Investments


How much to invest in each asset to earn 8 cents per Invested dollar and the investment risk is minimized

## Combinatorial Optimization

Communications


Assign frequencies to a set of radio links such that interferencies are minimized

Bioinformatics


Find a joint haplotype configuration for all members of the pedigree which maximizes the probability of data

## Constrained Optimization

## Power plant scheduling



Unit \# $\left.$\begin{tabular}{ccc}
Min Up <br>
Time

 

Min Down <br>
Time
\end{tabular} \right\rvert\,

Variables: $X_{1}, X_{2}, \ldots, X_{n} \quad$ Domains: ON, OFF
Constraints: $X_{1} \vee X_{2}, \quad \neg X_{3} \vee X_{4}$, min-uptime, min-downtime Power demand: Power $\left(X_{i}\right) \geq$ Demand

Objective: minimize TotalFuelConsumption $\left(X_{1}, \ldots, X_{n}\right)$

## Constraint Optimization Problems

A finite COP is a triple $R=\langle X, D, F\rangle$ where:

$$
\begin{aligned}
X & =\left\{x_{1}, \ldots, x_{n}\right\} \quad \text {-- variables } \\
D & =\left\{D_{1}, \ldots, D_{n}\right\} \quad-\text { domains } \\
F & =\left\{f_{\alpha_{1}}, \ldots, f_{\alpha_{m}}\right\}-\text { - cost functions }
\end{aligned}
$$

$f(A, B, D)$ has scope $\{A, B, D\}$

| $\mathbf{A}$ | $\mathbf{B}$ | $\mathbf{D}$ | Cost |
| :---: | :---: | :---: | :---: |
| 1 | 2 | 3 | 3 |
| 1 | 3 | 2 | 2 |
| 2 | 1 | 3 | $\infty$ |
| 2 | 3 | 1 | 0 |
| 3 | 1 | 2 | 5 |
| 3 | 2 | 1 | 0 |

Primal graph: $\left\{\begin{array}{l}\text { Variables - nodes } \\ \text { Functions - arcs / cliques }\end{array}\right.$

$$
F(a, b, c, d, f, g)=f_{1}(a, b, d)+f_{2}(d, f, g)+f_{3}(b, c, f)+f_{4}(a, c)
$$

Global Cost Function

$$
F(X)=\sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)
$$



## Constraint Networks

## Map coloring

Variables: countries (A, B, C, etc.)
Values: colors (red, green, blue)
Constraints: $A \neq B, \quad B \neq D, \quad A \neq D$, etc.

| A | B |
| :--- | :--- |
| red | green |
| red | blue |
| green | red |
| green | blue |
| blue | red |
| blue | green |



Constraint graph


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## Probabilistic Networks



## Monitoring Intensive-Care Patients

The "alarm" network - 37 variables, 509 parameters (instead of $2^{37}$ )


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## Genetic Linkage Analysis



- 6 individuals
- Haplotype: $\{2,3\}$
- Genotype: \{6\}
- Unknown


## Pedigree: 6 people, 3 markers



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## Influence Diagrams



Task: find optimal policy

$$
E=\max _{\Delta=\left(\delta_{1}, \ldots, \delta_{m}\right)} \sum_{x=\left(x_{1}, \ldots, x_{n}\right) i} \prod_{i} P_{i}(x) u(x)
$$

Chance variables: $X=x_{1}, \ldots, x_{n}$
Decision variables: $D=d_{1}, \ldots d_{m}$
CPDs for chance variables: $P_{i}=P\left(x_{i} \mid x_{\mathrm{pa}_{i}}\right), i=1, \ldots, n$
Reward components: $r=\left\{r_{1}, \ldots, r_{j}\right\}$
Utility function: $u(X)=\sum_{i} r_{i}(X)$

## Graphical Models

- A graphical model (X, D, F):
- $X=\left\{x_{1}, \ldots, x_{n}\right\} \quad$ variables
- $D=\left\{D_{1}, \ldots, D_{n}\right\} \quad$ domains
- $F=\left\{f_{\alpha_{1}}, \ldots, f_{\alpha_{m}}\right\}$ functions
- (constraints, CPTs, CNFs, ...)
- Operators
- Combination
- Elimination (projection)
- Tasks
- Belief updating: $\sum_{X \backslash Y} \prod_{j} P_{j}$
- MPE/MAP: $\max _{X} \prod_{j} P_{j}$
- Marginal MAP: $\max _{Y} \sum_{X \backslash Y} \prod_{j} P_{j}$
- CSP: $\prod_{j} C_{j}(x)$
- WCSP: $\min _{X} \sum_{j} f_{j}$
- MEU: $\max _{\Delta} \sum_{x} P(x) u(x)$

- All these tasks are NP-hard
- Exploit problem structure
- Identify special cases
- Approximate


## Example Domains for Graphical Models

- Web Pages and Link Analysis
- Communication Networks (Cell phone fraud detection
- Natual Language Processing (e.g., information extraction and semantic parsing)
- Battlespace Awarness
- Epidemiological Studies
- Citation Networks
- Intelligence Analysis (terrorist networks)
- Financial Transactions (money laundering)
- Computational Biology
- Object Recognition and Scene Analysis
- ...


## Combinatorial Optimization Tasks

- Most Probable Explanation (MPE), or Maximum A Posteriori (MAP)
- M Best MPE/MAP
- Marginal MAP (MMAP)
- Weighted CSPs (WCSP), Max-CSPs, Max-SAT
- Integer Linear Programs
- Maximum Expected Utility (MEU)


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- Introduction
- Graphical models
- Optimization tasks for graphical models
- Solving optimization problems by inference and search
- Inference
- Bounds and heuristics
- AND/OR Search
- Exploiting parallelism
- Software


## Solution Techniques

## AND/OR search

Search: Conditioning


Inference: Elimination

## Combination of Cost Functions

| $A$ | $\mathbf{B}$ | $\mathbf{f}(\mathbf{A}, \mathbf{B})$ |
| :---: | :---: | :---: |
| $b$ | $b$ | 6 |
| $b$ | $g$ | 0 |
| g | b | 0 |
| g | g | 6 |


| $\mathbf{B}$ | $\mathbf{C}$ | $\mathbf{f ( B , C )}$ |
| :---: | :---: | :---: |
| $b$ | $b$ | 6 |
| $b$ | $g$ | 0 |
| g | b | 0 |
| g | g | 6 |

## Elimination in a Cost Function

$\left.\begin{array}{|c|c|c|}\hline \mathbf{A} & \mathbf{B} & \mathbf{f ( A , B )} \\ \hline b & b & 4 \\ \hline b & g & 6 \\ \hline b & r & 1 \\ \hline g & b & 2 \\ \hline g & g & 6 \\ \hline g & r & 3 \\ \hline r & b & 1 \\ \hline r & g & 1 \\ \hline r & r & 6 \\ \hline\end{array}\right\}$ Elim(f,B)


## Conditioning in a Cost Function



## Conditioning vs. Elimination

## Conditioning (search)



Elimination (inference)


1 "denser" problem

## Outline

- Inference
- Variable Elimination, Bucket Elimination
- ANDIOR Search


## Computing the Optimal Cost Solution



$$
\text { OPT }=\min _{a, e, d, c, b} f(a)+\underbrace{f(a, b)}_{\text {Combination }}+f(a, c)+f(a, d)+\underbrace{f(b, c)+f(b, d)+f(b, e})+f(c, e)
$$

$$
\min _{a} f(a) \min _{e, d} f(a, d)+\min _{c} f(a, c)+f(c, e)+\min _{b} \underbrace{f(a, b)+f(b, c)+f(b, d)+f(b, e)}_{\lambda_{B}(a, d, c, e)}
$$

Variable Elimination

## Bucket Elimination

Algorithm elim-opt [Dechter, 1996]
Non-serial Dynamic Programming [Bertele \& Briochi, 1973]

$$
\mathrm{OPT}=\min _{a, e, d, c, b} f(a)+f(a, b)+f(a, c)+f(a, d)+f(b, c)+f(b, d)+f(b, e)+f(c, e)
$$



## Generating the Optimal Assignment

$$
\begin{array}{rl}
\mathbf{b}^{*}=\arg \min _{\mathbf{b}} & f\left(a^{*}, b\right)+f\left(b, c^{*}\right) \\
& +f\left(b, d^{*}\right)+f\left(b, e^{*}\right) \\
\mathbf{c}^{*}=\arg \min _{\mathbf{c}} & f\left(c, a^{*}\right)+f\left(c, e^{*}\right) \\
& +\lambda_{B \rightarrow C}\left(a^{*}, d^{*}, c, e^{*}\right)
\end{array}
$$

$$
\mathbf{d}^{*}=\arg \min _{\mathbf{d}} f\left(a^{*}, d\right)+\lambda_{C \rightarrow D}\left(a^{*}, d, e^{*}\right)
$$

$$
\mathbf{e}^{*}=\arg \min _{\mathbf{e}} \lambda_{D \rightarrow E}\left(a^{*}, e\right)
$$

$\mathbf{a}^{*}=\arg \min _{\mathbf{a}} f(a)+\lambda_{E \rightarrow A}(a)$

C: $\quad f(c, a) f(c, e) \quad \lambda_{B \rightarrow C}(a, d, c, e)$

D: $\quad f(a, d) \quad \lambda_{C \rightarrow D}(a, d, e)$
E: $\quad \lambda_{D \rightarrow E}(a, e)$

A: $\quad f(a) \quad \lambda_{E \rightarrow A}(a)$

Return: ( $\left.\mathbf{a}^{*}, \mathbf{b}^{*}, \mathbf{c}^{*}, \mathrm{~d}^{*}, \mathrm{e}^{*}\right)$

## Complexity of Bucket Elimination

Algorithm elim-opt [Dechter, 1996] Non-serial Dynamic Programming [Bertele \& Briochi, 1973]
$\mathrm{OPT}=\min _{a, e, d, c, b} f(a)+f(a, b)+f(a, c)+f(a, d)+f(b, c)+f(b, d)+f(b, e)+f(c, e)$


## Complexity of Bucket Elimination

Bucket Elimination is time and space

$$
O\left(r \exp \left(w^{*}(d)\right)\right)
$$

$w^{*}(d)$ : the induced width of the primal graph along ordering $d$
$r=$ number of functions
The effect of the ordering:

constraint graph

$w^{*}\left(d_{1}\right)=4$

$w^{*}\left(d_{2}\right)=2$

Finding the smallest induced width is hard!

