Gems of TCS

Heuristic Algorithms

Sasha Golovnev

February 25, 2021

Announcements

1. Deadline HW2 today
2. Next Tuesday:
   Nitin Vaidya
3. Next Thursday:
   last lecture on Algs
4. 3rd HW will be posted
   next Thursday
5. After this:
   Complexity
   Crypto,
   Learning
6. Post-Quantum Crypto talk:
   Noah SD (Cornell), Mar 5, 1pm

Heuristic Algorithms

- When exact algorithms are too slow, and approximate algorithm are not accurate enough

Heuristic Algorithms

- When exact algorithms are too slow, and approximate algorithm are not accurate enough
- We can use heuristic algorithms

Heuristic Algorithms

- When exact algorithms are too slow, and approximate algorithm are not accurate enough
- We can use heuristic algorithms
- Heuristic algorithms use practical methods that are not guaranteed/proved to be optimal or efficient

Heuristic Algorithms

- When exact algorithms are too slow, and approximate algorithm are not accurate enough
- We can use heuristic algorithms
- Heuristic algorithms use practical methods that are not guaranteed/proved to be optimal or efficient
- Some heuristic algorithms are fast but not guaranteed to find optimal solutions

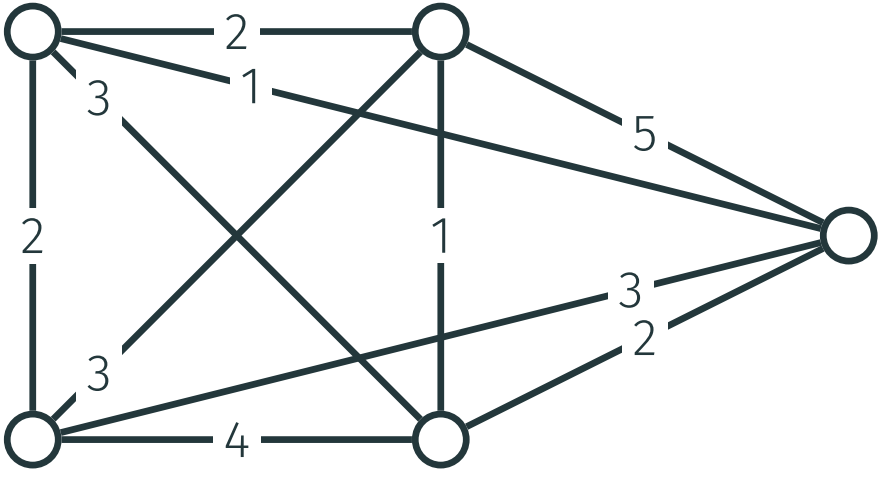
Heuristic Algorithms

- When exact algorithms are too slow, and approximate algorithm are not accurate enough
- We can use heuristic algorithms
- Heuristic algorithms use practical methods that are not guaranteed/proved to be optimal or efficient
- 1. Some heuristic algorithms are fast but not guaranteed to find optimal solutions
- 2. Some heuristic algorithms find optimal solutions but not guaranteed to be fast

Traveling Salesman

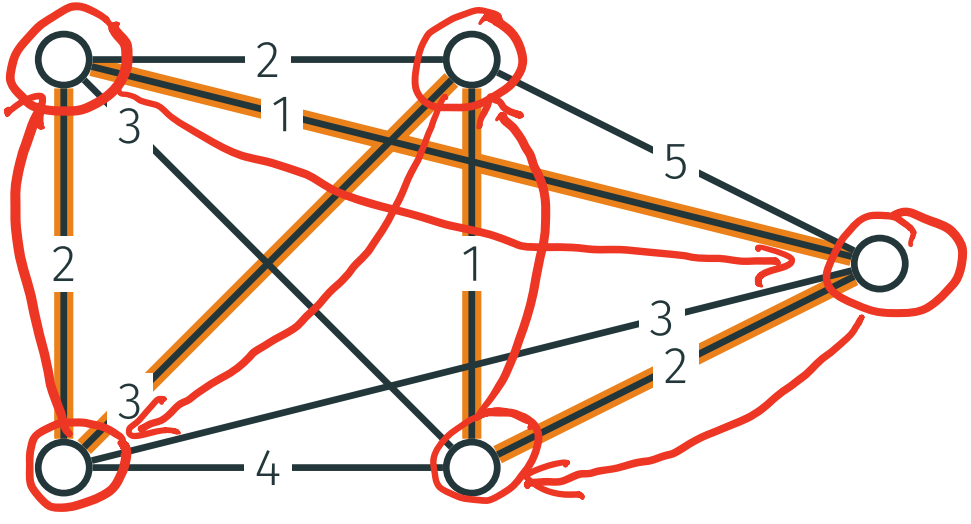
Traveling Salesman Problem

Given a complete weighted graph, find a cycle (or a path) of minimum total weight (length) visiting each node exactly once



