Stochastic Decision Diagrams

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Motivation

- Decision diagrams (DDs) have proved useful for solving **discrete optimization** problems.
  - Especially those with recursive **dynamic programming** (DP) models.

- Yet many (most) DP models are **stochastic**.
  - We therefore generalize DDs to **stochastic DDs** (SDDs) by adding probabilities to arcs.

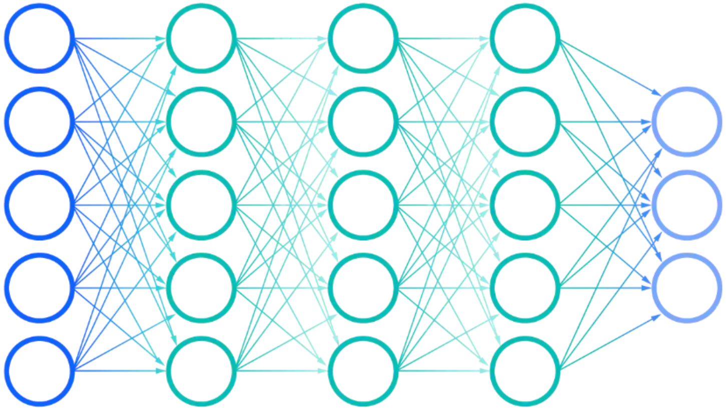
Motivation

- It's **no big deal** to put probabilities in a DD.
  - So why is this **interesting**?

- One reason:
  - It allows us to **extend DD-based relaxation techniques** to **stochastic** DP models.
  - Relaxation is **essential** to solving hard problems **to optimality**.

Review: Deterministic DDs

- A deterministic (binary) DD is a graphical representation of a **Boolean function**.
  - Often used for logic circuit design, product configuration.
  - Bounded-width DDs can represent **exponentially many** solutions.
  - **Same principle** lies behind “deep learning” and DP!



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  - **Same principle** lies behind "deep learning" and DP!

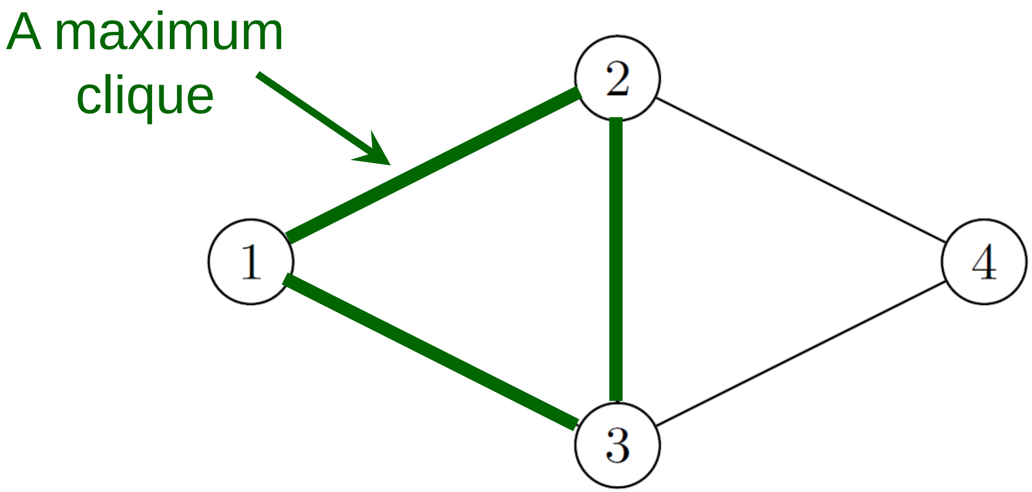
- A **weighted** DD can represent a discrete **optimization problem**.

Hadzic and JH (2006, 2007)

  - For example, the **maximum clique** problem...

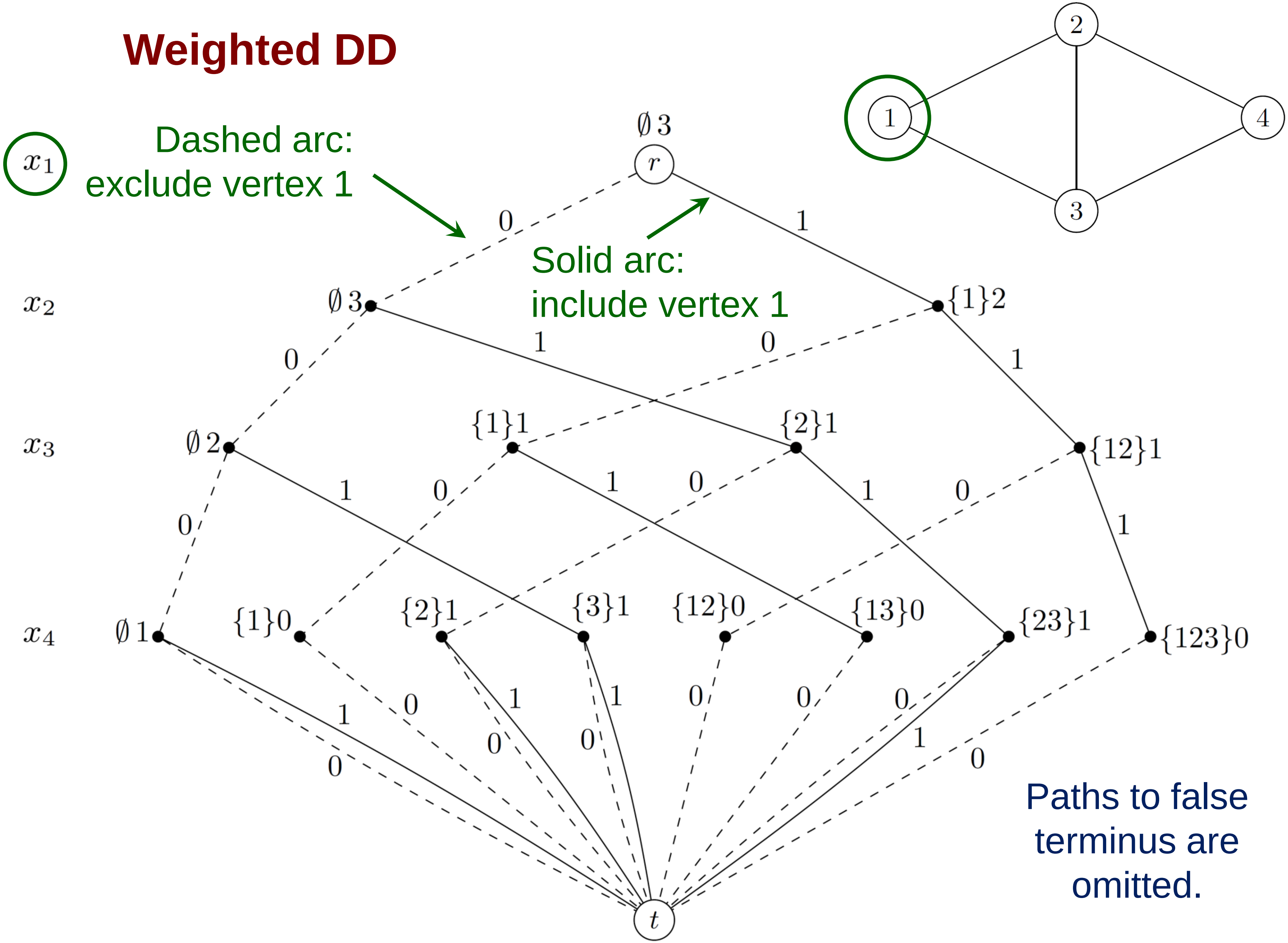
Maximum clique

Max clique example



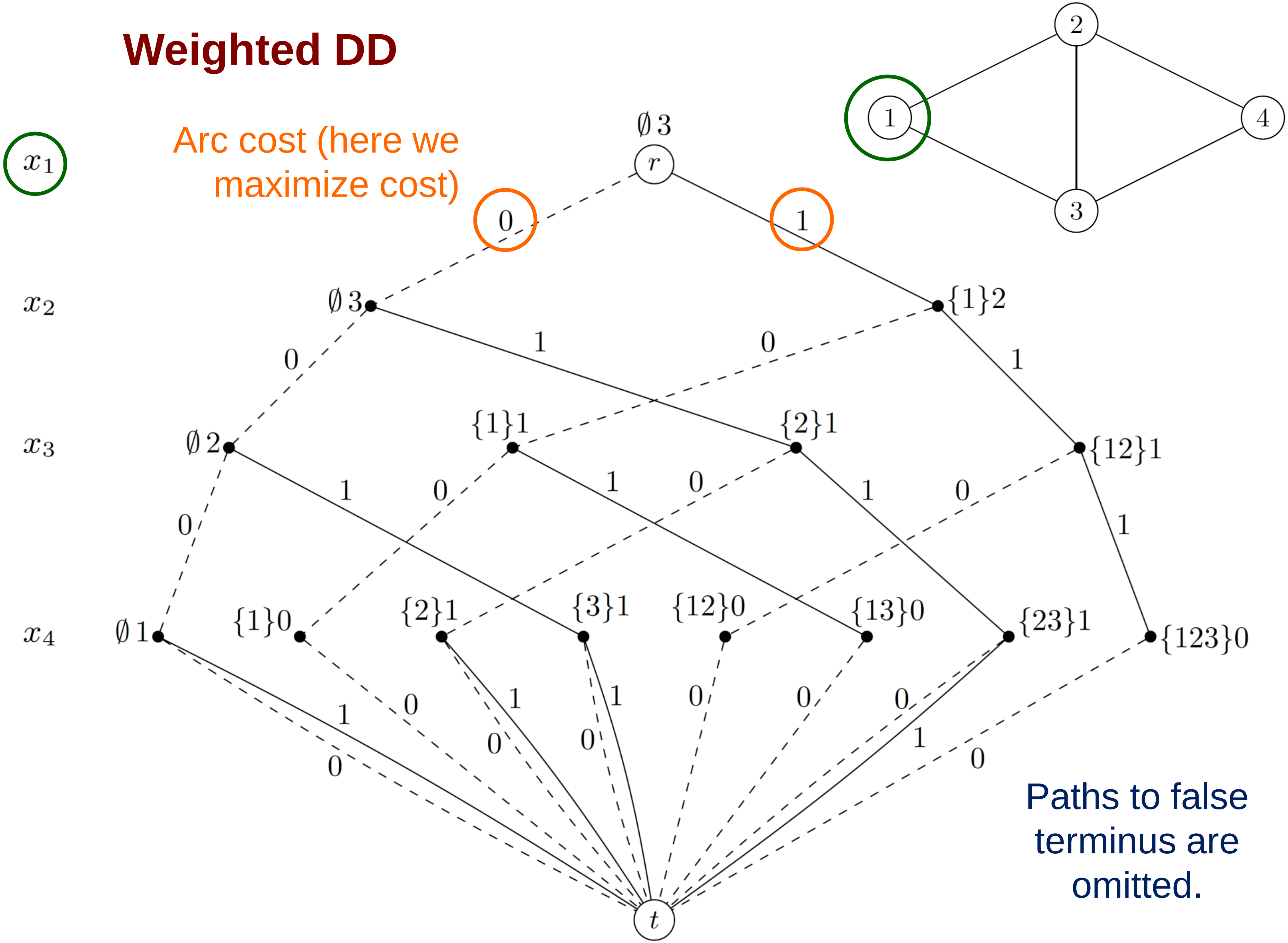
Let binary variable $x_i = 1$ when vertex i is in the clique.

Weighted DD



Dashed arc:
exclude vertex 1
Solid arc:
include vertex 1
x_1
x_2
x_3
x_4
r
t
$\emptyset\,3$
$\emptyset\,3$
$\{1\}2$
$\emptyset\,2$
$\{1\}1$
$\{2\}1$
$\{12\}1$
$\emptyset\,1$
$\{1\}0$
$\{2\}1$
$\{3\}1$
$\{12\}0$
$\{13\}0$
$\{23\}1$
$\{123\}0$
1
2
3
4
Paths to false
terminus are
omitted.