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## OR Search Spaces



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $\mathrm{f}_{6}$ | B | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ | E | F | $\mathrm{f}_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ |
| $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ |

$$
\text { Objective function: } F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)
$$



## OR Search Spaces



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $\mathrm{f}_{6}$ | B | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ | E | F | $\mathrm{f}_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ |
| $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ |

Objective function: $F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)$

A


Arc-cost is calculated based on cost functions with empty scope (conditioning)

## The Value Function



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $\mathrm{f}_{6}$ | B | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ | E | F | $\mathrm{f}_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ |
| $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{3}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{4}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{2}$ |

Objective function: $F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)$

A


E 0 $3 / 02 / 23 / 02 / 23 / 022 / 23 / 02 / 23 / 02 / 233 / 02 / 23 / 02 / 23 / 02 / 21 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 44$


Value of node = minimal cost solution below it

## The Optimal Solution



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $f$ |  | B | E | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ | E | F | ${ }_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 2 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 |  | 4 | 0 | 0 |  | 3 | 0 | 0 | 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 3 | 0 | 1 | 0 | 0 | 1 | 1 | 0 | 1 | 2 | 2 | 0 | 1 |  | 2 | 0 | 1 | 4 | 0 | 1 | 0 |
| 1 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 0 |
| 1 | 1 | 4 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 2 | 1 | 1 | 4 | 1 | 1 |  | 0 | 1 | 1 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 2 |

Objective function: $F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)$

A

 $3 / 02 / 23 / 02 / 23 / / 02 / 23 / 02 / 233 / 02 / 23 / / 02 / 23 / 02 / 23 / 02 / 21 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 411 / 20 / 41 / 20 / 41 / 20 / 41 / 20 / 44$

Value of node = minimal cost solution below it

## Basic Heuristic Search Schemes

Heuristic function $\tilde{f}\left(\hat{x}_{p}\right)$ computes a lower bound on the best extension of partial configuration $\hat{x}_{p}$ and can be used to guide heuristic search.
We focus on:

1. Branch-and-Bound

Use heuristic function $\tilde{f}\left(\hat{x}_{p}\right)$ to prune the depth-first search tree Linear space

$f(\hat{x})=U$

## 2. Best-First Search

Always expand the node with the lowest heuristic value $\tilde{f}\left(\hat{x}_{p}\right)$
Needs lots of memory


## Classic Depth-First Branch and Bound



Each node is a COP subproblem (defined by current conditioning)
$\mathrm{g}(\mathrm{n})$ : cost of the path from root to n

$$
\begin{aligned}
& \tilde{f}(n)=g(n)+\tilde{h}(n) \\
& \quad \text { (lower bound) }
\end{aligned}
$$

$$
\text { Prune if } \tilde{f}(n) \geq U B
$$

$\tilde{h}(n)$ : under-estimates optimal cost below n
(UB) Upper Bound = best solution so far

## Best-First vs. Depth-First Branch and Bound

- Best-First ( $\mathrm{A}^{*}$ ):
- Expands least number of nodes given h
- Requires storing full search tree in memory
- Depth-First BnB:
- Can use linear space
- If finds an optimal solution early, will expand the same search space as BestFirst (if search space is a tree)
- BnB can improve the heuristic function dynamically


## How to Generate Heuristics

- The principle of relaxed models
- Mini-Bucket Elimination
- Bounded directional consistency ideas
- Linear relaxations for integer programs


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- 
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- 


## Mini-Bucket Approximation

Split a bucket into mini-buckets => bound complexity

$$
\begin{gathered}
\text { bucket }(\mathrm{X})= \\
\underbrace{\left\{f_{1}, \ldots, f_{r}, f_{r+1}, \ldots, f_{n}\right\}}_{\lambda_{X}(\cdot)=\min _{x} \sum_{i=1}^{n} f_{i}(x, \ldots)} \\
\left\{f_{1}, \ldots, f_{r}\right\} \\
\lambda_{X}^{\prime}(\cdot)=\left(\min _{x} \sum_{i=1}^{r} f_{i}(\cdot)\right)+\left(\min _{x} \sum_{i=r+1}^{n} f_{i}(\cdot)\right) \\
\lambda_{X}^{\prime}(\cdot) \leq \lambda_{X}(\cdot)
\end{gathered}
$$

Exponential complexity decrease: $O\left(e^{n}\right) \rightarrow O\left(e^{r}\right)+O\left(e^{n-r}\right)$

## Mini-Bucket Elimination



## Mini-Bucket Elimination Semantics



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## Semantics of Mini-Buckets: Splitting a Node

Variables in different buckets are renamed and duplicated [Kask et al., 2001], [Geffner et al., 2007], [Choi et al., 2007], [Johnson et al. 2007]

Before Splitting:
Network $N$

After Splitting:
Network $N^{\prime}$


## MBE-MPE(i): Algorithm Approx-MPE

- Input: i - max number of variables allowed in a mini-bucket
- Output: [lower bound (P of a suboptimal solution), upper bound]

Example: approx-mpe(3) versus elim-mpe

[Dechter and Rish, 1997]

## Mini-Bucket Decoding


[Dechter and Rish, 2003]

## Properties of MBE(i)

- Complexity: $O(r \exp (i))$ time and $O(\exp (i))$ space
- Yields a lower-bound and an upper-bound
- Accuracy: determined by upper/lower (U/L) bound
- Possible use of mini-bucket approximations:
- As anytime algorithms
- As heuristics in search
- Other tasks (similar mini-bucket approximations):
- Belief updating, Marginal MAP, MEU, WCSP, MaxCSP [Dechter and Rish, 1997], [Liu and Ihler, 2011], [Liu and Ihler, 2013]


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- 
- 
- 


## Cost-Shifting

(Reparameterization) $-\lambda(\mathbf{B})$

| $\mathbf{B}$ | $\mathbf{C}$ | $\mathbf{f ( B , C )}$ |
| :---: | :---: | :---: |
| $b$ | $b$ | $6-3$ |
| $b$ | $g$ | $0-3$ |
| g | b | $0+1$ |
| g | g | $6+1$ |


| $\mathbf{B}$ | $\lambda(\mathbf{B})$ |
| :---: | :---: |
| $\mathbf{b}$ | 3 |
| $\mathbf{g}$ | -1 |


| $\mathbf{A}$ | $\mathbf{B}$ | $\mathbf{C}$ | $\mathbf{f ( A , B}, \mathbf{C})$ |
| :---: | :---: | :---: | :---: |
| $b$ | $b$ | $b$ | 12 |
| $b$ | $b$ | $g$ | 6 |
| $b$ | $g$ | $b$ | 0 |
| $b$ | $g$ | $g$ | 6 |
| $g$ | $b$ | $b$ | 6 |
| $g$ | $b$ | $g$ | 0 |
| $g$ | $g$ | $b$ | 6 |
| $g$ | $g$ | $g$ | 12 |

Modify the individual functions

- but -
keep the sum of functions unchanged


## Dual Decomposition


$F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}(x) \geq \sum_{\alpha} \min _{x} f_{\alpha}(x)$

- Bound solution using decomposed optimization
- Solve independently: optimistic bound


## Dual Decomposition


$F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}(x) \quad \geq \max _{\lambda_{i \rightarrow \alpha}} \sum_{\alpha} \min _{x}\left[f_{\alpha}(x)+\sum_{i \in \alpha} \lambda_{i \rightarrow \alpha}\left(x_{i}\right)\right]$

- Bound solution using decomposed optimization
- Solve independently: optimistic bound
- Tighten the bound by reparameterization
- Enforce lost equality constraints via Lagrange multipliers


## Dual Decomposition



$$
F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}(x) \quad \geq \max _{\lambda_{i \rightarrow \alpha}} \sum_{\alpha} \min _{x}\left[f_{\alpha}(x)+\sum_{i \in \alpha} \lambda_{i \rightarrow \alpha}\left(x_{i}\right)\right]
$$

Many names for the same class of bounds:

- Dual decomposition [Komodakis et al. 2007]
- TRW, MPLP
[Wainwright et al. 2005, Globerson \& Jaakkola 2007]
- Soft arc consistency [Cooper \& Schiex 2004]
- Max-sum diffusion [Warner 2007]


## Dual Decomposition



$$
F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}(x) \quad \geq \max _{\lambda_{i \rightarrow \alpha}} \sum_{\alpha} \min _{x}\left[f_{\alpha}(x)+\sum_{i \in \alpha} \lambda_{i \rightarrow \alpha}\left(x_{i}\right)\right]
$$

Many ways to optimize the bound:

- Sub-gradient descent [Komodakis et al. 2007; Jojic et al. 2010]
- Coordinate descent [Warner 2007; Globerson \& Jaakkola 2007; Sontag et al. 2009; Ihler et al. 2012]
- Proximal optimization [Ravikumar et al. 2010]
- ADMM
[Meshi \& Globerson 2011; Martins et al. 2011; Forouzan \& Ihler 2013]


## Mini-Bucket as Dual Decomposition



## Mini-Bucket as Dual Decomposition

$$
\begin{aligned}
& \min _{a, c, b}\left[f(a, b)+f(b, c)-\lambda_{B \rightarrow C}(a, c)\right]=0 \\
& \min _{d, e, b}\left[f(b, d)+f(b, e)-\lambda_{B \rightarrow D}(d, e)\right]=0
\end{aligned}
$$



## Mini-Bucket as Dual Decomposition

$$
\begin{array}{r}
\min _{a, c, b}\left[f(a, b)+f(b, c)-\lambda_{B \rightarrow C}(a, c)\right]=0 \\
\min _{d, e, b}\left[f(b, d)+f(b, e)-\lambda_{B \rightarrow D}(d, e)\right]=0 \\
\min _{a, e, c}\left[\lambda_{B \rightarrow C}(a, c)+f(a, c)+f(c, e)\right. \\
\left.-\lambda_{C \rightarrow E}(a, e)\right]=0
\end{array}
$$