Traveling Salesman Problem

Given a complete weighted graph, find a cycle (or a path) of minimum total weight (length) visiting each node exactly once



length: 9

Nearest Neighbors

- Going to the nearest unvisited node at every iteration?

Nearest Neighbors

- Going to the nearest unvisited node at every iteration?
- Efficient, works reasonably well in practice

$O(n^2)$

Nearest Neighbors

- Going to the nearest unvisited node at every iteration?
- Efficient, works reasonably well in practice
- For general graphs, may produce a cycle that is much worse than an optimal one

Nearest Neighbors

- Going to the nearest unvisited node at every iteration?
- Efficient, works reasonably well in practice
- For general graphs, may produce a cycle that is much worse than an optimal one
- For Euclidean instances, the resulting cycle may be about $\log n$ times worse than an optimal one

Nearest Neighbors: Bad Case

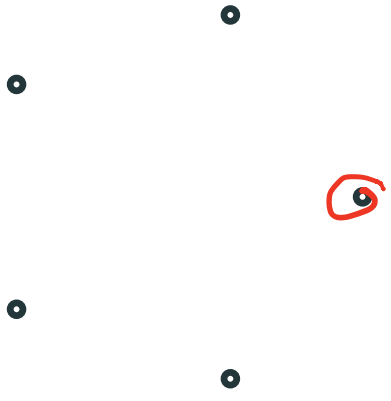
- How to fool the nearest neighbors heuristic?

Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2

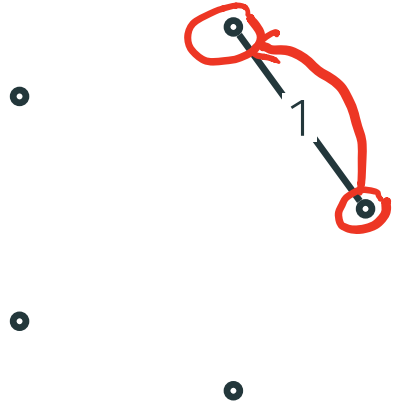
Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:



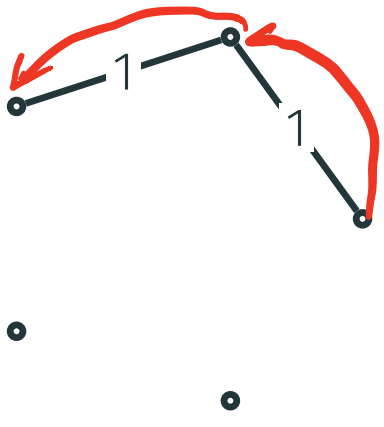
Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:



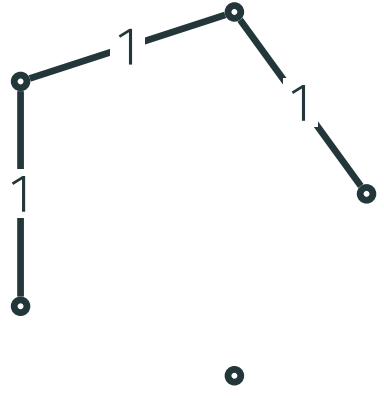
Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:



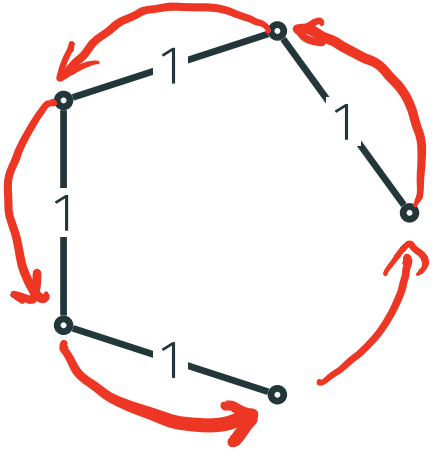
Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:



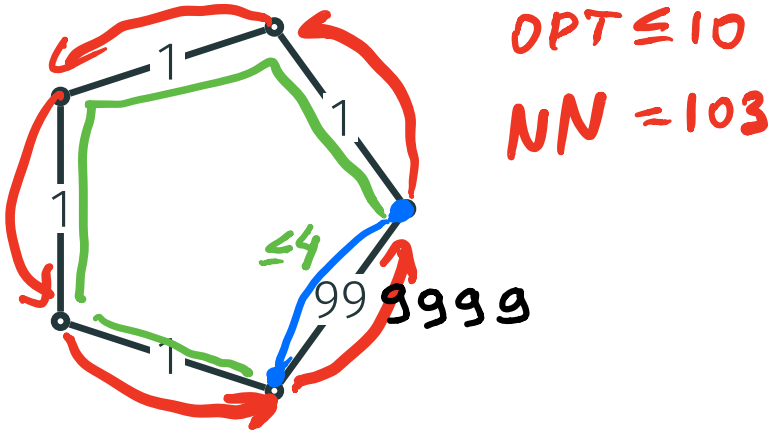
Nearest Neighbors: Bad Case

- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:

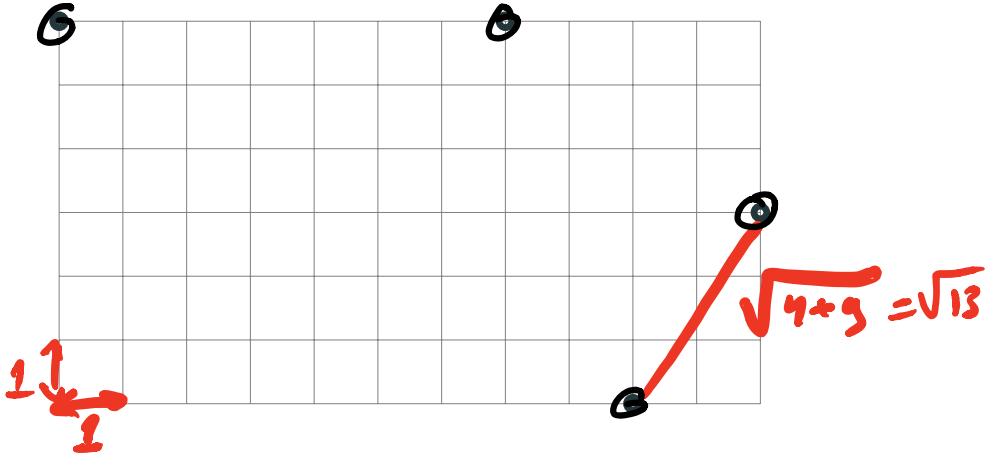


Nearest Neighbors: Bad Case

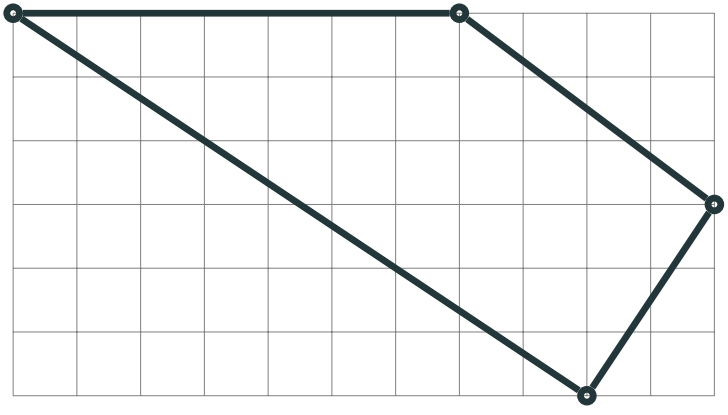
- How to fool the nearest neighbors heuristic?
- Assume that the weights of almost all the edges in the graph are equal to 2
- And we start to construct a cycle:



Suboptimal Solution for Euclidean TSP

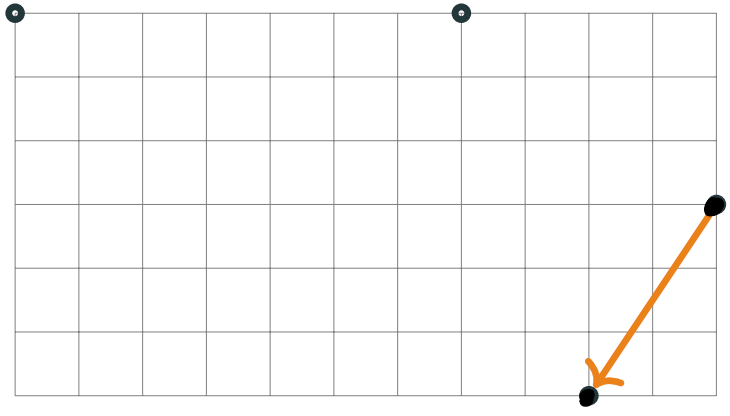


Suboptimal Solution for Euclidean TSP



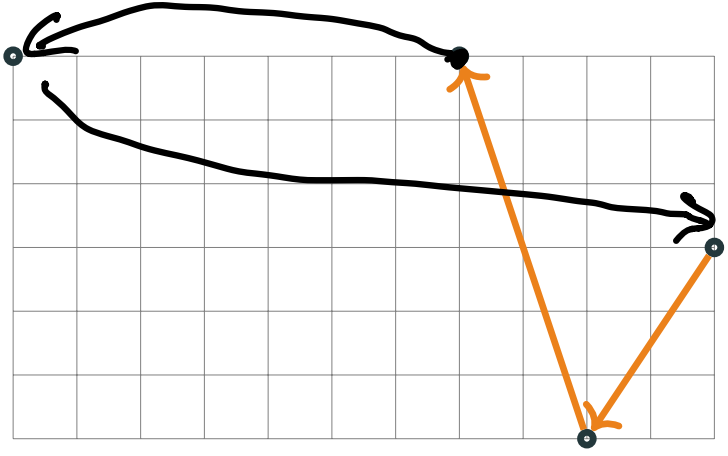
$\mathrm{OPT} \approx 26.42$

Suboptimal Solution for Euclidean TSP



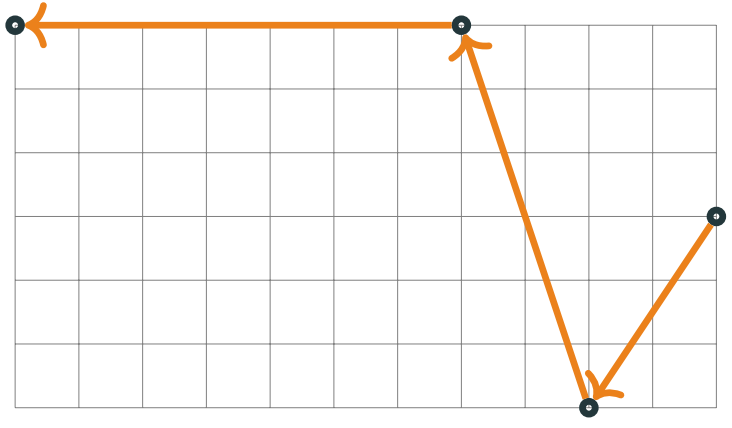
$\mathrm{OPT} \approx 26.42$

Suboptimal Solution for Euclidean TSP



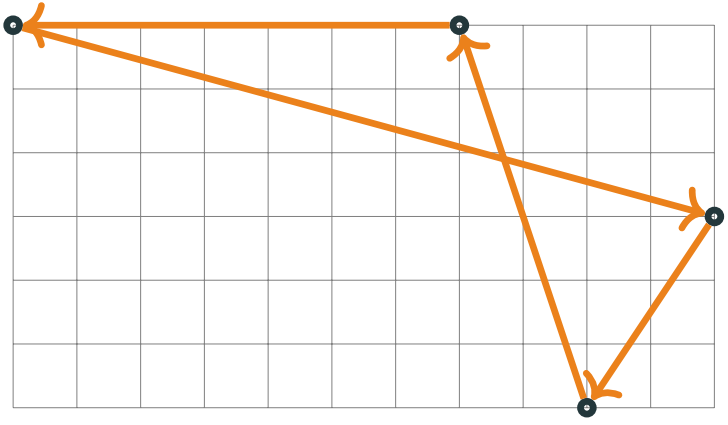
$\mathrm{OPT} \approx 26.42$

Suboptimal Solution for Euclidean TSP



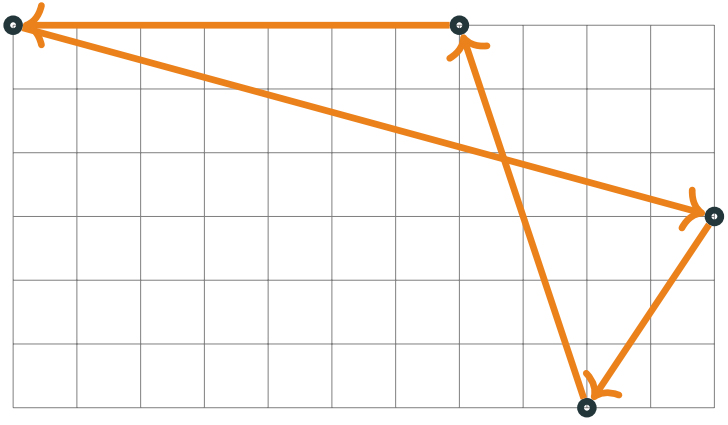
$\mathrm{OPT} \approx 26.42$

Suboptimal Solution for Euclidean TSP



$\mathrm{OPT} \approx 26.42$

Suboptimal Solution for Euclidean TSP



OPT ≈ 26.42

NN ≈ 28.33