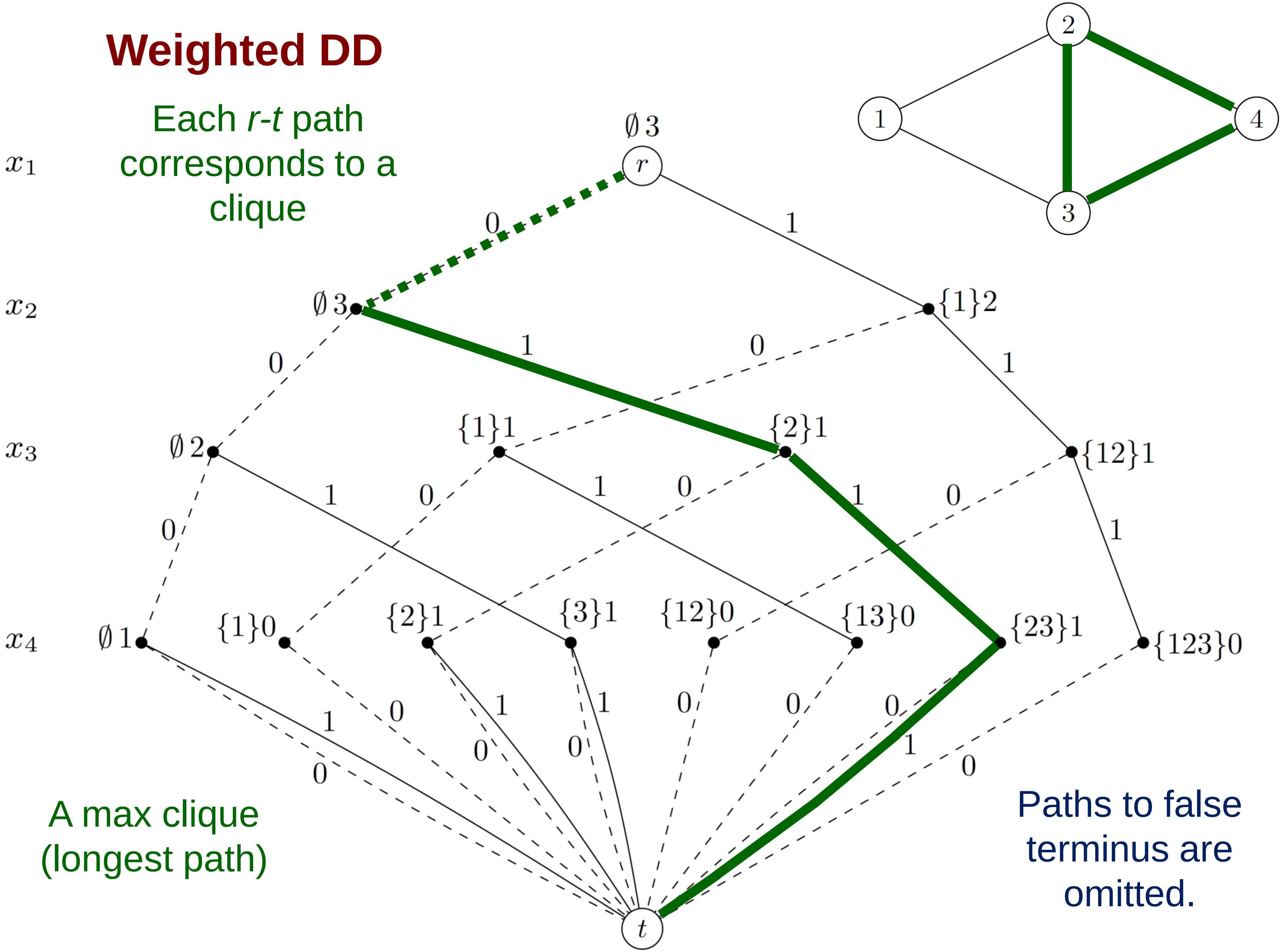
Weighted DD



Paths to false terminus are omitted.

Weighted DD

Each *r-t* path corresponds to a clique

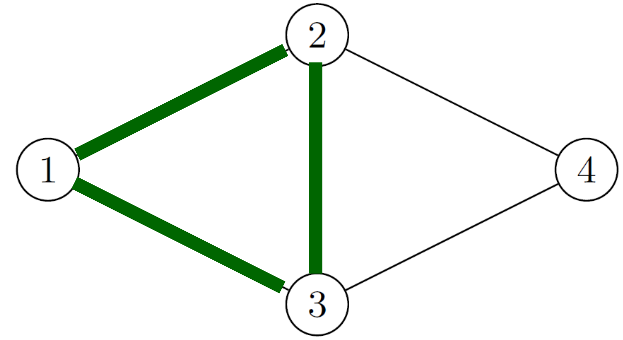


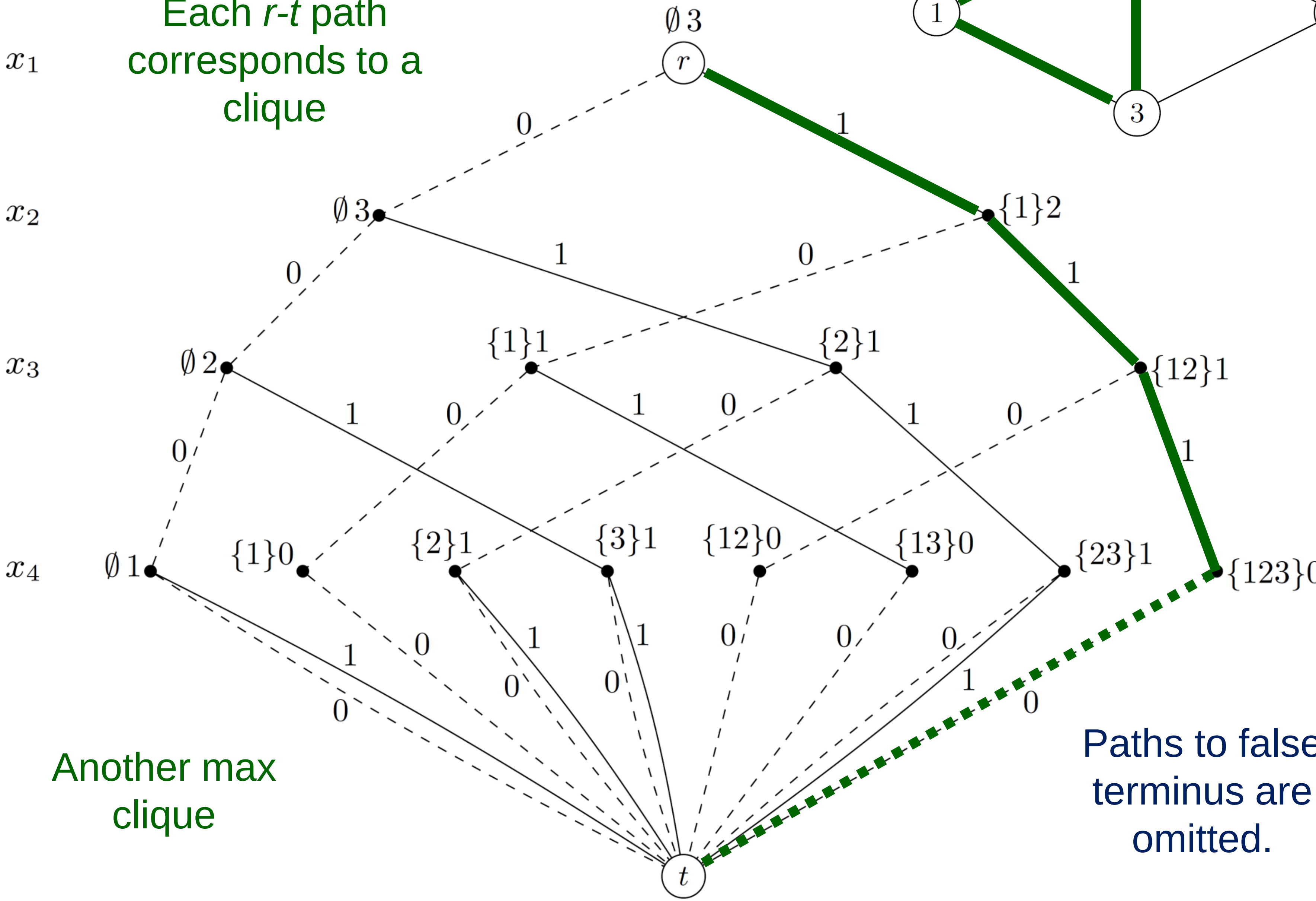
A max clique (longest path)

Paths to false terminus are omitted.

Weighted DD

Each *r*-*t* path corresponds to a clique





Another max clique

Paths to false terminus are omitted.

Dynamic Programming

- The **state transition graph** of a dynamic programming (DP) problem can be interpreted as a DD.
  - By associating states with nodes of the DD.
  - This opens the door to using DD **relaxation** techniques to obtain bounds for DPs.

Andersen, Hadzic, JH, Tiedemann (2007)
Bergman, Cire, van Hoeve, JH (2013)

  - …and to solving the DPs by **branch and bound**.

Bergman, Cire, van Hoeve, JH (2014)

  - For example, the **maximum clique** problem...

Deterministic DDs

Max clique DP model

State variable $S_i = \{\text{vertices selected so far in stage } i\}$.

The recursion is

$$h_i(S_i) = \max\left\{h_{i+1}(S_i),\ \ 1 + h_{i+1}\big(S_i \cup \{i\}\big)\right\},\ \ i = n, \ldots, 1$$

$x_i = 0$

$x_i = 1$

cost to go

(max number of vertices that can be added to the clique, given that the vertices in S_i have been added so far)

Deterministic DDs

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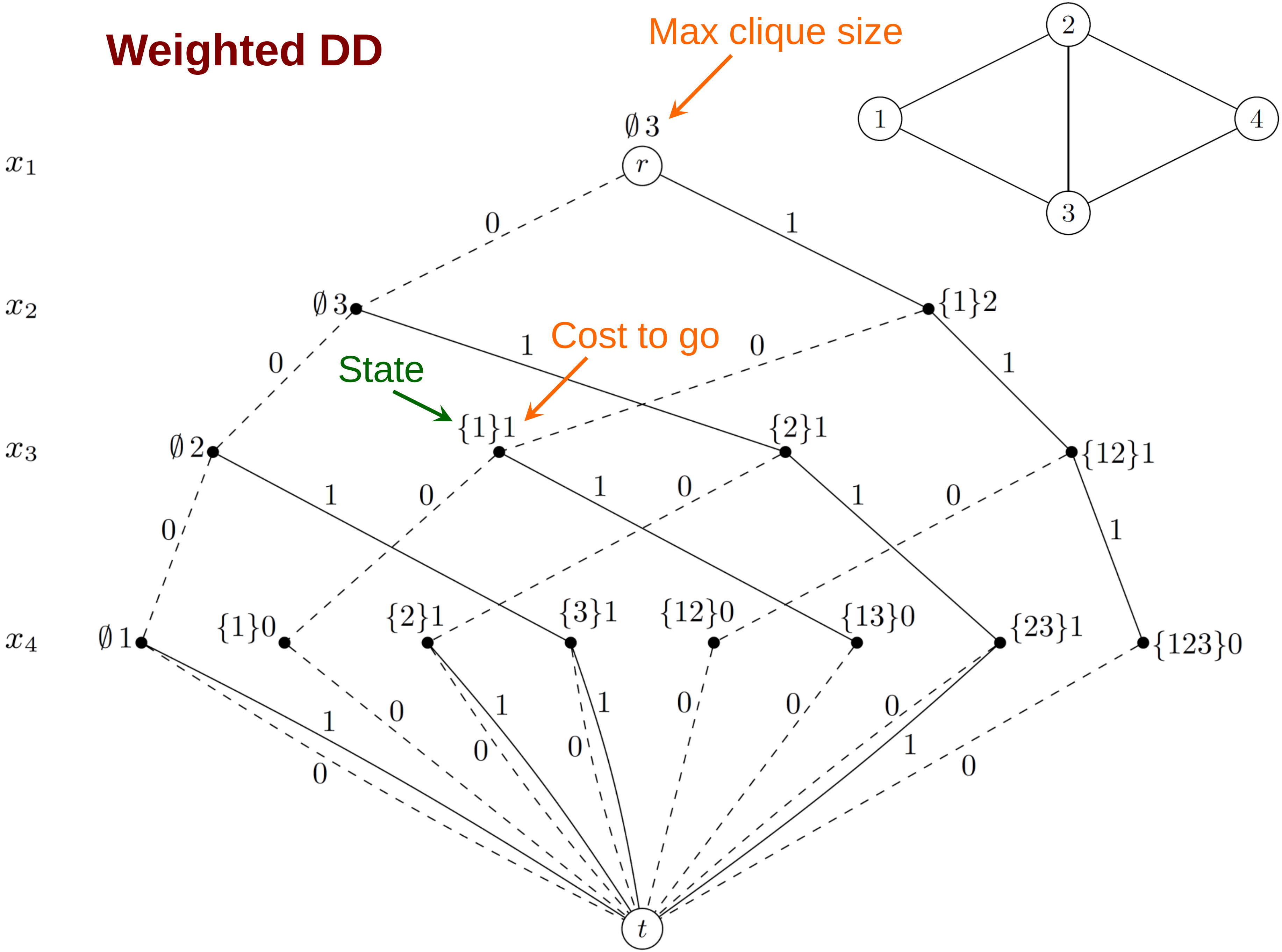
In general,