## Mini-Bucket as Dual Decomposition

$$
\begin{array}{r}
\min _{a, c, b}\left[f(a, b)+f(b, c)-\lambda_{B \rightarrow C}(a, c)\right]=0 \\
\min _{d, e, b}\left[f(b, d)+f(b, e)-\lambda_{B \rightarrow D}(d, e)\right]=0 \\
\min _{a, e, c}\left[\lambda_{B \rightarrow C}(a, c)+f(a, c)+f(c, e)\right. \\
\left.-\lambda_{C \rightarrow E}(a, e)\right]=0 \\
\min _{a, d}\left[f(a, d)+\lambda_{B \rightarrow D}(d, e)\right. \\
\left.-\lambda_{D \rightarrow E}(a, e)\right]=0
\end{array}
$$



## Mini-Bucket as Dual Decomposition

$$
\begin{array}{r}
\min _{a, c, b}\left[f(a, b)+f(b, c)-\lambda_{B \rightarrow C}(a, c)\right]=0 \\
\min _{d, e, b}\left[f(b, d)+f(b, e)-\lambda_{B \rightarrow D}(d, e)\right]=0 \\
\min _{a, e, c}\left[\lambda_{B \rightarrow C}(a, c)+f(a, c)+f(c, e)\right. \\
\left.-\lambda_{C \rightarrow E}(a, e)\right]=0 \\
\min _{a, d}\left[f(a, d)+\lambda_{B \rightarrow D}(d, e)\right. \\
\left.-\lambda_{D \rightarrow E}(a, e)\right]=0 \\
\min _{a, e}\left[\lambda_{C \rightarrow E}(a, e)+\lambda_{D \rightarrow E}(a, e)\right. \\
\left.-\lambda_{E \rightarrow A}(a)\right]=0
\end{array}
$$



## Mini-Bucket as Dual Decomposition

$$
\begin{aligned}
& \min _{a, c, b}\left[f(a, b)+f(b, c)-\lambda_{B \rightarrow C}(a, c)\right]=0 \\
& \min _{d, e, b}\left[f(b, d)+f(b, e)-\lambda_{B \rightarrow D}(d, e)\right]=0 \\
& \min _{a, e, c}\left[\lambda_{B \rightarrow C}(a, c)+f(a, c)+f(c, e)\right. \\
& \left.-\lambda_{C \rightarrow E}(a, e)\right]=0 \\
& \min _{a, d}\left[f(a, d)+\lambda_{B \rightarrow D}(d, e)\right. \\
& \left.-\lambda_{D \rightarrow E}(a, e)\right]=0 \\
& \begin{aligned}
\min _{a, e}\left[\lambda_{C \rightarrow E}(a, e)+\lambda_{D \rightarrow E}\right. & (a, e) \\
& \left.-\lambda_{E \rightarrow A}(a)\right]=0
\end{aligned} \\
& \begin{aligned}
\min _{a, e}\left[\lambda_{C \rightarrow E}(a, e)+\lambda_{D \rightarrow E}\right. & (a, e) \\
& \left.-\lambda_{E \rightarrow A}(a)\right]=0
\end{aligned} \\
& \min _{a}\left[f(a)+\lambda_{E \rightarrow A}(a)\right]=L
\end{aligned}
$$

## Mini-Bucket as Dual Decomposition

- Downward pass as cost-shifting
- Can also do cost-shifting within mini-buckets
- "Join graph" message passing
- "Moment matching" version: one message update within each bucket during downward sweep.



## Anytime Approximation

anytime-mpe( $\varepsilon$ )

Initialize: $i=i_{0}$
While time and space resources are available
$i \leftarrow i+i_{\text {step }}$
$U \leftarrow$ upper bound computed by approx - mpe(i)
$L \leftarrow$ lower bound computed by approx - mpe(i)
keep the best solution found so far
if $1 \leq \frac{U}{L} \leq 1+\varepsilon$, return solution
end
return the largest $L$ and the smallest $U$

## Anytime Approximation




- Can tighten the bound in various ways
- Cost-shifting
- Increase i-bound
(improve consistency between cliques)
(higher order consistency)
- Simple moment-matching step improves bound significantly


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- Can tighten the bound in various ways
- Cost-shifting
- Increase i-bound
(improve consistency between cliques)
(higher order consistency)
- Simple moment-matching step improves bound significantly


## Weighted Mini-Bucket

## ( for summation bounds )

Exact bucket elimination:
$\lambda_{B}(a, c, d, e)=\sum_{b}[f(a, b) \cdot f(b, c) \cdot f(b, d) \cdot f(b, e)]$
$\leq\left[\sum_{b}^{w_{1}} f(a, b) f(b, c)\right] \cdot\left[\sum_{b}^{w_{2}} f(b, d) f(b, e)\right]$
$=\lambda_{B \rightarrow C}(a, c)$

- $\lambda_{B \rightarrow D}(d, e)$
(mini-buckets)
where $\sum_{x}^{w} f(x)=\left[\sum_{x} f(x)^{1 / w}\right]^{w}$
is the weighted or "power" sum operator

By Holder's inequality,

$$
\begin{aligned}
& \sum_{x}^{w} f_{1}(x) f_{2}(x) \leq\left[\sum_{x}^{w_{1}} f_{1}(x)\right]\left[\sum_{x}^{w_{2}} f_{2}(x)\right] \\
& \text { where } w_{1}+w_{2}=w \text { and } w_{1}>0, w_{2}>0
\end{aligned}
$$

$$
\text { (lower bound if } w_{1}>0, w_{2}<0 \text { ) }
$$

## Weighted Mini-Bucket

- Related to conditional entropy decomposition [Globerson \& Jaakkola 2008] but, with an efficient, "primal" bound form
- We can optimize the bound over:
- Cost-shifting
- Weights
- Again, involves message passing on JG
- Similar, one-pass "moment matching" variant

Join graph:


## WMB for Marginal MAP

Weighted mini-bucket is applicable more generally, since

$$
\begin{cases}\lim _{w \rightarrow 0^{+}} \sum_{x}^{w} f(x)=\max _{x} f(x) & (f(x) \geq 0) \\ \lim _{w \rightarrow 0^{-}} \sum_{x}^{w} f(x)=\min _{x} f(x) & (\mathrm{w}=\text { "temperature" })\end{cases}
$$

So, when w=0+, WMB reduces to max-inference.

For marginal MAP problems, just use different w's:

$$
\max _{x_{B}} \sum_{x_{A}} \prod_{j} f_{j}(x)=\sum_{x_{B}}^{0^{+}} \sum_{x_{A}}^{1} \prod_{j} f_{j}(x)
$$



## WMB for Marginal MAP

$$
\left.\begin{array}{rl}
\lambda_{B \rightarrow C}(a, c) & =\sum_{b}^{w_{1}} f(a, b) f(b, c) \\
\lambda_{B \rightarrow D}(d, e) & =\sum_{b}^{w_{2}} f(b, d) f(b, e) \\
& \left(w_{1}+w_{2}=1\right)
\end{array}\right] \begin{aligned}
& \\
& \lambda_{E \rightarrow A}(a)=\max _{e} \lambda_{C \rightarrow E}(a, e) \lambda_{D \rightarrow E}(a, e) \\
& U=\max _{a} f(a) \lambda_{E \rightarrow A}(a)
\end{aligned}
$$

Can optimize over cost-shifting and weights

Marginal MAP:

$U=$ upper bound (single-pass "MM" or with iterative message passing)

## Outline

- 
- 
- Bounds and heuristics
- Basics of search: DFS versus BFS
- Mini-Bucket Elimination
- Weighted Mini-Buckets and Iterative Cost-Shifting
- Generating Heuristics using Mini-Bucket Elimination
- 
- 


## Generating Heuristics for Graphical Models

Given a cost function:

$$
f(a, \ldots, e)=f(a)+f(a, b)+f(a, c)+f(a, d)+f(b, c)+f(b, d)+f(b, e)+f(c, e)
$$

define an evaluation function over a partial assignment as the cost of its best extension:
$f^{*}(\hat{a}, \hat{e}, D)=\min _{b, c} F(\hat{a}, b, c, D, \hat{e})$


$$
=g(\hat{a}, \hat{e}, D)+h^{*}(\hat{a}, \hat{e}, D)
$$


[Kask and Dechter, 2001]

## Static Mini-Bucket Heuristics

Given a partial assignment, $[\hat{a}=1, \hat{e}=0]$
(weighted) mini-bucket gives an admissible heuristic:
mini-buckets


cost to go:

$$
\begin{aligned}
\tilde{h}(\hat{a}, \hat{e}, D)= & \lambda_{C \rightarrow E}(\hat{a}, \hat{e}) \\
& +f(\hat{a}, D)+\lambda_{B \rightarrow D}(D, \hat{e})
\end{aligned}
$$

(admissible: $\tilde{h}(\hat{a}, \hat{e}, D) \leq h^{*}(\hat{a}, \hat{e}, D)$ ) cost so far:

$$
g(\hat{a}, \hat{e})=f(A=\hat{a})
$$

## Properties of the Heuristic

- MB heuristic is monotone, admissible
- Computed in linear time
- IMPORTANT
- Heuristic strength can vary by MB(i)
- Higher i-bound $\rightarrow$ more pre-processing $\rightarrow$ more accurate heuristic $\rightarrow$ less search
- Allows controlled trade-off between preprocessing and search


## Dynamic Mini-Bucket Heuristics

- Rather than pre-compile, compute the heuristics, dynamically, during search
- Dynamic MB: use the Mini-Bucket algorithm to produce a bound for any node during search
- Dynamic MBTE: compute heuristics simultaneously for all un-instantiated variables using Mini-Bucket-Tree Elimination (MBTE)
- MBTE is an approximation scheme defined over cluster trees. It outputs multiple bounds for each variable and value extension at once


## Outline

- Bounds and heuristics
- ANDIOR Search


## Outline

- 
- 
- 
- AND/OR Search
- AND/OR Search Spaces
- AND/OR Branch and Bound
- Best-First AND/OR Search
- Advanced Searches and Tasks