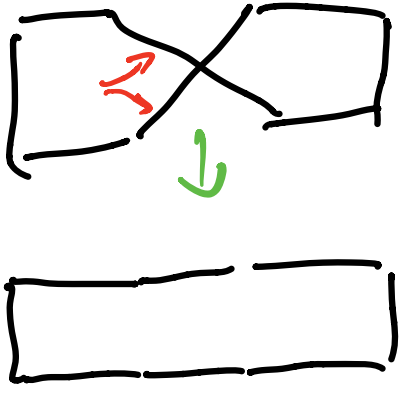
Local Search

Another Heuristic

- s ← some initial solution — any cycle that visits each vertex exactly once $1 \to 2 \to 3 \to \dots \to n$

Local Search

- $s \leftarrow$ some initial solution
- while it is possible to change 2 edges in s to get a better cycle s':



Local Search

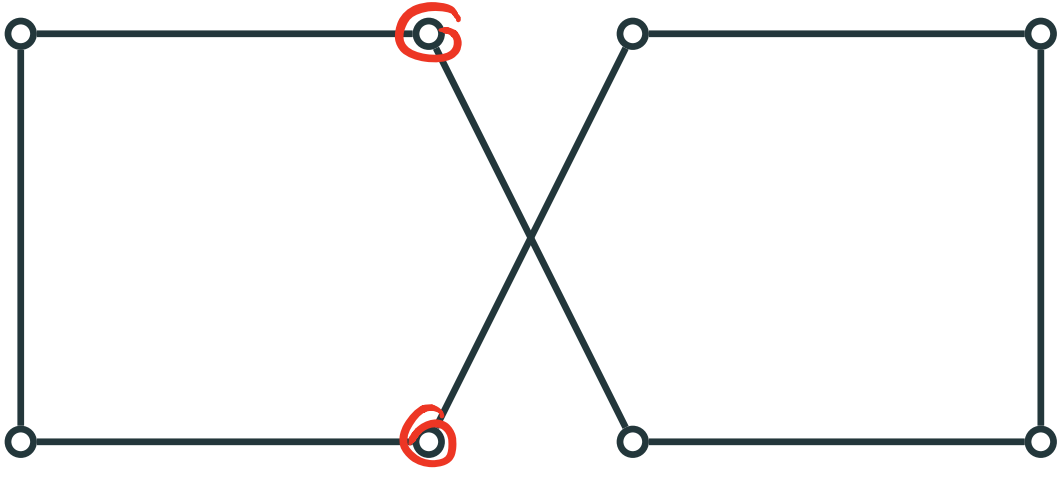
- $s \leftarrow$ some initial solution
- while it is possible to change 2 edges in s to get a better cycle s':
    - $s \leftarrow s'$

Local Search

- $s \leftarrow$ some initial solution
- while it is possible to change 2 edges in s to get a better cycle s':
    - $s \leftarrow s'$
- return s