$$h_i(\boldsymbol{S}_i) = \min_{\underbrace{x_i}_{\text{control}}}\left\{\underbrace{c_i(\boldsymbol{S}_i, x_i)}_{\text{immediate cost}} + \underbrace{h_{i+1}}_{\text{cost to go}}\big(\underbrace{\phi_i(\boldsymbol{S}_i, x_i)}_{\text{state transition function}}\big)\right\},\ \ i = n, \ldots, 1$$

Weighted DD



Max clique size
Cost to go
State
x_1
x_2
x_3
x_4
$\emptyset\,3$
r
$\emptyset\,3$
$\{1\}2$
$\emptyset\,2$
$\{1\}1$
$\{2\}1$
$\{12\}1$
$\emptyset\,1$
$\{1\}0$
$\{2\}1$
$\{3\}1$
$\{12\}0$
$\{13\}0$
$\{23\}1$
$\{123\}0$
t
1
2
3
4

Deterministic MDDs

Job sequencing example

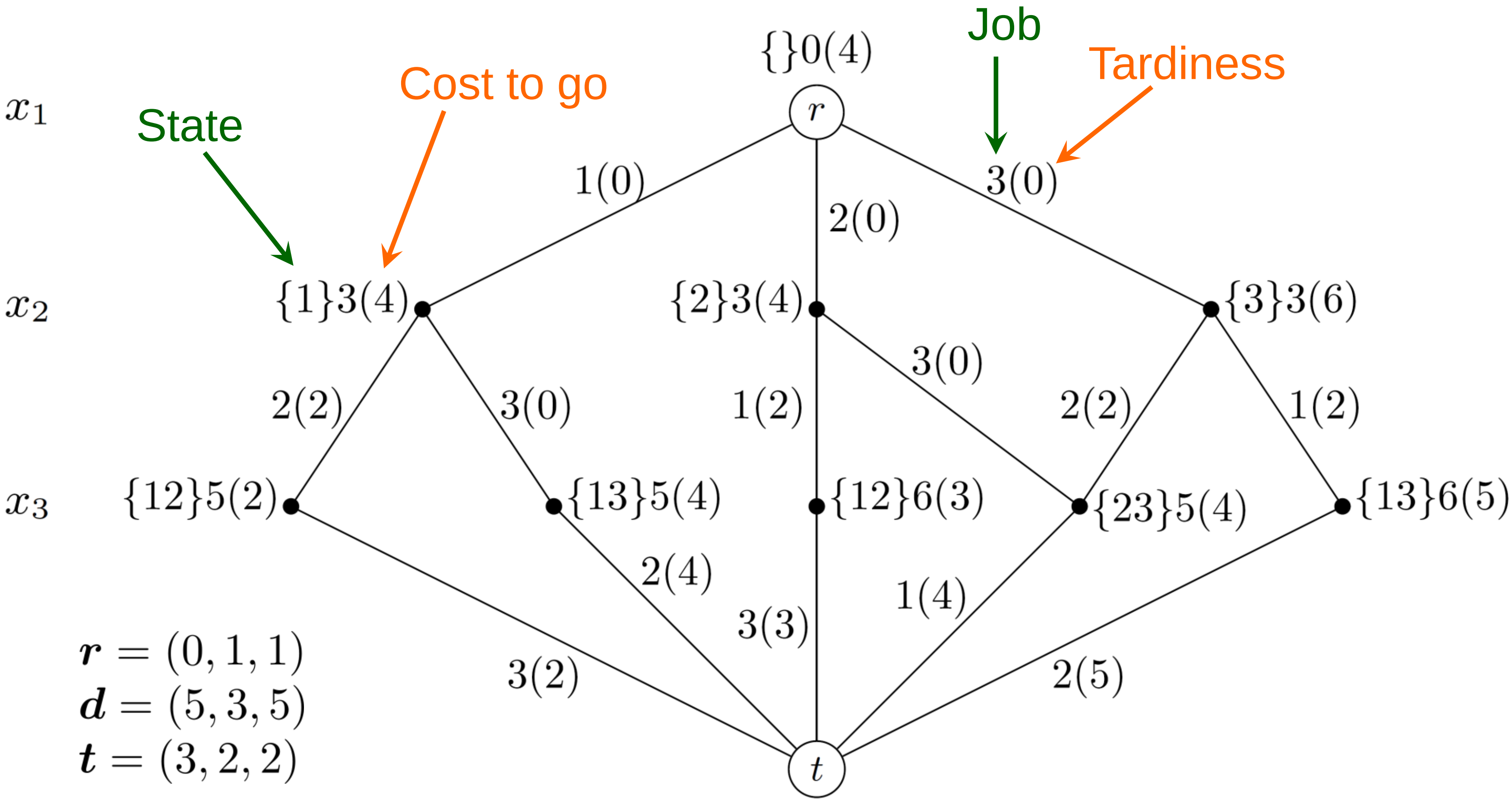
Let control x_i be ith job in sequence.

Time window $[r_i, d_i]$ and processing time t_i for each job i.

Minimize total tardiness.

Weighted DD

State $= (S_i, f_i)$, where
$S_i = \{\text{jobs sequenced so far}\}$, $f_i =$ finish time of previous job



$\boldsymbol{r} = (0, 1, 1)$
$\boldsymbol{d} = (5, 3, 5)$
$\boldsymbol{t} = (3, 2, 2)$

Deterministic DDs

Job sequencing DP model

State is (S_i, f_i).

The recursion is

$$h_i(S_i, f_i) = \min_{x_i \notin S_i} \Big\{ c_i(S_i, f_i) + h_{i+1}\big(\phi_i((S_i, f_i), x_i)\big) \Big\}$$

where

$$c_i\big((S_i, f_i), x_i\big) = \max\big\{0,\ \max\{r_{x_i}, f_i\} + t_{x_i} - d_{x_i}\big\}$$

$$\phi_i\big((S_i, f_i), x_i\big) = \big(S_i \cup \{x_i\}, \max\{r_{x_i}, f_i\} + t_{x_i}\big)$$

Dynamic Programming

- Note: a state transition graph is a **different concept** than a DD.
  - A DD does not need **state information**.

Dynamic Programming

- Note: a state transition graph is a **different concept** than a DD.
  - A DD does not need **state information.**
- The DD perspective yields advantages:
  - A DD can be often be **reduced** by identifying isomorphic portions of the DD that are associated with different states.

    Bryant (1986 etc.)
    - This occasionally results in **radical** simplification (e.g., inventory management).

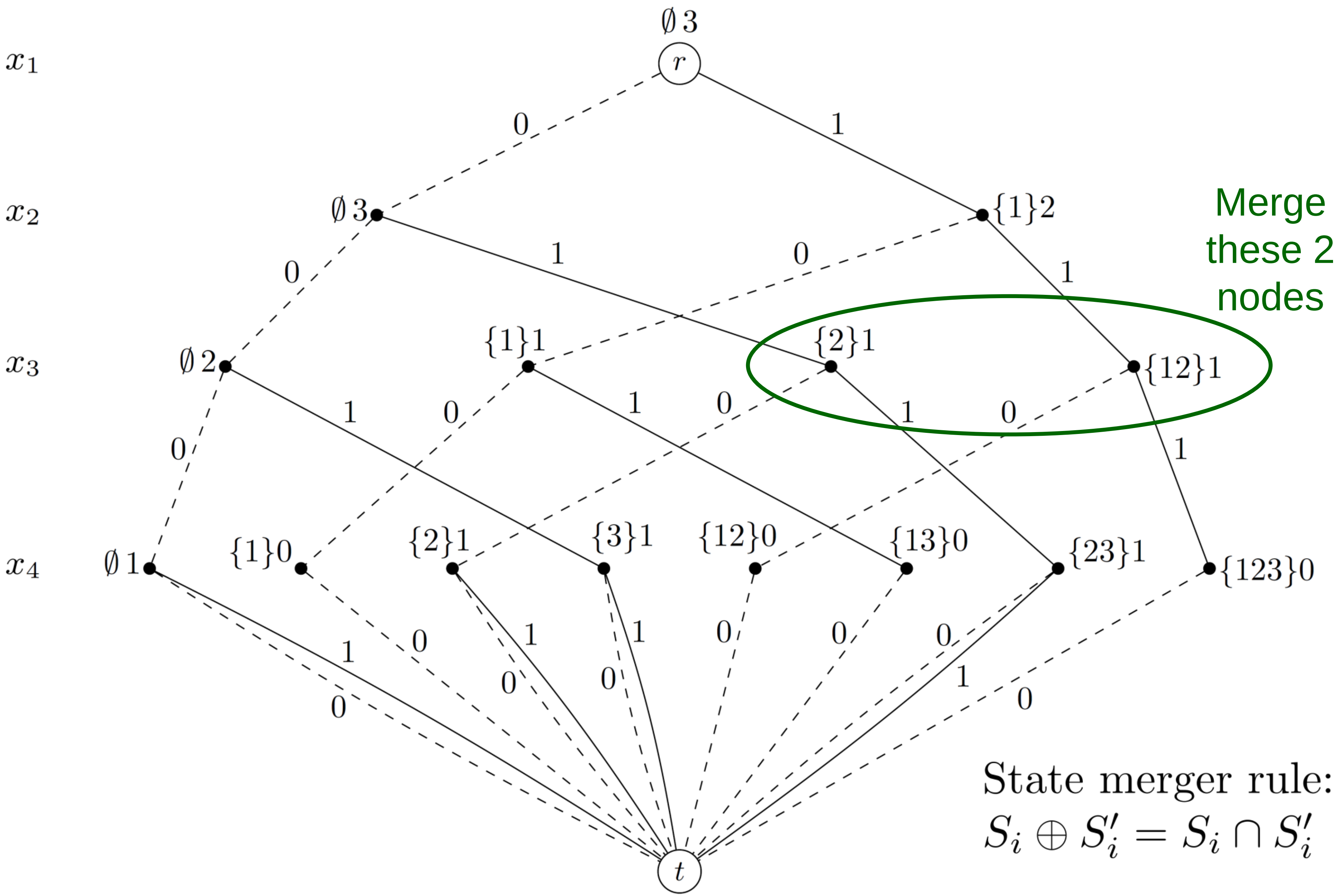
      JH (2013)
  - DP can benefit from **relaxation techniques** that have been developed for DDs…

Relaxed DDs

- A **relaxed** DD represents a superset of feasible solutions.
  - Can provide a **bound** on the optimal value.
- Created during top-down compilation of the DD.
  - By **node merger** or **node splitting**.
  - We focus on **node merger**.
  - Mergers result in **smaller DD** but weaker bound.
  - Can obtain bound of **any desired quality** by controlling width of relaxed DD.