## Solution Techniques

## AND/OR search

Search: Conditioning


Inference: Elimination

## Classic OR Search Space



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $f$ |  | B | E | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ | E | F | ${ }_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 2 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 |  | 4 | 0 | 0 |  | 3 | 0 | 0 | 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 3 | 0 | 1 | 0 | 0 | 1 | 1 | 0 | 1 | 2 | 2 | 0 | 1 |  | 2 | 0 | 1 | 4 | 0 | 1 | 0 |
| 1 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 0 |
| 1 | 1 | 4 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 2 | 1 | 1 | 4 | 1 | 1 |  | 0 | 1 | 1 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 2 |

$$
\text { Objective function: } F^{*}=\min _{X} \sum_{i} f_{i}(X)
$$

## A



## The AND/OR Search Tree



Pseudo tree
[Freuder and Quinn, 1985]


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[Dechter and Mateescu, 2007]

## The AND/OR Search Tree



Pseudo tree


## Weighted AND/OR Search Tree



| A | B | $\mathrm{f}_{1}$ | A | C | $\mathrm{f}_{2}$ | A | E | $\mathrm{f}_{3}$ | A | F | $\mathrm{f}_{4}$ | B | C | $\mathrm{f}_{5}$ | B | D | $f_{6}$ | B | E | $\mathrm{f}_{7}$ | C | D | $\mathrm{f}_{8}$ |  | F | $\mathrm{f}_{9}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 2 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 3 | 0 | 0 | 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 3 | 0 | 1 | 0 | 0 | 1 | 1 | 0 | 1 | 2 | 0 | 1 | 2 | 0 | 1 | 4 | 0 | 1 | 0 |
| 1 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 0 |
| 1 | 1 | 4 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 2 | 1 | 1 | 4 | 1 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 2 |

Objective function: $F^{*}=\min _{X} \sum_{i} f_{i}(X)$


## Node Value (bottom-up evaluation)

OR - minimization
AND - summation

## AND/OR versus OR Spaces



## AND/OR versus OR Spaces

| width depth | OR space |  | AND/OR space |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Time (sec) | Nodes | Time (sec) | AND nodes | OR nodes |
| 5 | 10 | 3.15 | $2,097,150$ | 0.03 | 10,494 | 5,247 |
| 4 | 9 | 3.13 | $2,097,150$ | 0.01 | 5,102 | 2,551 |
| 5 | 10 | 3.12 | $2,097,150$ | 0.03 | 8,926 | 4,463 |
| 4 | 10 | 3.12 | $2,097,150$ | 0.02 | 7,806 | 3,903 |
| 5 | 13 | 3.11 | $2,097,150$ | 0.10 | 36,510 | 18,255 |

Random graphs with 20 nodes, 20 edges and 2 values per node

## Complexity of AND/OR Tree Search

## AND/OR tree

## OR tree

## Space

$O(n)$
$O(n)$

## Time

$$
\begin{aligned}
& O\left(n d^{t}\right) \\
O\left(n d^{\left(w^{*} \log n\right)}\right) & O\left(d^{n}\right)
\end{aligned}
$$

[Freuder \& Quinn85], [Collin, Dechter \& Katz91], [Bayardo \& Miranker95], [Darwiche01]

$$
\begin{array}{ll}
d=\text { domain size } & n=\text { number of variables } \\
t=\text { depth of pseudo tree } & w^{*}=\text { induced width }
\end{array}
$$

## Constructing Pseudo Trees

- AND/OR serch algorithms are influenced by the quality of the pseudo tree
- Finding minimal induced width / depth pseudo tree is NP-hard
- Heuristics
- Min-Fill (min induced width)
- Hypergraph partitioning (min depth)


## Constructing Pseudo Trees

- Min-Fill [kjaerulff, 1990]
- Depth-first traversal of the induced graph obtained along the min-fill elimination order heuristic
- Variables ordered according to smallest "fill-set"
- Hypergraph Partitioning [Karypis and Kumar, 2000]
- Functions are vertices in the hypergraph and variables are hyperedges
- Recursive decomposition of the hypergraph while minimizing the separator size at each step
- Using state-of-the-art software package hMeTiS


## Quality of the Pseudo Trees

| Network | hypergraph |  | min-fill |  |
| :--- | :---: | :---: | :---: | :---: |
|  | $W^{*}$ | depth | $w^{\star}$ | depth |
| barley | 7 | 13 | 7 | 23 |
| diabetes | 7 | 16 | 4 | 77 |
| link | 21 | 40 | 15 | 53 |
| mildew | 5 | 9 | 4 | 13 |
| munin1 | 12 | 17 | 12 | 29 |
| munin2 | 9 | 16 | 9 | 32 |
| munin3 | 9 | 15 | 9 | 30 |
| munin4 | 9 | 18 | 9 | 30 |
| water | 11 | 16 | 10 | 15 |
| pigs | 11 | 20 | 11 | 26 |

Bayesian Networks Repository

| Network | hypergraph |  | min-fill |  |
| :--- | :---: | :---: | :---: | :---: |
|  | $w^{*}$ | depth | $w^{*}$ | depth |
| spot5 | 47 | 152 | 39 | 204 |
| spot28 | 108 | 138 | 79 | 199 |
| spot29 | 16 | 23 | 14 | 42 |
| spot42 | 36 | 48 | 33 | 87 |
| spot54 | 12 | 16 | 11 | 33 |
| spot404 | 19 | 26 | 19 | 42 |
| spot408 | 47 | 52 | 35 | 97 |
| spot503 | 11 | 20 | 9 | 39 |
| spot505 | 29 | 42 | 23 | 74 |
| spot507 | 70 | 122 | 59 | 160 |

SPOT5 Benchmark

## From Search Trees to Search Graphs

- Any two nodes that root identical subtrees or subgraphs can be merged


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## From Search Trees to Search Graphs

- Any two nodes that root identical subtrees or subgraphs can be merged


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## Merging Based on Contexts

- One way of recognizing nodes that can be merged (based on the graph structure)
- context $(X)=$ ancestors of $X$ in the pseudo tree that are connected to $X$ or to descendants of $X$



## AND/OR Search Graph



| A |  | $f_{a b}$ | A | C |  | A | E | $f_{\text {ae }}$ | A | F |  | af | B |  |  |  | B | I | $f_{b d}$ | B |  |  |  | C | D | $\mathrm{f}_{\mathrm{cd}}$ | E |  | ef |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 2 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 |  | 3 | 0 | 0 | 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 3 | 0 | 1 | 0 | 0 | 0 | 1 |  | 1 | 0 | 1 | 2 | 0 | 1 | 12 | 2 | 0 | 1 | 4 | 0 | 1 | 0 |
| 1 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 2 | 1 | 0 | 0 | 0 | 1 | 0 | 2 | 2 | 1 | 0 | 1 | 1 | 0 |  | 1 | 1 | 0 | 0 | 1 | 0 | 0 |
| 1 | 1 | 4 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 2 | 2 | 1 | 1 |  | 4 | 1 | 1 | 0 | 1 | 1 |  | 0 | 1 | 1 | 0 | 1 | 1 | 2 |

Objective function: $F^{*}=\min _{x} \sum_{\alpha} f_{\alpha}\left(x_{\alpha}\right)$


Cache table for D

## How Big Is The Context?

- Theorem: The maximum context size for a pseudo tree is equal to the treewidth of the graph along the pseudo tree.

(CKHABEJLNODPMFG)


## Complexity of AND/OR Graph Search

## AND/OR graph <br> OR graph

## Space

$O\left(n d^{w^{*}}\right)$
$O\left(n d^{p w^{*}}\right)$

## Time

$$
O\left(n d^{w^{*}}\right) \quad O\left(n d^{p w^{*}}\right)
$$

d = domain size
$\mathrm{w}^{*}=$ induced width
$\mathrm{n}=$ number of variables
pw* = pathwidth

$$
w^{*} \leq p w^{*} \leq w^{*} \log n
$$

## All Four Search Spaces



Full OR search tree
126 nodes


Full ANDIOR search tree
54 AND nodes


Context minimal OR search graph
28 nodes


## Context minimal AND/OR search graph

18 AND nodes

## Outline

- Bounds and heuristics
- AND/OR Search
- AND/OR Branch and Bound
- 
- 
- 
- 


## Classic Depth-First Branch and Bound



Each node is a COP subproblem (defined by current conditioning)
$\mathrm{g}(\mathrm{n})$ : cost of the path from root to n

$$
\begin{aligned}
& \tilde{f}(n)=g(n)+\tilde{h}(n) \\
& \quad \text { (lower bound) }
\end{aligned}
$$

$$
\text { Prune if } \tilde{f}(n) \geq U B
$$

$\tilde{h}(n)$ : under-estimates optimal cost below n
(UB) Upper Bound = best solution so far

## Partial Solution Tree



Pseudo tree

( $\mathrm{A}=0, \mathrm{~B}=0, \mathrm{C}=0, \mathrm{D}=0$ )


Extension( $\left.T^{\prime}\right)$ - solution trees that extend $T^{\prime}$

## Exact Evaluation Function



$$
f^{*}\left(T^{\prime}\right)=w(A, 0)+w(B, 1)+w(C, 0)+w(D, 0)+v(D, 0)+v(F)
$$

## Exact Evaluation Function



| $B$ | $D$ | $E$ | $f_{3}(B D E)$ |
| :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | 6 |
| 0 | 0 | 1 | 4 |
| 0 | 1 | 0 | 8 |
| 0 | 1 | 1 | 5 |
| 1 | 0 | 0 | 9 |
| 1 | 0 | 1 | 3 |
| 1 | 1 | 0 | 7 |
| 1 | 1 | 1 | 4 |



$$
f\left(T^{\prime}\right)=w(A, 0)+w(B, 1)+w(C, 0)+w(D, 0)+h(D, 0)+h(F)=12 \leq f^{*}\left(T^{\prime}\right)
$$

## AND/OR Branch and Bound Search



## AND/OR Branch and Bound (AOBB)

- Associate each node $n$ with a heuristic lower bound $h(n)$ on $v(n)$
- EXPAND (top-down)
- Evaluate $f\left(T^{\prime}\right)$ and prune search if $f\left(T^{\prime}\right) \geq$ UB
- Generate successors of the tip node n
- UPDATE (bottom-up)
- Update value of the parent $p$ of $n$
- OR nodes: minimization
- AND nodes: summation


## AND/OR Branch and Bound with Caching

- Associate each node n with a heuristic lower bound $h(n)$ on $v(n)$
- EXPAND (top-down)
- Evaluate $f\left(T^{\prime}\right)$ and prune search if $f\left(T^{\prime}\right) \geq$ UB
- If not in cache, generate successors of the tip node $n$
- UPDATE (bottom-up)
- Update value of the parent $p$ of $n$
- OR nodes: minimization
- AND nodes: summation
- Cache value of $n$ based on context


## Breadth-Rotating AOBB

- AND/OR decomposition vs. depth-first search:
- Compromises anytime property of AOBB.
solved optimally


## Breadth-Rotating AOBB

- AND/OR decomposition vs. depth-first search:
- Compromises anytime property of AOBB.
- Breadth-Rotating AOBB:
- Combined breadth/depth-first schedule.
- Maintains depth-first complexity.
- Superior experimental results.



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- Won PASCAL'11 Inference Challenge MPE track.


## Mini-Bucket Heuristics for AND/OR Search

- The depth-first and best-first AND/OR search algorithms use $h(n)$ that can be computed:
- Static Mini-Bucket Heuristics
- Pre-compiled
- Reduced computational overhead
- Less accurate
- Static variable ordering
- Dynamic Mini-Bucket Heuristics
- Computed dynamically, during search
- Higher computational overhead
- High accuracy
- Dynamic variable ordering


## Bucket Elimination



Ordering: $(A, B, C, D, E, F, G)$


Exact evaluation of $(A=a, B=b)$ below $C$ : $h^{*}(a, b, C)=h^{D}(a, b, C)+h^{E}(b, C)$

## Static Mini-Bucket Heuristics



$$
\begin{aligned}
h(a, b, C) & =h^{D}(a)+h^{D}(b, C)+h^{E}(b, C) \\
& \leq h^{\star}(a, b, C)
\end{aligned}
$$

## Dynamic Mini-Bucket Heuristics



Ordering: (A, B, C, D, E, F, G)


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## Dynamic Variable Orderings

- Variable ordering heuristics
- Semantic-based
- Aim at shrinking the size of the search space based on context and current value assignments
- e.g., min-domain, min-dom/wdeg, min reduced cost
- Graph-based
- Aim at maximizing the problem decomposition
- e.g., pseudo tree arrangement


## Partial Variable Orderings (PVO)



Primal graph


Variable Groups/Chains:

- $\{A, B\}$
- $\{C, D\}$
- $\{\mathrm{E}, \mathrm{F}\}$

Instantiate $\{\mathrm{A}, \mathrm{B}\}$ before $\{C, D\}$ and $\{E, F\}$

* $\{A, B\}$ is a separator/chain

Variables on chains in the pseudo tree can be instantiated dynamically, based on some semantic ordering heuristic

* Similar idea is exploited by BTD (Backtracking with Tree Decomposition) [Jegou and Terrioux, 2004]


## Full Dynamic Variable Ordering (DVO)



Domains $\quad D_{A}=\{0,1\} \quad D_{B}=\{0,1,2\}$ $\mathrm{D}_{\mathrm{E}}=\{0,1,2,3\}$
$\mathrm{D}_{\mathrm{C}}=\mathrm{D}_{\mathrm{D}}=\mathrm{D}_{\mathrm{F}}=\mathrm{D}_{\mathrm{G}}=\mathrm{D}_{\mathrm{H}}=\mathrm{D}_{\mathrm{E}}$
Cost functions

| $A$ | $B$ | $f(A B)$ | $A$ | $E$ | $f(A E)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | $\mathbf{3}$ | 0 | 0 | 0 |
| 0 | 1 | 8 | 0 | 1 | $\mathbf{5}$ |
| 0 | 2 | $\mathbf{8}$ | 0 | 2 | $\mathbf{1}$ |
| 1 | 0 | 4 | 0 | 3 | $\mathbf{4}$ |
| 1 | 1 | 0 | 1 | 0 | $\mathbf{8}$ |
| 1 | 2 | 6 | 1 | 1 | $\mathbf{8}$ |
|  |  |  | 1 | 2 | 0 |
|  |  |  | 1 | 3 | $\mathbf{5}$ |



* Similar idea exploited in \#SAT [Bayardo and Pehoushek, 2000]


## Dynamic Separator Ordering (DSO)



Constraint Propagation may create singleton variables in P1 and P2 (changing the problem's structure), which in turn may yield smaller separators

* Similar idea exploited in SAT [Li and val Beek, 2004]


## Backtrack with Tree Decomposition


tree decomposition ( $\mathrm{w}=2$ )

## BTD:

- AND/OR graph search (caching on separators)
- Partial variable ordering (dynamic inside clusters)
- Maintaining local consistency



## Backtrack with Tree Decomposition

- Before the search
- Merge clusters with a separator size > p
- Time O(k exp(w*)), Space O(exp(p))
- More freedom for variable ordering heuristics
- Properties
- BTD(-1) is Depth-First Branch and Bound
- BTD(0) solves connected components independently
- BTD(1) exploits bi-connected components
- BTD(s) is Backtrack with Tree Decomposition (s: largest separator size)


## Outline

- 
- 
- 
- AND/OR Search
- 
- AND/OR Branch and Bound
- Best-First AND/OR Search
- Advanced Searches and Tasks


## Outline

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## Basic Heuristic Search Schemes

Heuristic function $\tilde{f}\left(\hat{x}_{p}\right)$ computes a lower bound on the best extension of partial configuration $\hat{x}_{p}$ and can be used to guide heuristic search.
We focus on:

1. Branch-and-Bound

Use heuristic function $\tilde{f}\left(\hat{x}_{p}\right)$ to prune the depth-first search tree Linear space

$f(\hat{x})=U$

## 2. Best-First Search

Always expand the node with the lowest heuristic value $\tilde{f}\left(\hat{x}_{p}\right)$
Needs lots of memory


## Best-First Principle

- Best-first search expands first the node with the best heuristic evaluation function among all nodes encountered so far
- Never expands nodes whose cost is beyond the optimal one, unlike depth-first algorithms [Dechter and Pearl, 1985]
- Superior among memory intensive algorithms employing the same heuristic evaluation function


## Best-First AND/OR Search (AOBF)

- Maintains the explicated AND/OR search graph in memory
- Top-Down Step (EXPAND)
- Trace down marked connectors from root
- E.g., best partial solution tree
- Expand a tip node $n$ by generating its successors n'
- Associate each successor with heuristic estimate $h\left(n^{\prime}\right)$
- Initialize $\mathbf{q ( n )}=\mathbf{h ( n ' )}$ (q-value $\mathrm{q}(\mathrm{n})$ is a lower bound on $v(n)$


## - Bottom-Up Step (UPDATE)

- Update node values $q(n)$
- OR nodes: minimization
- AND nodes: summation
- Mark the most promissing partial solution tree from the root
- Label the nodes as SOLVED:
- OR node is SOLVED if marked child is SOLVED
- AND node is SOLVED if all children are SOLVED
- Terminate when root node is SOLVED
[Marinescu and Dechter, 2006; 2009]


## AOBF versus AOBB

- AOBF with the same heuristic as AOBB is likely to expand the smallest search space
- This translates into significant time savings
- AOBB can use far less memory by avoiding for example dead-caches, whereas AOBF keeps in memory the explicated search graph
- AOBB is anytime, whereas AOBF is not


## Recursive Best-First AND/OR Search

- AND/OR search algorithms (AOBB and AOBF)
- AOBB (depth-first): memory efficient but may explore many suboptimal subspaces
- AOBF (best-first): explores the smallest search space but may require huge memory
- Recursive best-first search for AND/OR graphs
- Requires limited memory (even linear)
- Nodes are explored in best-first order
- Main issue: some nodes will be re-expanded (want to minimize this)


## Recursive Best-First AND/OR Search

- Transform best-first search (AO* like) into depth-first search using a threshold controlling mechanism (explained next)
- Based on Korf's classic RBFS
- Adapted to the context minimal AND/OR graph
- Nodes are still expanded in best-first order
- Node values are updated in the usual manner based on the values of their successors
- OR nodes by minimization
- AND nodes by summation
- Some nodes will be re-expanded
- Use caching (limited memory) based on contexts
- Use overestimation of the threshold to minimize node re-expansions


## RBFAOO - Example (1)



- Expand OR node A by generating its AND successors: $(A, 0)$ and (A,1)
- Best successor is $(\mathrm{A}, 0)$
- Set threshold $\theta(A, 0)=4$ - indicates next best successor is (A,1)
- We can backtrack to $(\mathrm{A}, 1)$ if the updated cost of the subtree below $(\mathrm{A}, 0)$ exceeds the threshold $\theta=4$


## RBFAOO - Example (2)



- Expand AND node $(A, 0)$ by generating its OR successors: $B$ and $C$
- Update node value $\mathrm{q}(\mathrm{A}, 0)=\mathrm{h}(\mathrm{B})+\mathrm{h}(\mathrm{C})=3-$ threshold OK


## RBFAOO - Example (3)



- Expand OR node $B$ by generating its AND successor: $(B, 0)$
- Update node values $q(B)=4$ and $q(A, 0)=6-$ threshold NOT OK


## RBFAOO - Example (4)



- Backtrack to $(\mathrm{A}, 0)$ and select next best node $(\mathrm{A}, 1)$
- Set threshold $\theta(A, 1)=6$ (updated value of the left subtree)
- Cache (minimize re-expansion) or discard left subtree


## RBFAOO - Overestimation



- Some of the nodes in the subtree below $(\mathrm{A}, 0)$ may be re-expanded
- Simple overestimation scheme for minimizing the node re-expansions
- Inflate the threshold with some small $\delta$ : $\theta^{\prime}=\theta+\delta(\delta>0)$
- In practice, we determine $\delta$ experimentally (e.g., $\delta=1$ worked best)


## Empirical Evaluation




Grid and Pedigree benchmarks; Time limit 1 hour.