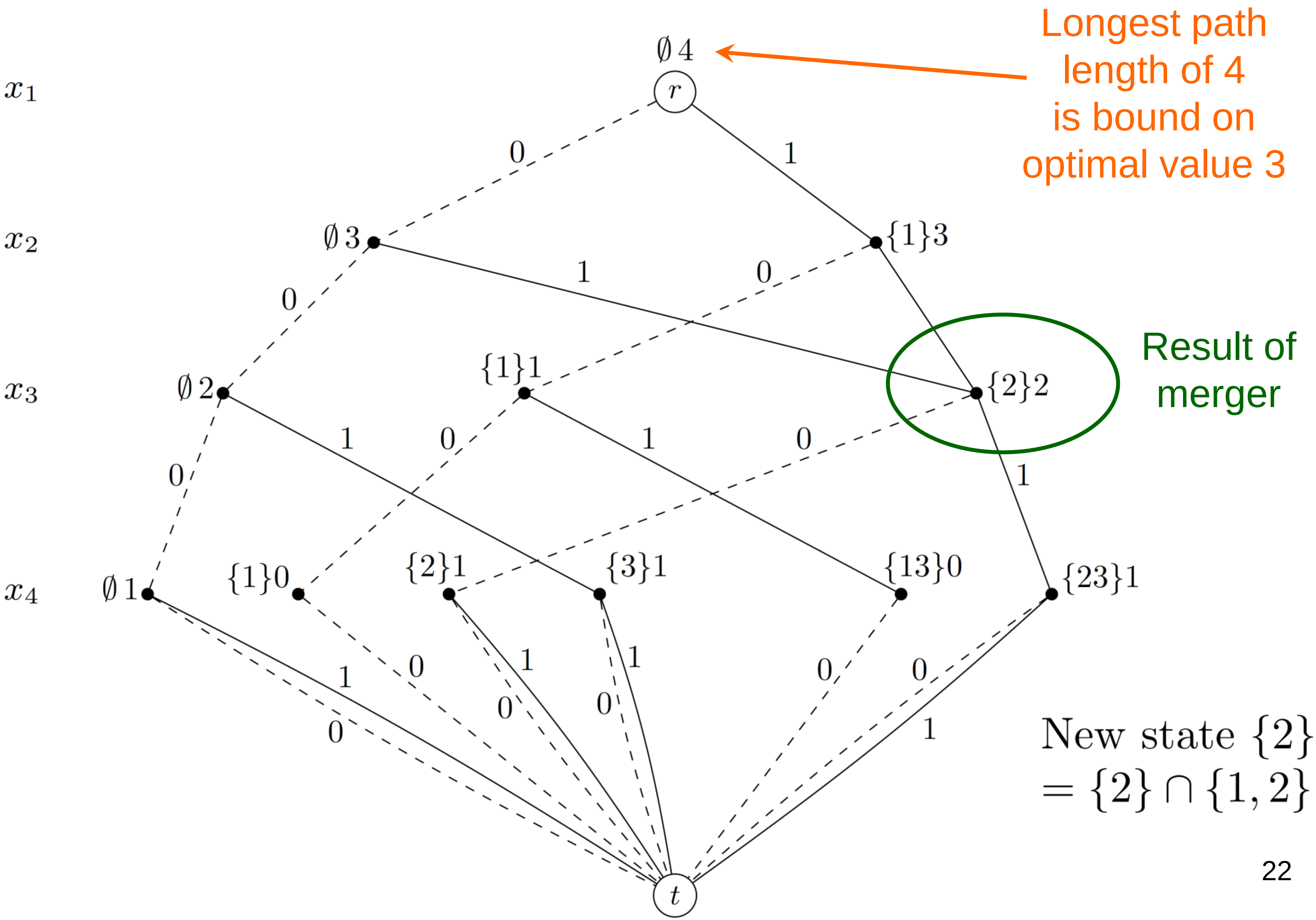
Andersen, Hadzic, JH, Tiedemann (2007)
Bergman, Cire, van Hoeve, JH (2013)

Weighted DD for max clique

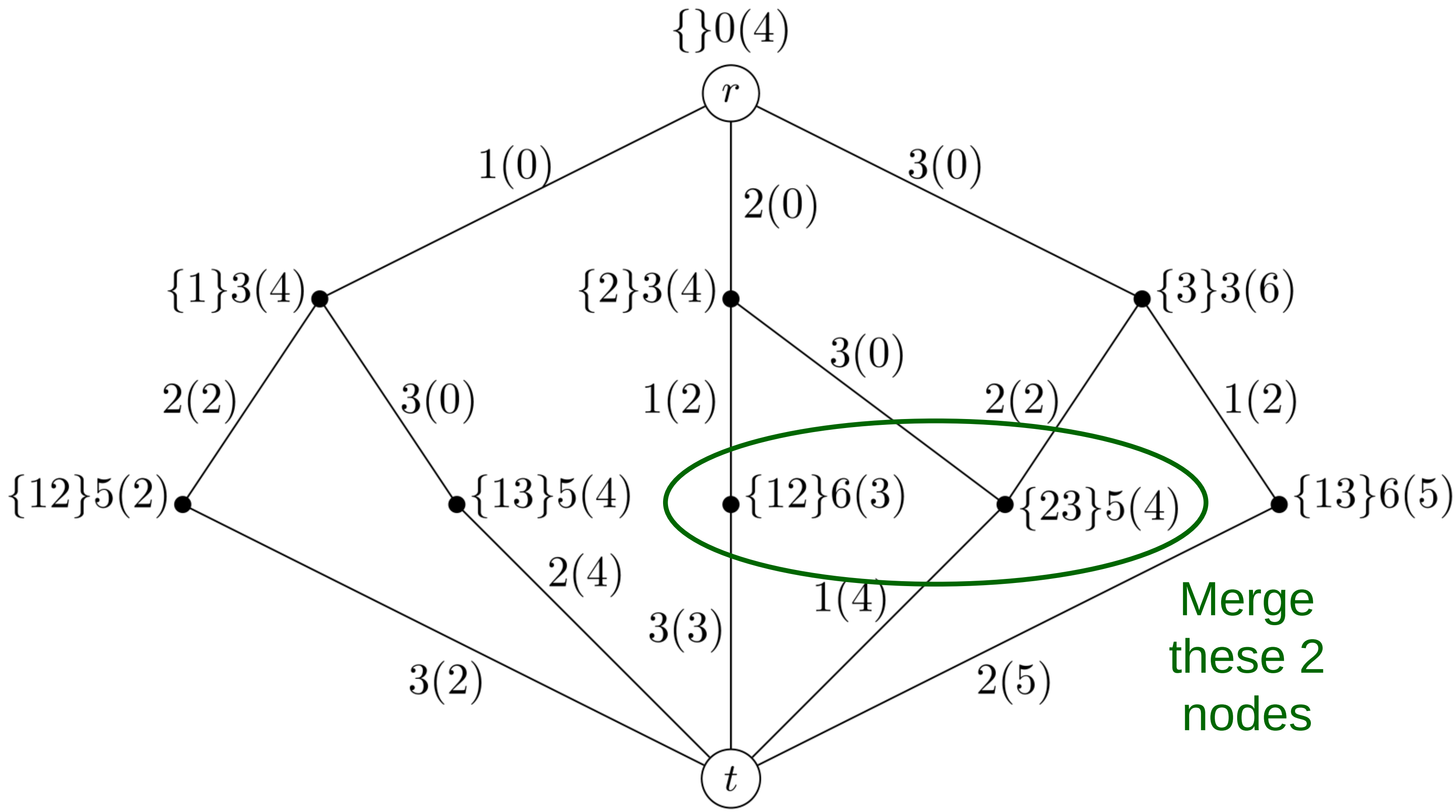


State merger rule:
$S_i \oplus S_i' = S_i \cap S_i'$

Relaxed DD for max clique

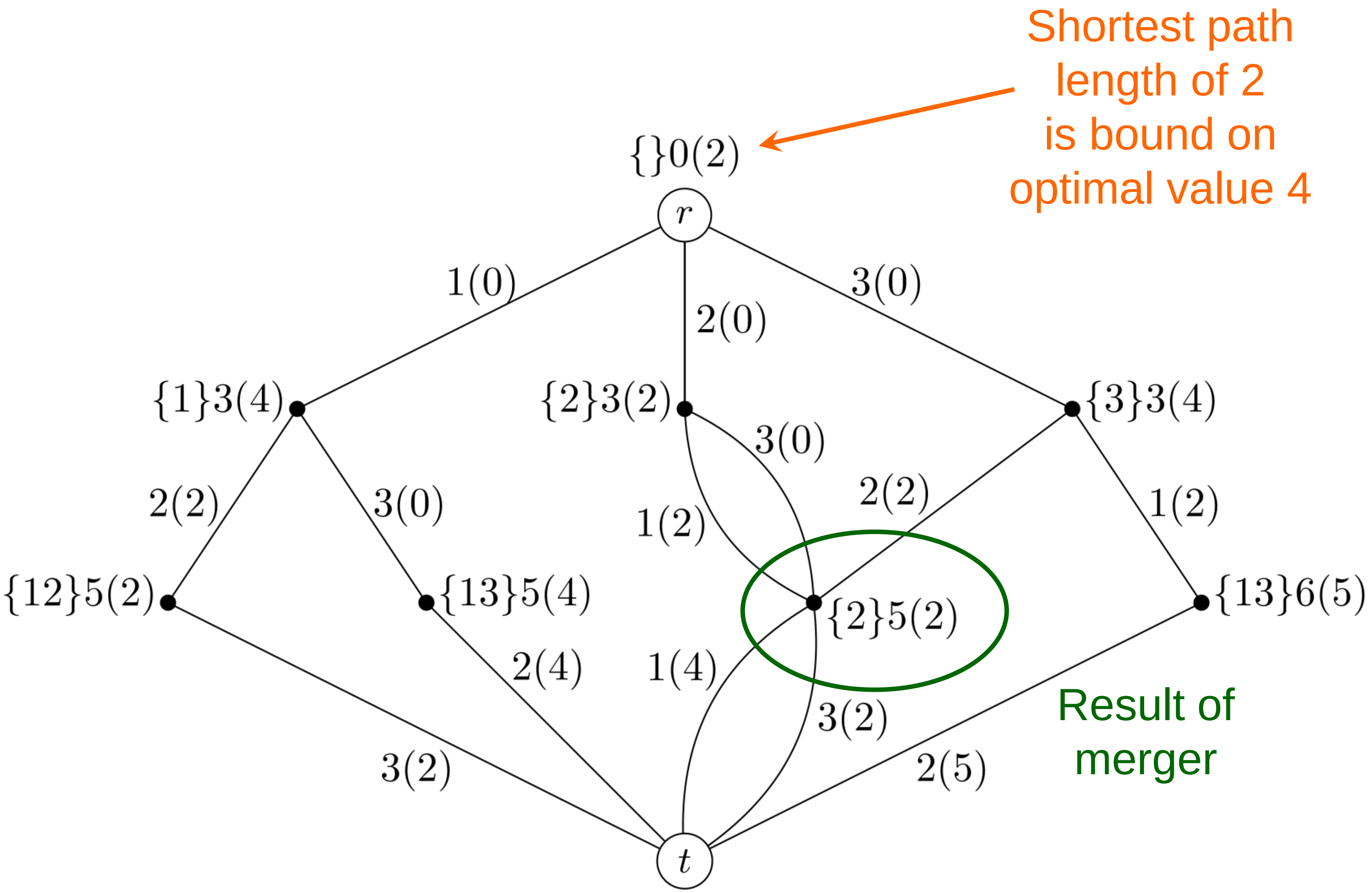


Weighted DD for job sequencing



State merger rule: $(S_i, f_i) \oplus (S_i', f_i') = \big((S_i \cap S_i'), \min\{f_i, f_i'\}\big)$

Relaxed DD for job sequencing



$$\text{New state } (\{2\}, 5) = (\{1, 2\} \cap \{2, 3\}, \min\{6, 5\})$$

Traditional state space relaxation

- Requires creation of alternate (smaller) state space for every problem.