## Outline

- 
- 
- 
- AND/OR Search
- 
- 
- 
- Advanced Searches and Tasks


## Marginal MAP

- Occurs in many applications involving hidden variables
- Seeks a partial configuration of variables with maximum marginal probability
- Complexity: NPPP-complete
- State-of-the-art is DFS BnB (over the MAP variables)
- Guided by unconstrained join-tree based upper bounds
- Advances
- AND/OR Branch and Bound and Best-First AND/OR Search algorithms
- Heuristics based on Weighted Mini-Buckets
- WMB-MM: single pass with cost-shifting by moment matching
- WMB-JG: iterative updates by message passing along the join-graph


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## AND/OR Search Space for MMAP


constrained pseudo tree

## AND/OR Search Space for MMAP



- Node types
- OR (MAP): max
- OR (SUM): sum
- AND: multiplication
- Arc weights
- derived from input F
- Problem decomposition over MAP variables


## AND/OR Search Algorithms

- AOBB: Depth-First AND/OR Branch and Bound
- Depth-first traversal of the AND/OR search graph
- Prune only at OR nodes that correspond to MAP variables
- Cost of MAP assignment obtained by searching the SUM sub-problem
- AOBF: Best First AND/OR Search
- Best-first (AO*) traversal of the AND/OR space corresponding to the MAP variables
- SUM subproblem solved exactly
- RBFAOO: Recursive Best-First AND/OR Search
- Recursive best-first traversal of the AND/OR graph
- For SUM subproblems, the threshold is set to $\infty$ (equivalent to depthfirst search)
[Marinescu, Dechter and Ihler; 2014; 2015] ${ }^{\text {ICAI } 2015}$


## Quality of the Upper Bounds



Average relative error wrt tightest upper bound. 10 iterations for WMB-JG(i).

## AOBB versus BB




Number of instances solved and median CPU time (sec). 10 iterations for WMB-JG(i).

## AOBF/RBFAOO versus AOBB




Number of instances solved and median CPU time (sec). Time limit 1 hour.

## Searching for M Best Solutions

- New inference and search based algorithms for the task of finding the $m$ best solutions
- Search: m-A*, m-BB
- Inference: elim-m-opt, BE+m-BF
- Extended m-A* and m-BB to AND/OR search spaces for graphical models, yielding m-AOBB and m-AOBF
- Competitive and often superior to alternative (approximate) approaches based on LP relaxations
- e.g., [Fromer and Globerson, 2009], [Batra, 2012]


## Searching for M Best Solutions



## Empirical Evaluation



Grid instances; Time limit $=3 \mathrm{~h}$; Memory bound $=4 \mathrm{~GB}$

## Hybrid of Variable Elimination and Search

- Tradeoff space and time


## Search Basic Step: Conditioning

Variable Branching by Conditioning


## Search Basic Step: Conditioning

Variable Branching by Conditioning

Select a variable


## Search Basic Step: Conditioning

 Variable Branching by Conditioning

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## Search Basic Step: Conditioning

 Variable Branching by Conditioning

## The Cycle-Cutset Scheme

## Condition until Treeness

- Cycle-cutset
- i-cutset
- C(i)-size of i-cutset

<Tree part
(F) (E)
(C)
(D)


Space: $\exp (\mathrm{i})$, Time: $\mathbf{O}(\exp (\mathbf{i}+\mathrm{c}(\mathrm{i}))$
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## Eliminate First



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## Eliminate First



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## Eliminate First



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## Hybrid Variants

- Condition, condition, condition, ... and then only eliminate (w-cutset, cycle-cutset)
- Eliminate, eliminate, eliminate, ... and then only search
- Interleave conditioning and elimination steps (elim-cond(i), VE+C)


## Interleaving Conditioning and Elimination



## Interleaving Conditioning and Elimination



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## Interleaving Conditioning and Elimination



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## Interleaving Conditioning and Elimination



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## Interleaving Conditioning and Elimination



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## Interleaving Conditioning and Elimination



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## Interleaving Conditioning and Elimination



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## Boosting Search with Variable Elimination

- At each search node
- Eliminate all unassigned variables with degree $\leq p$
- Select an assigned variable A
- Branch on the values of A
- Properties
- BB+VE(-1) is Depth-First Branch and Bound
- $\mathrm{BB}+\mathrm{VE}(\mathrm{w})$ is Variable Elimination
- $\mathrm{BB}+\mathrm{VE}(1)$ is similar to Cycle-Cutset
- $\mathrm{BB}+\mathrm{VE}(2)$ is well suited with soft local consistencies (add binary constraints only, independent of elimination order)


## Mendelian Error Detection



- Given a pedigree and partial observations (genotypings)
- Find the erroneous genotypings, such that their removal restores consistency
- Checking consistency is NP-complete [Aceto et al, 2004]
- Minimize the number of genotypings to be removed
- Maximize the joint probability of true genotypes (MPE/MAP)

$$
\text { Pedigree problem size: } n \leq 20,000 ; k=3-66 ; e(3) \leq 30,000
$$

## Pedigree

- toulbar2 v0.5 with EDAC and binary branching
- Minimize the number of genotypings to be removed
- CPU time to find and prove optimality on a 3 GHz computer with 16 GB


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## Outline

- Bounds and heuristics

- Exploiting parallelism


## Outline



- Exploiting parallelism
- Distributed and parallel search


## Contributions

- Propose parallel $A O B B$, first of its kind.
- Runs on computational grid.
- Extends parallel tree search paradigm.
- Two variants with different parallelization logic.
- Analysis of schemes' properties:
- Performance considerations and trade-offs.
- Granularity vs. overhead and redundancies.
- Large-scale experimental evaluation:
- Good parallel performance in many cases.
- Analysis of some potential performance pitfalls.


## Context and Related Work

- Task parallelism (vs. data parallelism):
- Extensive computation on small input.


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- Task parallelism (vs. data parallelism):
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- Computational grid framework:
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- Parallel tree search ("stack splitting"):
- Typically uses shared memory for dynamic load balancing and cost bound updates for BaB.
- Not feasible in grid setup.
- Motivation: Superlink Online.
- Distributed linkage (likelihood) computation.


## Parallel AOBB Illustrated

- Master process applies partial conditioning to obtain parallel subproblems.



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8 independent subproblem search spaces

## Fixed-depth Parallel AOBB

- Algorithm receives cutoff depth $d$ as input:
- Expand nodes centrally until depth $d$.
- At depth $d$, submit to grid job queue.


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## Variable-depth Parallel AOBB

- Given subproblem count $p$ and estimator $N$ :
- Iteratively deepen frontier until size $p$ reached:
- Pick subproblem $n$ with largest estimate $N(n)$ and split.
- Submit subproblems into job queue by descending complexity estimates.


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## Aside: Modeling AOBB Complexity

- Model number of nodes $N(n)$ in subproblem as exp. function of subproblem features $\varphi_{i}(n)$ :

$$
N(n)=\exp \left(\sum_{i} \lambda_{i} \varphi_{i}(n)\right)
$$

## Aside: Modeling AOBB Complexity

- Model number of nodes $N(n)$ in subproblem as exp. function of subproblem features $\varphi_{i}(n)$ :

$$
N(n)=\exp \left(\sum_{i} \lambda_{i} \varphi_{i}(n)\right)
$$

- Logarithm yields linear regression problem.
- Minimize MSE with Lasso regularization. [Tibshirani]

$$
\frac{1}{m} \sum_{j=1}^{m}\left(\sum_{i} \lambda_{i} \varphi_{i}\left(n_{k}\right)-\log N\left(n_{k}\right)\right)^{2}+\alpha \sum_{i}\left|\lambda_{i}\right|
$$

- Full details:
- "A Case Study in Complexity Estimation: Towards Parallel Branch-and-Bound over Graphical Models", UAI 2012.


## 35 Subproblem Features <br> Subproblem variable statistics (static):

## - Characterize subproblem:

- Static, structural properties:
- Number of variables.
- Avg. and max. width.
- Height of sub pseudo tree.
- State space bound SS .
- Dynamic, runtime properties:
- Upper and lower bound on subproblem cost.
- Pruning ratio and depth of small AOBB probe.
- only $5 n$ nodes, very fast.

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1: Number of variables in subproblem
2-6: Min, Max, mean, average, and std. dev. of variable domain sizes in subproblem.
Pseudo tree depth/leaf statistics (static):
7: Depth of subproblem root in overall search space.
8-12: Min, max, mean, average, and std. dev. of depth of subproblem pseudo tree leaf nodes, counted from subproblem root
13: Number of leaf nodes in subproblem pseudo tree
Pseudo tree width statistics (static):
14-18: Min, max, mean, average, and std. dev. of induced width of variables within subproblem.
19-23: Min, max, mean, average, and std. dev. of induced width of variables within subproblem, conditioned on subproblem root context.
State space bound (static):
24: State space size upper bound on subproblem search space size.
Subproblem cost bounds (dynamic):
25: Lower bound $L$ on subproblem solution cost, derived from current best overall solution.
26: Upper bound $U$ on subproblem solution cost, provided by mini bucket heuristics.
27: Difference $U-L$ between upper and lower bound, expressing "constrainedness" of the subproblem.
Pruning ratios (dynamic), based on running AOBB for $5 n$ node expansions:

28: Ratio of nodes pruned using the heuristic
29: Ratio of nodes pruned due of determinism (zero probabilities, e.g.)
30: Ratio of nodes corresponding to pseudo tree leaf. AOBB sample (dynamic), based on running AOBB for $5 n$ node expansions:

31: Average depth of terminal search nodes within probe
32: Average node depth within probe (denoted $\bar{d}$ ).
33: Average branching degree, defined as $\sqrt[d]{5 n}$
Various (static):
34: Mini bucket $i$-bound parameter
35: Max. subproblem variable context size minus mini bucket $i$-bound.

## Example Estimation Results

- Across subproblems from several domains.
- Hold out test data for model learning.










## Assessing Parallel Performance

- Sequential AOBB performance baseline:
- $T_{\text {seq }}$ : sequential runtime.
- $N_{\text {seq }}$ : number of sequential node expansions.