Christofides, Mingozzi, Toth (1981)
Baldacci, Mingozzi, Roberti (2012)

  - General practice is to use **approximate DP** instead.

Powell (2011)

Traditional state space relaxation

- Advantages of DD-based relaxation**.**
  - Uses **same state variables** as original problem.
  - This allows DD-based **branch-and-bound** method to solve problem.

Bergman, Cire, van Hoeve, JH (2014)

  - Relaxation constructed **dynamically**.
  - Can be **tightened** by filtering, Lagrangian relaxation.

Bergman, Cire, van Hoeve (2015); JH (2017, 2019)

  - Can be sized to provide bound of **any desired quality**.

Stochastic DDs

- A stochastic decision diagram (SDD) has **probabilistic** transitions to the next layer.
  - A control can have several possible **outcomes**, each with a known probability.
  - The outcome determines which arc is followed.

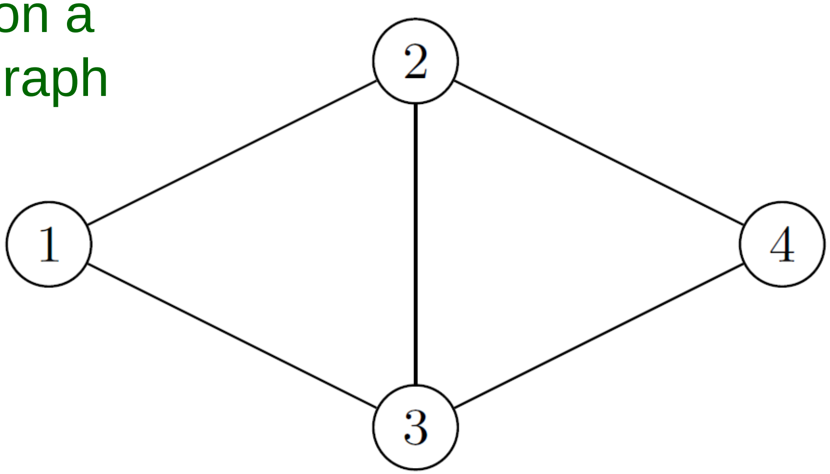
Stochastic DDs

- A stochastic decision diagram (SDD) has **probabilistic** transitions to the next layer.
  - A control can have several possible **outcomes**, each with a known probability.
  - The outcome determines which arc is followed.
- A solution is now a **policy**.
  - The control in a given layer depends on the **state** (node).
  - We **learn** from previous decisions
  - Original occurrence of learning in optimization?

Stochastic DDs

Max clique example

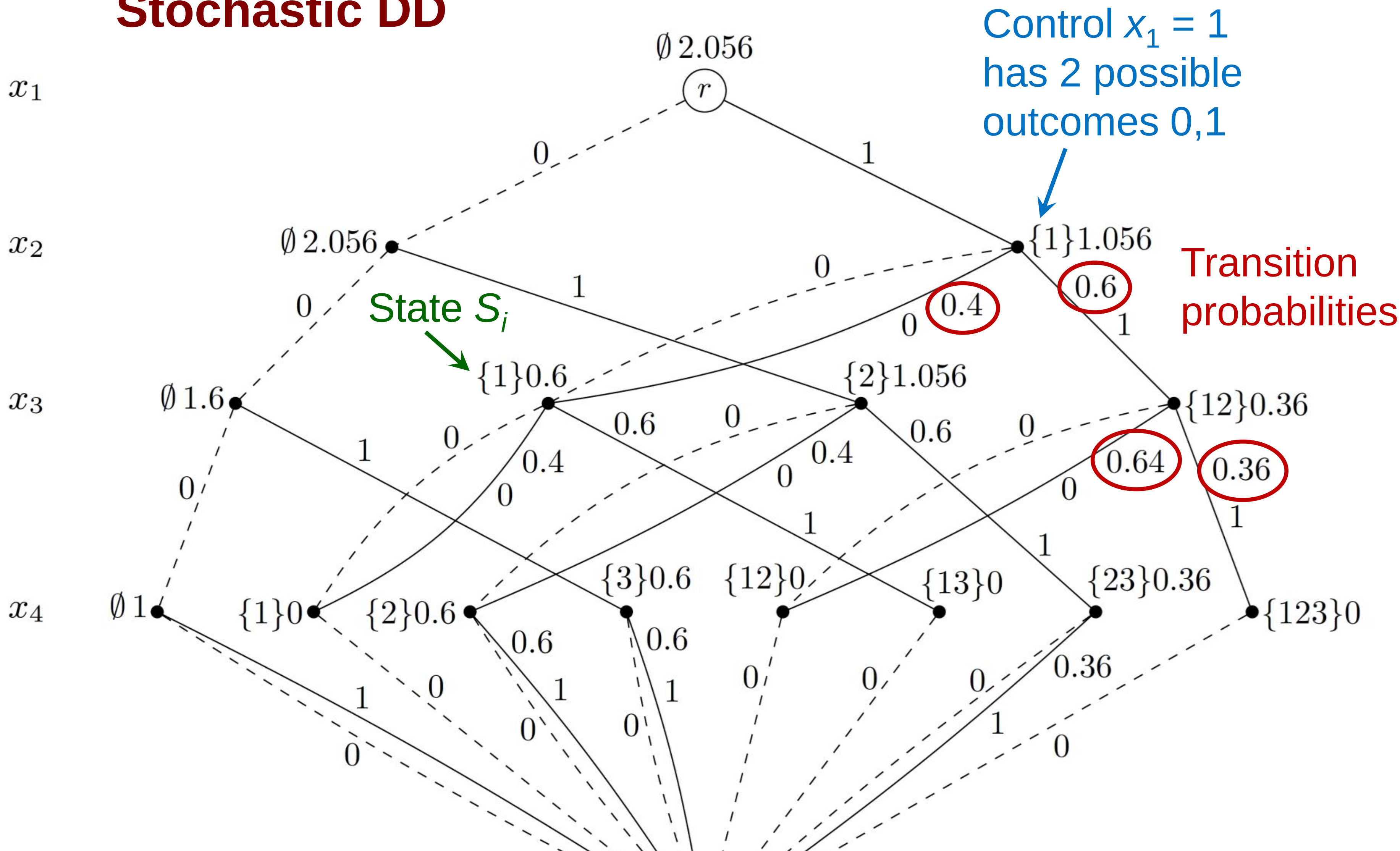
Defined on a random graph



Each arc has probability 0.6

Objective is to maximize expected clique size.

Stochastic DD

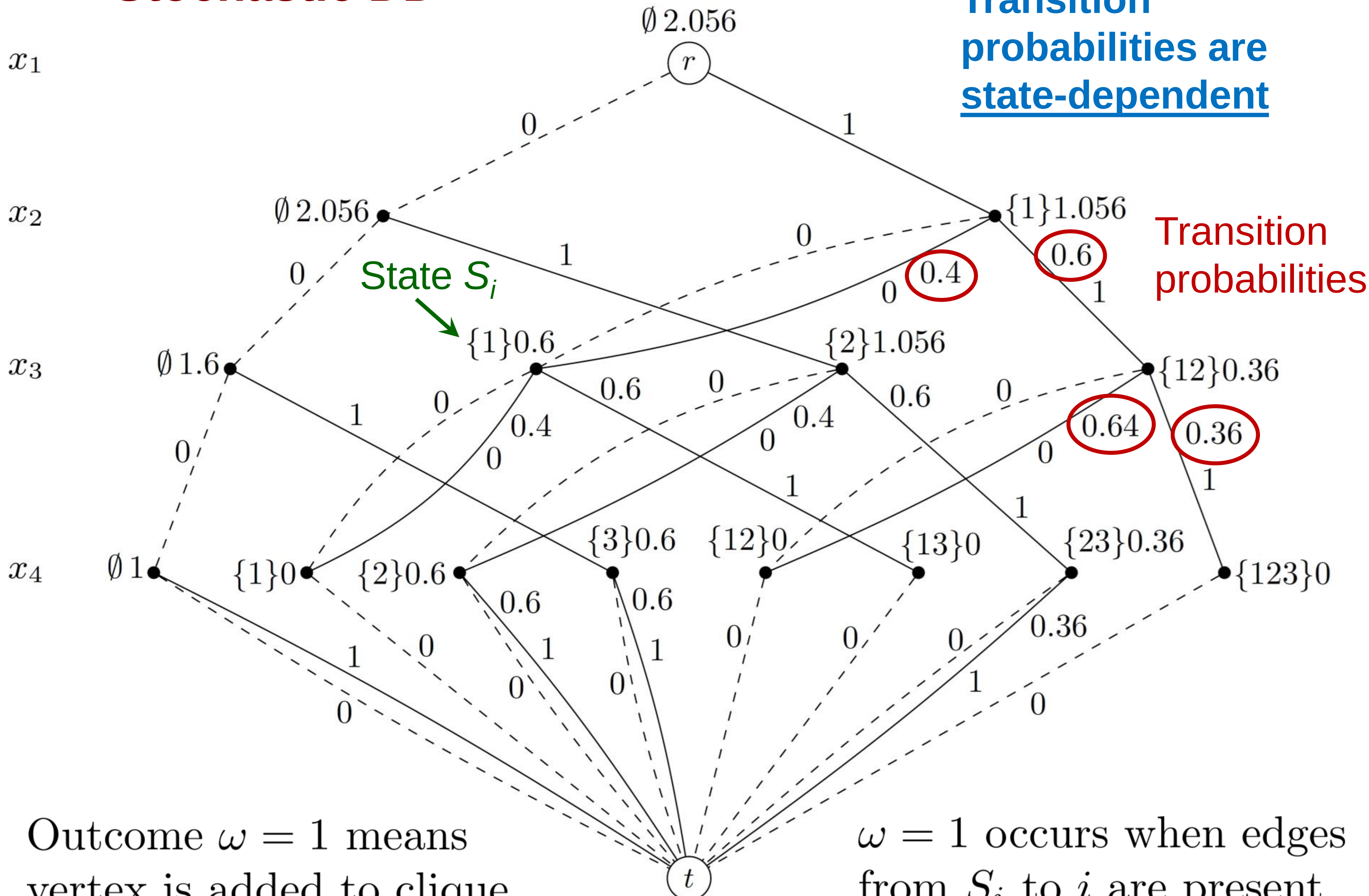


Outcome $\omega = 1$ means vertex is added to clique

$\omega = 1$ occurs when edges from S_i to i are present.

Stochastic DD

Transition probabilities are <u>state-dependent</u>



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Stochastic DDs

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The recursion is

$$h_i(S_i) = \max \left\{ \underbrace{h_{i+1}(S_i)}_{x_i = 0},\ \underbrace{\big(1 - p(S_i)\big) h_{i+1}(S_i) + p(S_i) h_{i+1}\big(S_i \cup \{i\}\big)}_{x_i = 1} \right\}$$

where $p(S_i)$ = probability that vertex i can be added to clique

Stochastic DDs

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$x_i = 0$ $\qquad$ $x_i = 1$

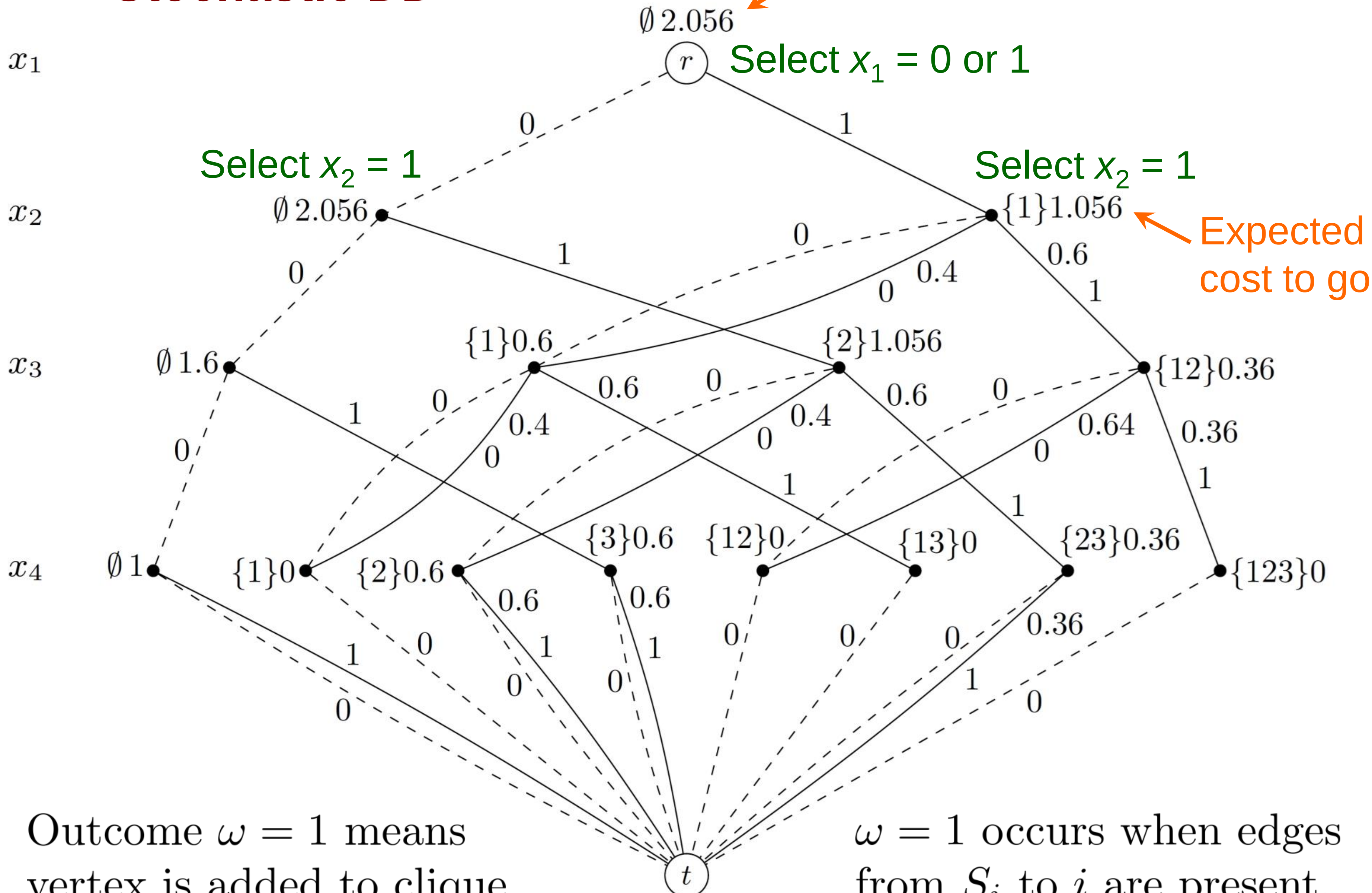
where $p(S_i)$ = probability that vertex i can be added to clique

In general,

$$h_i(\boldsymbol{S}_i) = \min_{x_i}\left\{\sum_{\omega} p_{i\omega}(\boldsymbol{S}_i, x_i)\Big[c_{i\omega}(\boldsymbol{S}_i, x_i) + h_{i+1}\big(\phi_{i\omega}(\boldsymbol{S}_i, x_i)\big)\Big]\right\}$$

where $p_{i\omega}(\boldsymbol{S}_i, x_i)$ = prob. of outcome ω given control x_i in state $\boldsymbol{S}_i$ and similarly for $c_{i\omega}(\boldsymbol{S}_i, x_i)$ and $\phi_{i\omega}(\boldsymbol{S}_i, x_i)$

Stochastic DD



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Relaxed SDDs

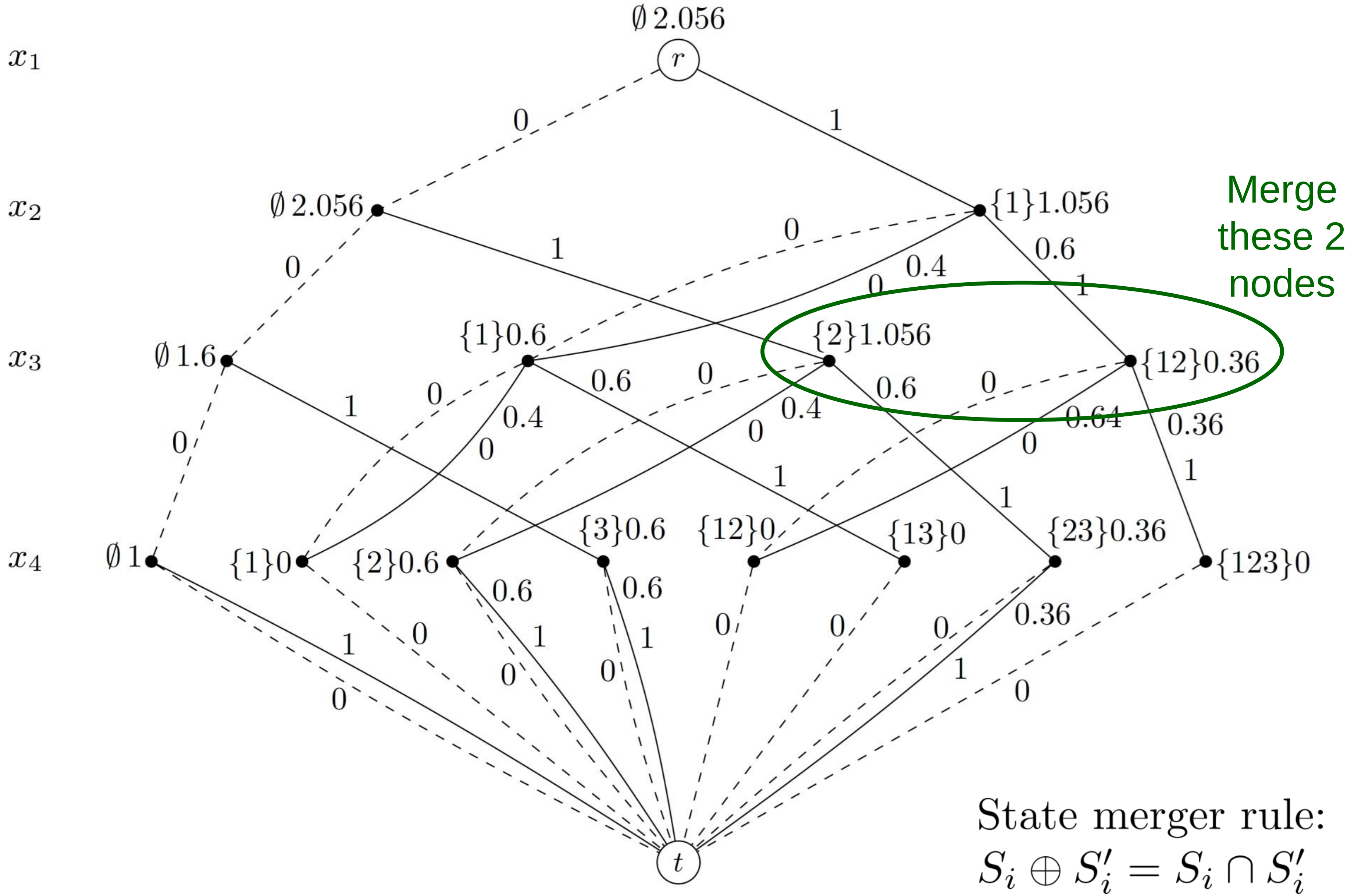
- A relaxed SDD is one that provides a **valid bound** on optimal expected cost.
  - **Unclear** how to define relaxation in terms of **individual solutions**.
  - …since solutions are **policies** defined on the **entire SDD**, and a relaxed SDD may have very different structure.

Stochastic diagram $\bar{D}$ relaxes diagram D when $\bar{D}$ and D have the same variables, controls, and possible outcomes, and when optimal cost of $\bar{D} \leq$ optimal cost of D.

Relaxed SDDs

- We will relax SDDs by node merger.
  - We will also provide **sufficient conditions** under which a given merger operation yields a valid relaxed SDD.
  - Conditions must account for **policy-based** solutions rather than simple control sequences.
  - Examples…

Stochastic DD for max clique



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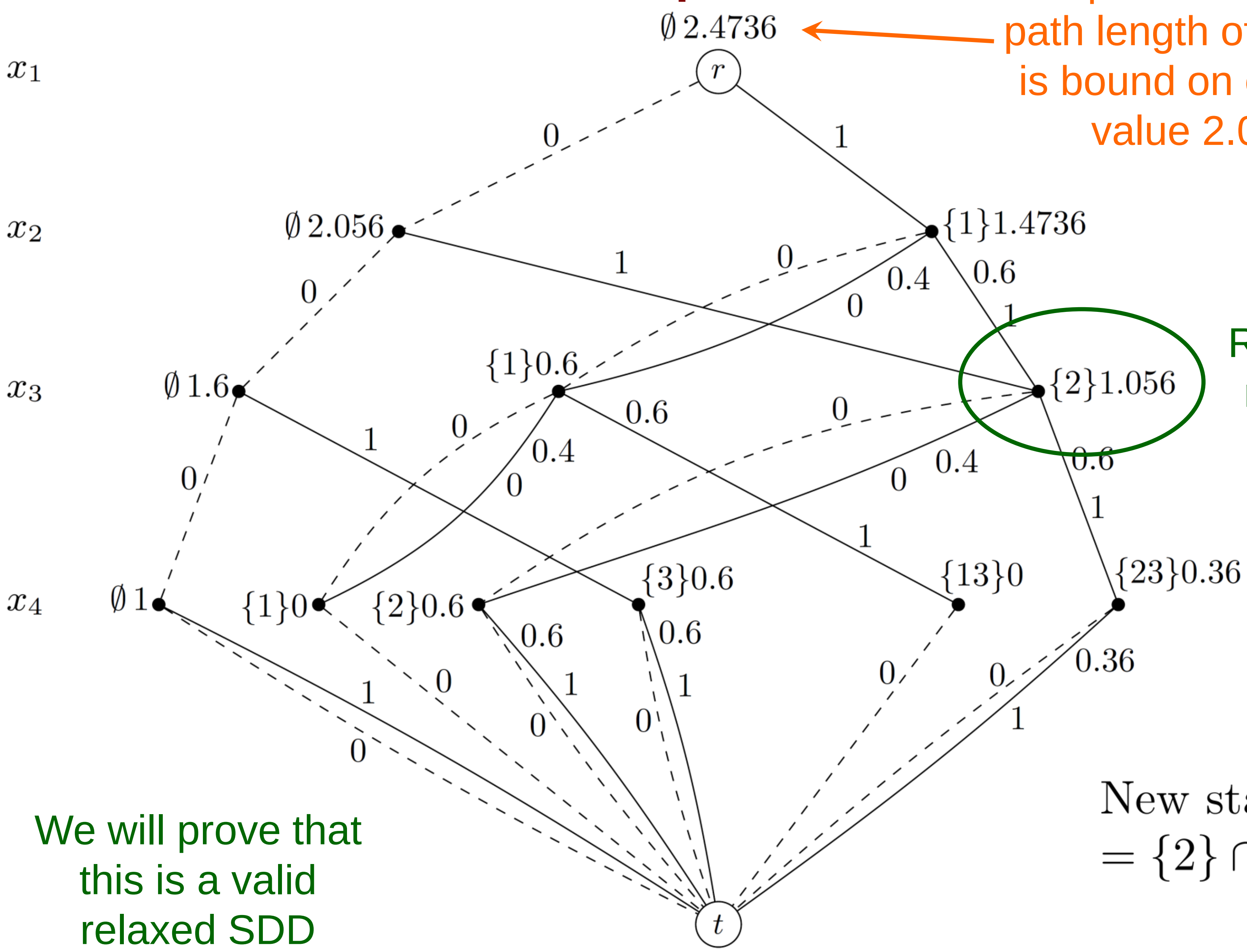

We will prove that this is a valid relaxed SDD

New state $\{2\}$
$= \{2\} \cap \{1, 2\}$

Relaxed SDDs

Stochastic job sequencing DP model

Stochastic element is processing time (state independent).
Let $t_{j\omega}$ = job j processing time in outcome ω.
Let $p_{j\omega}$ probability of outcome ω for job j.