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- $T_{\text {par }}$ : parallel runtime including central preprocessing.
- $\mathrm{S}_{\text {par }}$ : Parallel speedup $T_{\text {seq }} / T_{p a r}$.


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- $\mathrm{S}_{p a r}$ : Parallel speedup $T_{\text {seq }} / T_{p a r}$.
- $N_{p a r}$ : Node expansions across all subproblems.
- $O_{p a r}$ : Relative parallel overhead $N_{p a r} / N_{s e q}$.


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- $O_{p a r}$ : Relative parallel overhead $N_{p a r} / N_{\text {seq }}$.
- $U_{\text {par: }}$ Avg. processor utilization, relative to longest.


## Performance Considerations

- Amdahl's Law [1967]:
- "If a fraction $p$ of a computation can be sped up by a factor or $s$, the overall speedup cannot exceed $1 /(1-p+p / s)$."
- Example: 20 minute computation, 30 sec preprocessing. Best speedup 40x (regardless of parallel CPUs).


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- Example: 20 minute computation, 30 sec preprocessing. Best speedup 40x (regardless of parallel CPUs).
- Implication of overhead $O_{p a r}$ :
- Proposition: assuming parallel overhead o and execution on $p$ CPUs, speedup is bounded by $p / o$.
- Example: 500 CPUs, overhead $2 \rightarrow$ best speedup 250.
- In practice even lower due to load balancing, communication delaysfe ettqrs


## Parallel AOBB Performance Factors

- Distributed System Overhead:
- Master preprocessing and parallelization decision.
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- Communication and scheduling delays.


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- Impacted pruning, lack of bounds propagation.
- Local search for near-optimal initial bound.
- Loss of caching across parallel subproblems.
- Analyzed subsequently.


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- Distributed System Overhead:
- Master preprocessing and parallelization decision.
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- Parallel search space redundancies:
- Impacted pruning, lack of bounds propagation.
- Local search for near-optimal initial bound.
- Loss of caching across parallel subproblems.
- Analyzed subsequently.
- Parallel AOBB is not "embarrassingly parallel".


## Redundancy Analysis



## Redundancy Analysis



$[\mathrm{BC}](\mathrm{D}) \quad \mathrm{F}:[\mathrm{BE}]$
[D] G
(H) ${ }^{\text {EFF] }}$


## Redundancy Analysis



$[\mathrm{BC}] \mathrm{D}, \mathrm{F},[\mathrm{BE}]$
[D] G
(H) $[\mathrm{EF}]$


## Redundancy Analysis




## Redundancy Analysis



## Redundancy Analysis



## Redundancy Analysis



## Redundancy Analysis



## Redundancy Analysis


(B)


## Redundancy Analysis


d=1


## Redundancy Analysis


d=1


## Redundancy Analysis


d=1


## Redundancy Analysis


d=1


## Redundancy Analysis


$[D]$
(H) $[\mathrm{EF}]$

B




0101010101010101010101020001010101010100101010101

$$
\{A=0, B=0\} \quad\{A=0, B=0\} \quad\{A=0, B=1\} \quad\{A=0, B=1\} \quad\{A=1, B=0\} \quad\{A=1, B=0\} \quad\{A=1, B=1\} \quad\{A=1, B=1\}
$$

## Redundancy Analysis


[D]
H $[\mathrm{EF}]$


## Redundancy Analysis


(A)


$[\mathrm{D}]$
(H) $[\mathrm{EF}]$

B


## Redundancy Analysis

(A)


## Redundancy Quantied

- Definitions:
- $w_{d}(X)$ is size of context of $X$ below level $d$.
- $\pi_{d}(X)$ is ancestor of $X$ at level $d$.
- Underlying parallel search space size SS $_{p a r}$ :

$$
S S_{p a r}(d)=\sum_{j=0}^{d} \sum_{X^{\prime} \in L_{j}} k^{w\left(X^{\prime}\right)+1}+\sum_{j=d+1}^{h} \sum_{X^{\prime} \in L_{j}} k^{w\left(\pi_{d}\left(X^{\prime}\right)\right)+w_{d}\left(X^{\prime}\right)+1}
$$

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- Underlying parallel search space size $S S_{p a r}$ :

$-S S_{p a r}(0)=S S_{p a r}(h)=S S_{s e q}$.
$-S S_{p a r}(d) \geq S S_{p a r}(0)$ for all $d$.


## Redundancy vs. Parallelism

- Assume parallelism with sufficient CPUs.
- Consider conditioning space + max. subproblem.

| Example revisited: | $d$ |  |  |  |  |  |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| parallel space $S S_{\text {par }}(d)$ | 50 | 78 | 102 | 70 | 50 | 50 |
| conditioning space | 0 | 2 | 6 | 22 | 38 | 50 |
| no. of subproblems | 1 | 2 | 8 | 8 | 6 | 0 |
| max. parallel subproblem | 50 | 38 | 14 | 6 | 2 | - |
| cond. space + max. subprob | 50 | 40 | 20 | 28 | 40 | 50 |

## Redundancy vs. Parallelism

- Assume parallelism with sufficient CPUs.
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| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
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## Redundancy vs. Parallelism

- Assume parallelism with sufficient CPUs.
- Consider conditioning space + max. subproblem.

|  | $d$ |  |  |  |  |  |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example revisited: | 0 | 1 | 2 | 3 | 4 | 5 |
| parallel space $S S_{\text {par }}(d)$ | 50 | 78 | 102 | 70 | 50 | 50 |
| conditioning space | 0 | 2 | 6 | 22 | 38 | 50 |
| no. of subproblems | 1 | 2 | 8 | 8 | 6 | 0 |
| max. parallel subproblem | 50 | 38 | 14 | 6 | 2 | - |
| cond. space + max. subprob | 50 | 40 | 20 | 28 | 40 | 50 |

## Redundancy vs. Parallelism

- Assume parallelism with sufficient CPUs.
- Consider conditioning space + max. subproblem.

- But: doesn't capture explored search space.
- Can pruning compensate for redundancies?


## Empirical Evaluation

- Parallel experiments over 75 benchmarks.
- Instances from four classes, with varying $i$-bound.
- $T_{\text {seq }}$ from under 1 hour to over 2 weeks.
- Run with 20, 100, and 500 parallel CPUs.


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- Apply different fixed-depth cutoff depths $d$.
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## Empirical Evaluation

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- Experimental Methodology:
- Apply different fixed-depth cutoff depths $d$.
- Use subproblem count $p$ as var-depth input.
- ~91 thousand CPU hours - over 10 years!
- Over 1400 parallel runs.
- Can only summarize s@mers aspects here.


## Example Results

- Record overall parallel runtime / speedup.
- Lots of data!

|  |  |  |  | Cutoff depth $d$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| instance | $i$ | $T_{\text {seq }}$ | \#cpu | 2 | 4 | 6 | 8 | 10 | 12 |
|  |  |  |  | fix $\operatorname{var}$ | fix $\operatorname{var}$ | fix var | fix $\operatorname{var}$ | fix var | fix $\quad$ var |
| $\begin{aligned} & \text { lF3-15-59 } \\ & \begin{array}{l} n=3730 \\ k=31 \\ w=31 \end{array} \\ & h=84 \end{aligned}$ | 19 | 43307 |  | ( $p=4$ ) | ( $p=20$ ) | ( $p=80$ ) | ( $p=476$ ) | ( $p=1830$ ) | ( $p=6964$ ) |
|  |  |  | 20 | 1585815694 | 59095470 | 36492845 | 27442501 | 34823505 | 72227238 |
|  |  |  | 100 | 1585815694 | 59095470 | 34342247 | $1494 \quad 723$ | 928741 | 15401536 |
|  |  |  | 500 | 1585815694 | 59095470 | 34342247 | $1414 \quad 573$ | 692260 | 415399 |
| $\begin{aligned} & \text { ped44 } \\ & \begin{array}{l} n=811 \\ k==85 \\ w=65 \end{array} \\ & h \end{aligned}$ |  | 95830 |  | $(p=4)$ | ( $p=16$ ) | ( $p=112$ ) | ( $p=560$ ) | ( $p=2240$ ) | ( $p=8960$ ) |
|  |  |  | 20 | 2677626836 | 97169481 | 67416811 | 79597947 | 101039763 | 1241812472 |
|  |  |  | 100 | 2677626836 | 97169481 | 23443586 | 17991700 | 21262276 | $2545 \quad 2543$ |
|  |  |  | 500 | 2677626836 | 97169481 | 16593586 | 583886 | 536905 | 569824 |
| $\begin{aligned} & \text { ped7 } \\ & \begin{array}{l} n=1068 \\ k=106 \\ w=32 \\ h=90 \end{array} \end{aligned}$ | 6118383 |  |  | $(p=4)$ | ( $p=32$ ) | ( $p=160$ ) | ( $p=640$ ) | ( $p=1280$ ) | ( $p=3840$ ) |
|  |  |  | 20 | 3538758872 | 1233858121 | 90318515 | 96547319 | 87057582 | 82367693 |
|  |  |  | 100 | 3538758872 | 1195658121 | 51227690 | 48602306 | 39291814 | 26441649 |
|  |  |  | 500 | 3538758872 | 1195658121 | 49847690 | 43592086 | 32941301 | 1764943 |

## Example Results

- Record overall parallel runtime / speedup.
- Lots of data!