Transition probabilities are <u>state-independent</u>

The recursion is

$$h_i(S_i, f_i) = \min_{x_i \notin S_i} \left\{ \sum_{\omega} p_{i\omega}(S_i, x_i)\big[c_{i\omega}(S_i, f_i) + h_{i+1}\big(\phi_{i\omega}((S_i, f_i), x_i)\big)\big] \right\}$$

where

$$c_{i\omega}\big((S_i, f_i), x_i\big) = \max\left\{0,\ \max\{r_{x_i}, f_i\} + t_{x_i\omega} - d_{x_i}\right\}$$

$$\phi_{i\omega}\big((S_i, f_i), x_i\big) = \big(S_i \cup \{x_i\}, \max\{r_{x_i}, f_i\} + t_{x_i\omega}\big)$$

We can use the same node merger operation as before.

Node Merger in SDDs

We need a concept of **one state relaxing another**.

Relaxation must have the property that state $\bar{\boldsymbol{S}}_i$ **relaxes** state $\boldsymbol{S}_i$ only if

$$p_{i\omega}(\bar{\boldsymbol{S}}_i, x_i)c_{i\omega}(\bar{\boldsymbol{S}}_i, x_i) \leq p_{i\omega}(\boldsymbol{S}_i, x_i)c_{i\omega}(\boldsymbol{S}_i, x_i)$$

for any control x_i and any outcome ω.

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for any control x_i and any outcome ω.

Max clique problem: $\bar{S}_i$ relaxes S_i when $\bar{S}_i \subseteq S_i$.

Job sequencing problem: $(\bar{S}_i, \bar{f}_i)$ relaxes (S_i, f_i) when $\bar{S}_i \subseteq S_i$ and $\bar{f}_i \leq f_i$.

These definitions satisfy the property.

Node Merger in SDDs

Jointly sufficient conditions under which node merger yields a relaxed SDD:

(C1) State $\boldsymbol{S}_i \oplus \boldsymbol{S}_i'$ relaxes both $\boldsymbol{S}_i$ and $\boldsymbol{S}_i'$.

(C2) If state $\bar{\boldsymbol{S}}_i$ relaxes state $\boldsymbol{S}_i$, then $\phi_{i\omega}(\bar{\boldsymbol{S}}_i, x_i)$ relaxes $\phi_{i\omega}(\boldsymbol{S}_i, x_i)$ for any ω, x_i.

Note: (C1) and (C2) are sufficient for deterministic DDs

JH (2017)

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(C3) If state $\bar{\boldsymbol{S}}_i$ relaxes state $\boldsymbol{S}_i$, then given any control x_i and any set of numbers $\{\eta_\omega \mid \text{all } \omega\}$, there is a control $\bar{x}_i$ such that

$$\sum_\omega p_{i\omega}(\bar{\boldsymbol{S}}_i, \bar{x}_i)\big(c_{i\omega}(\bar{\boldsymbol{S}}_i, \bar{x}_i) + \eta_\omega\big) \leq \sum_\omega p_{i\omega}(\boldsymbol{S}_i, x_i)\big(c_{i\omega}(\boldsymbol{S}_i, x_i) + \eta_\omega\big)$$

Note: (C1) and (C2) are sufficient for deterministic DDs

JH (2017)

Node Merger in SDDs

- Key to proofs: work with **fully articulated** SDDs.
  - All states are represented, even those that are reached with zero probability.
  - Node merger becomes rearrangement of probabilities.

Lemma. If condition (C2) is satisfied, and $\bar{\boldsymbol{S}}_i$ relaxes $\boldsymbol{S}_i$, then cost to go of $\bar{\boldsymbol{S}}_i \leq$ cost to go of $\boldsymbol{S}_i$.

Proof by backward induction on layers.

Node Merger in SDDs

Theorem. If **(C1)-(C3)** are satisfied, then node merger yields a relaxed SDD.

Proof by forward induction on layers of partially compiled SDDs.

Node Merger in SDDs

Theorem. If **(C1)-(C3)** are satisfied, then node merger yields a relaxed SDD.

Proof by forward induction on layers of partially compiled SDDs.

Corollary. The **max clique** state merger operation yields a relaxed SDD.

The operation satisfies (C1)–(C3), but the proof is nontrivial due to the strength of condition (C3).

Node Merger in SDDs

Theorem. If **probabilities are state-independent**, then a merger operation that satisfies (C1) and (C2) alone yields a relaxed SDD.

Corollary. The **job sequencing** merger operation yields a relaxed SDD.

Probabilities are state-independent, and it is easy to show the merger operation satisfies (C1)–(C2).

Computational Experiments

- **Major barrier to computational testing:**
  - We **don’t know** optimal solutions of nontrivial stochastic DDs.
  - We need **optimal** (or very good) solutions to judge the quality of bounds from DDs.

Computational Experiments

- **Approach 1:** Use deterministic **max clique** instances in DIMACS library…
  - …and **add edge** probabilities.
- **Why?**
  - Relaxed DDs provide good bounds for the **deterministic** problem.
  - Better than **full cutting plane resources** of MIP.

Bergman, Cire, van Hoeve, JH (2013)

Computational Experiments

- **Approach 1:** Use deterministic **max clique** instances in DIMACS library…
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Bergman, Cire, van Hoeve, JH (2013)

- **However…**
  - Can't compare with **optimal** solutions
    - 2 exceptions, 1 of which required **24 hours** to solve.

Computational Experiments

- **Approach 2: Random** instances.
  - **Sized** to be tractable and nontrivial.
  - Exact solutions found with **complete SDDs**, since state space enumeration is the only available method.

Computational Experiments

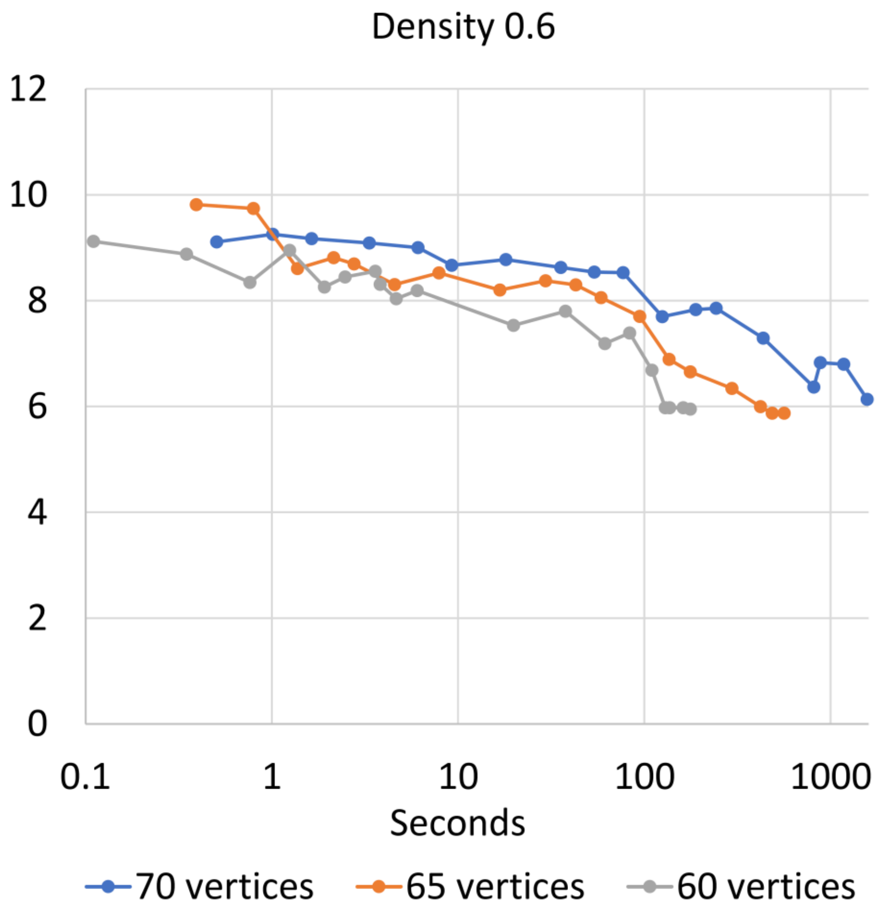
- **Merger heuristic…**
  - Standard method: Merge **less attractive** nodes first
  - …as measured by path lengths to root node in deterministic problem.

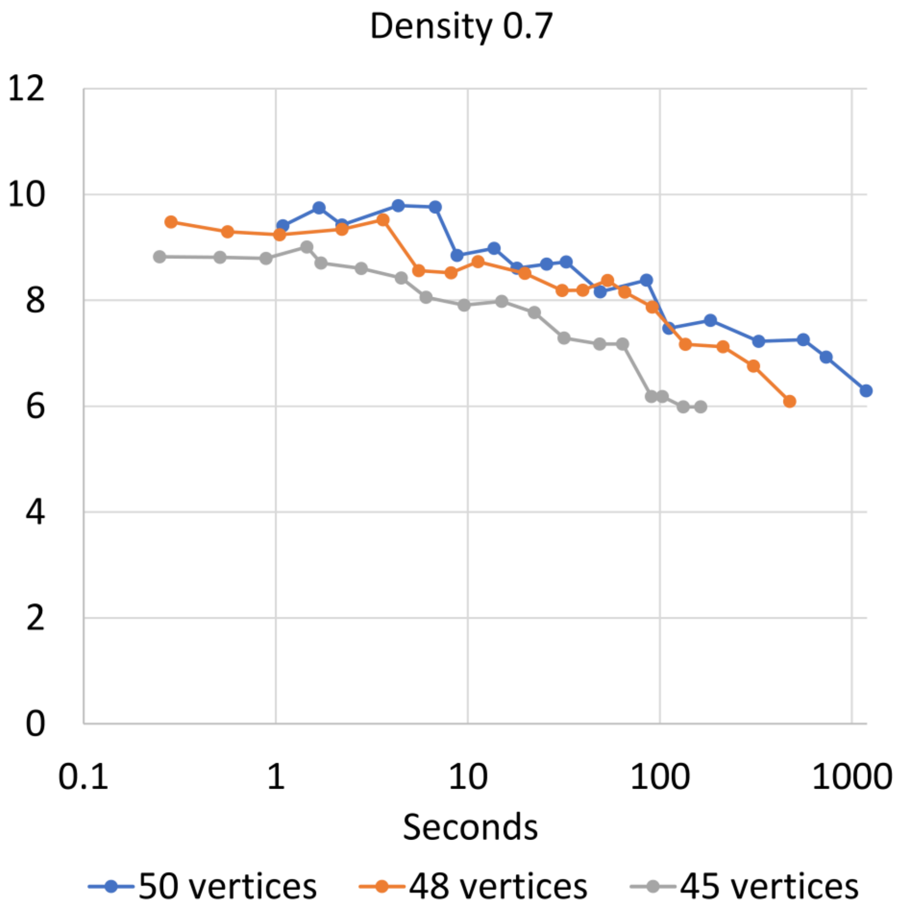
- **Control size** of relaxed SDD by limiting **width**.
  - Width = max number of nodes in a layer.

Random instances

Solved to optimality

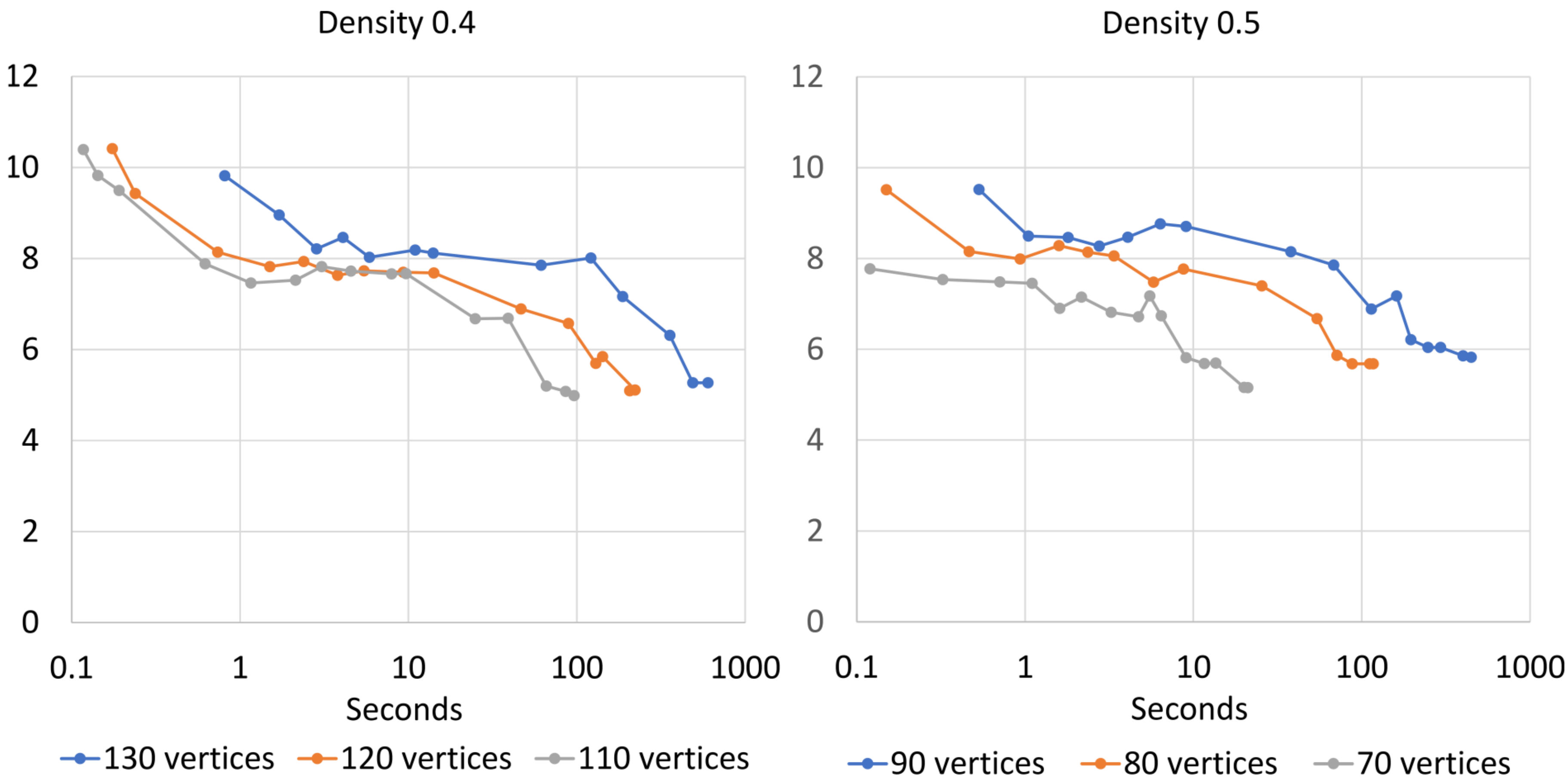
Bound vs time





Random instances

Solved to optimality



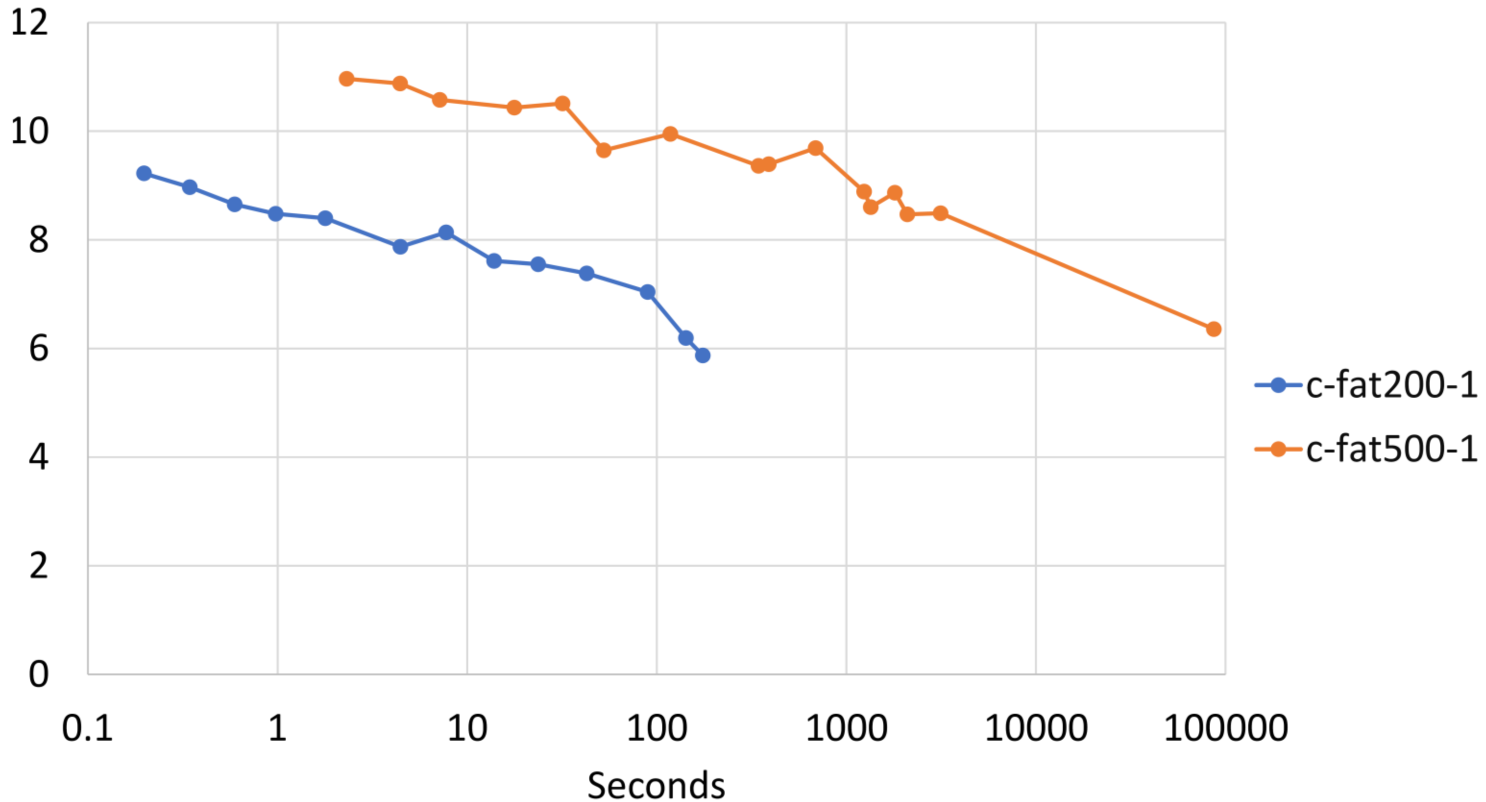
DIMACS instances

Instance	Vertices	Density	Instance	Vertices	Density
brock200_1	200	0.7417	hamming6-2	64	0.8906
cfat200-1	200	0.0767	johnson8-4-4	70	0.7571
cfat500-1	500	0.0357	keller4	171	0.6453
c125.9	125	0.8913	p_hat300-1	300	0.2430
DSJC500_5	500	0.5010	san200_0.7_1	200	0.6965
gen200_p0.9_44	200	0.8955	sanr_0.7	200	0.6934

2 DIMACS instances

Solved to optimality

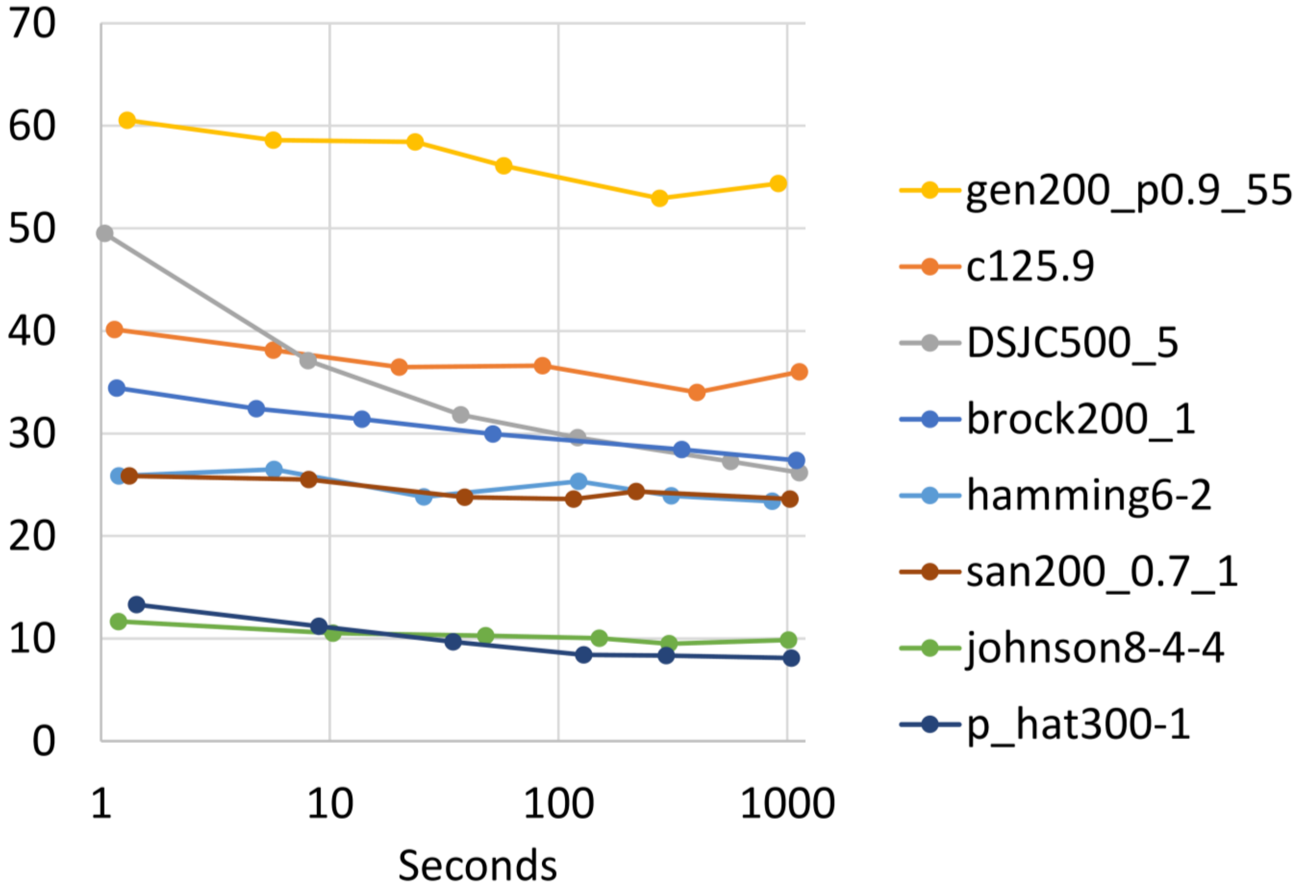
Bound vs time



DIMACS instances

Not solved to optimality

Bound vs time



Computational Experiments

- Bound quality degrades **gradually** with reduction in SDD width/time investment**.**
  - Even reduction down to a **few seconds**.
  - Indicates that SDDs can provide **useful bounds** for DP models.

- Roughly **logarithmic** relationship**.**
  - In most cases.
  - May allow estimate of how bound will **improve** with greater time investment.

Research Issues

- Use SDD bounds to solve moderate-sized problems by **branch and bound.**
  - Based on previous experience with deterministic problems**.**

- Use relaxed SDDs to compute bounds for **approximate DP**.
  - Find solution with traditional approximate DP, which **estimates** costs to go.
  - Use relaxed SDDs to compute **bounds** on costs to go, using same controls as in approximate DP solution.