| instance | $i$ | $T_{\text {seq }}$ | \#cpu | Cutoff depth $d$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | 2 | 4 | 6 | 8 | 10 | 12 |
|  |  |  |  | fix var | fix var | fix var | fix var | fix var | fix var |
| IF3-15-59 |  |  |  | $(p=4)$ 2 | ${ }^{(p=20)}$ | ( $p=80$ ) | ( $p=476$ ) | ( $p=1830$ ) | ( $p=6964$ ) |
|  |  | 43307 | 20 | 2.732 .76 | $7.33-7.92$ | 11.8715 .22 | 15.7817 .32 | 12.4412 .36 | $6.00 \quad 5.98$ |
| $\begin{aligned} & n=3 \\ & k=3 \\ & w=31 \end{aligned}$ |  | 43307 | 100 | 2.732 .76 | 7.33 | 12.6119 .27 | $28.99 \quad 59.90$ | $46.67 \quad 58.44$ | $28.12 \quad 28.19$ |
| $h=84$ |  |  | 500 | 2.732 .76 | $7.33 \quad 7.92$ | 12.6119 .27 | $30.63 \quad 75.58$ | 62.58166 .57 | 104.35108 .54 |
|  |  |  |  | ( $p=4$ ) | ( $p=16$ ) | ( $p=112$ ) | ( $p=560$ ) | ( $p=2240$ ) | ( $p=8960$ ) |
|  |  | 95830 | 20 | 3.583 .57 | 9.8610 .11 | 14.2214 .07 | 12.0412 .06 | $9.49 \quad 9.82$ | $7.72 \quad 7.68$ |
| $n=81$ $k=4$ $w=25$ |  | 95830 | 100 | 3.583 .57 | 9.8610 .11 | 40.8826 .72 | $53.27 \quad 56.37$ | 45.0842 .10 | $37.65 \quad 37.68$ |
| ${ }^{w} h=65$ |  |  | 500 | 3.583 .57 | 9.8610 .11 | 57.7626 .72 | 164.37108 .16 | 178.79105 .89 | 168.42116 .30 |
|  |  |  |  | ( $p=4$ ) | ( $p=32$ ) | ( $p=160$ ) | ( $p=640$ ) | ( $p=1280$ ) | ( $p=3840$ ) |
| $\frac{\mathrm{ped}}{n=1068}$ |  | 8383 | 20 | 3.352 .01 | $9.59 \quad 2.04$ | 13.1113 .90 | $\begin{array}{lll}12.26 & 16.17\end{array}$ | 13.6015 .61 | 14.3715 .39 |
|  |  | 8383 | 100 | 3.352 .01 | $9.90 \quad 2.04$ | 23.1115 .39 | $24.36 \quad 51.34$ | $30.13 \quad 65.26$ | $44.77 \quad 71.79$ |
| $h=90$ |  |  | 500 | 3.352 .01 | $9.90 \quad 2.04$ | 23.7515 .39 | $27.16 \quad 56.75$ | $35.94 \quad 90.99$ | 67.11125 .54 |

## Example: LargeFam3-15-59, $i=19$

- Sequential runtime

$$
T_{\text {seq }}=43,307 \mathrm{sec} .
$$



## Example: LargeFam3-15-59, $i=19$

- Sequential runtime $T_{\text {seq }}=43,307 \mathrm{sec}$.

(Fixed-depth)

(Variable-depth)



## Example: Pedigree7, $i=6$

- Sequential runtime $T_{\text {seq }}=118,383 \mathrm{sec}$.



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(Fixed-depth)
ped7, $i=6,20$ CPUs, fixed $d=5$

(Variable-depth)



## Example: Pedigree7, $i=6$

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ped7, $i=6,20$ CPUs, fixed $d=5$



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(Fixed-depth)



## Example: LargeFam3-16-56, $i=15$

- Sequential runtime

$$
T_{\text {seq }}=1,891,710 \mathrm{sec} .
$$

IF3-16-56, i=15


## Example: LargeFam3-16-56, $i=15$

- Sequential runtime $T_{\text {seq }}=1,891,710 \mathrm{sec}$.
(Fixed-depth)
IF3-16-56, $\mathrm{i}=15,100$ CPUs, fixed $\mathrm{d}=7$
IF3-16-56, $\mathrm{i}=15$



## Example: LargeFam3-16-56, $i=15$

- Sequential runtime $T_{\text {seq }}=1,891,710 \mathrm{sec}$.
(Fixed-depth)

IF3-16-56, $\mathrm{i}=15$


## Example: Pdb1huw, $i=3$

- Sequential runtime

$$
T_{\text {seq }}=545,249 \mathrm{sec} .
$$



## Example: Pdb1huw, $i=3$

- Sequential runtime
$T_{\text {seq }}=545,249 \mathrm{sec}$.

(Fixed-depth)
pdb1huw, $i=3,100$ CPUs, fixed $d=4$

(Variable-depth)



## Example: Pdb1huw, $i=3$

- Sequential runtime
$T_{\text {seq }}=545,249 \mathrm{sec}$.

(Fixed-depth) pdb1huw, $i=3,100$ CPUs, fixed $d=4$



## Example: 75-25-1, $i=14$

- Sequential runtime

$$
T_{\text {seq }}=15,402 \mathrm{sec} .
$$



## Example: 75-25-1, $i=14$

- Sequential runtime $T_{\text {seq }}=15,402 \mathrm{sec}$.

(Fixed-depth)

(Variable-depth)



## Example: 75-25-1, $i=14$

- Sequential runtime $T_{\text {seq }}=15,402 \mathrm{sec}$.

(Fixed-depth)



## Underlying vs. Explored Search Space

- Compute $S S_{p a r}$ bound (ahead of time).
- Plot against $N_{p a r}$ for different $i$-bounds.


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ped7





## Underlying vs. Explored Search Space <br> - Compute $S S_{p a r}$ bound (ahead of time).

- Plot against $N_{p a r}$ for different $i$-bounds.



IF3-15-59

pdb1huw

pdb1kao


75-25-1


75-26-10


## Redundancies and Overhead $O_{p a r}$

- Assess parallel redundancies in practice.
- Node expansion overhead $O_{p a r}=N_{p a r} / N_{s e q}$.


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ped7


IF3-13-58


IF3-15-59




## Redundancies and Overhead $O_{p a r}$

- Assess parallel redundancies in practice.
- Node expansion overhead $O_{p a r}=N_{p a r} / N_{\text {seq }}$.


IF3-13-58


IF3-15-59

pdb1huw



75-25-3


75-26-10


## Parallel Scaling Summary

- Plot speedup against CPU count.
- Trade off load balancing vs. overhead:
- \#subproblems $\approx 10 \times$ \#CPUs


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## Fixed-depth vs. Variable-depth

- Compare speedup of the two parallel schemes.
- Count cases that are 10\% and 50\% better.

|  | margin | fix var | fix var | fix var | fix var | fix var | fix var |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $d=2$ | $d=4$ | $d=6$ | $d=8$ | $d=10$ | $d=12$ |
| Pedigree | 10\% | 2016 | $40 \quad 30$ | 3841 | $24 \quad 49$ | $28 \quad 40$ | $12 \quad 28$ |
|  | 50\% | $\begin{array}{lr} \mathbf{2 0} & 12 \\ (116 & \text { total }) \end{array}$ | 2715 | 3015 | $16 \quad 22$ | $20 \quad 9$ | $\begin{array}{cc} 4 & 13 \\ (88 & \text { total }) \end{array}$ |
|  |  |  | (116 total) | (116 total) | (116 total) | (108 total) |  |
|  |  | $d=2$ | $d=4$ | $d=6$ | $d=8$ | $d=10$ | $d=12$ |
| LargeFam | 10\% | $32 \quad 12$ | $21 \quad 30$ | 1151 | 752 | 547 | 832 |
|  | 50\% | 120 | $\begin{array}{cr} 15 & 10 \\ (84 \text { total }) \\ \hline \end{array}$ | $\begin{array}{cc} 8 & \mathbf{2 8} \\ (84 \text { total) } \\ \hline \end{array}$ | $\begin{array}{cr} 3 & \mathbf{3 6} \\ (76 & \text { total }) \\ \hline \end{array}$ | $\begin{array}{cr} 1 & \mathbf{3 0} \\ (76 \text { total) } \end{array}$ | $\begin{array}{cc} 5 & \mathbf{2 2} \\ (76 \text { total }) \end{array}$ |
|  |  | (84 total) |  |  |  |  |  |
|  |  | $d=1$ | $d=2$ | $d=3$ | $d=4$ | $d=5$ | $d=6$ |
| Pdb | 10\% | $0 \quad 0$ | $5 \quad 39$ | $0 \quad 33$ | $0 \quad 20$ | $0 \quad 4$ | $0 \quad 4$ |
|  | 50\% | 0 0 | $\begin{array}{cr} 4 & \mathbf{3 0} \\ (44 \text { total) } \end{array}$ | $\begin{array}{cr} 0 & \mathbf{2 8} \\ (36 \text { total }) \end{array}$ | $\begin{array}{cr} 0 & \mathbf{1 6} \\ \text { (20 total) } \end{array}$ | $\begin{array}{ll} 0 & 4 \\ (4 \text { total) } \end{array}$ | $\begin{array}{lr} 0 & 4 \\ (4 \text { total }) \end{array}$ |
|  |  | (44 total) |  |  |  |  |  |
|  |  | $d=2$ | $d=4$ | $d=6$ | $d=8$ | $d=10$ | $d=12$ |
| Grid | 10\% | 2013 | 129 | 178 | 2710 | $20 \quad 9$ | $12 \quad 19$ |
|  | 50\% | $12 \quad 4$ | $\begin{gathered} 10 \\ (60 \text { total }) \end{gathered}$ | $\begin{array}{cc} \mathbf{9} & 3 \\ (60 \text { total }) \\ \hline \end{array}$ | $\begin{array}{lr} 11 & 3 \\ (60 \text { total }) \end{array}$ | $\begin{array}{cr} 5 & \mathbf{6} \\ (60 \text { total }) \\ \hline \end{array}$ | $\begin{array}{rr} 5 & \mathbf{8} \\ (60 \text { total }) \end{array}$ |
|  |  | (60 total) |  |  |  |  |  |

## Outline

- Bounds and heuristics
- ANDIOR Search
- Explolting parallelism
- Software
- UAI Probabilistic Inference Competition


## Software

- aolib
- http://graphmod.ics.uci.edu/group/Software (standalone AOBB, AOBF solvers)
- daoopt
- https://github.com/lotten/daoopt (distributed and standalone AOBB solver)


## UAI Probabilistic Inference Competitions

- 2006
- 2008
- 2011
- 2014

(daoopt)

(merlin)

MPE/MAP

MMAP

## Conclusion

- Only a few principles
- Inference and search should be combined
- Time-space tradeoff
- AND/OR search should be used
- Caching in search should be used
- Parallel search should be used if a distributed environment is available