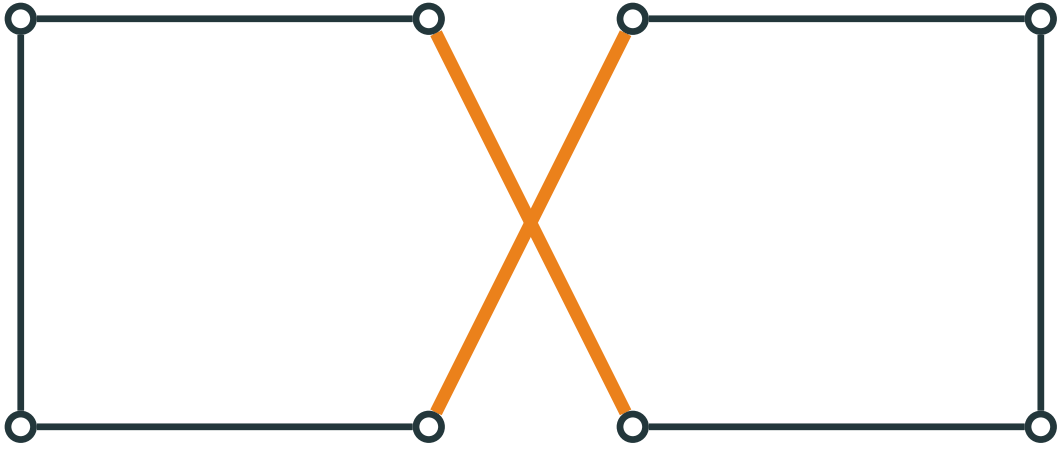
Example

Changing two edges in a suboptimal solution:



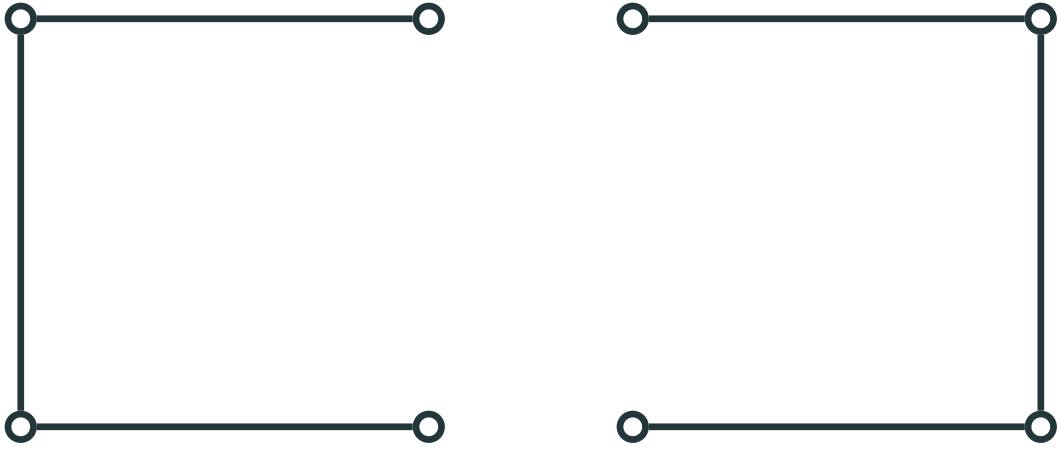
Example

Changing two edges in a suboptimal solution:



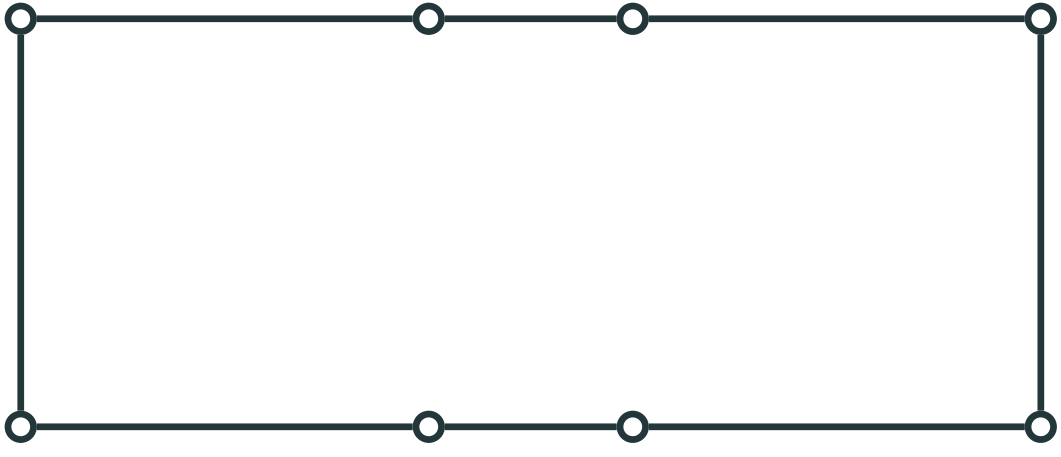
Example

Changing two edges in a suboptimal solution:



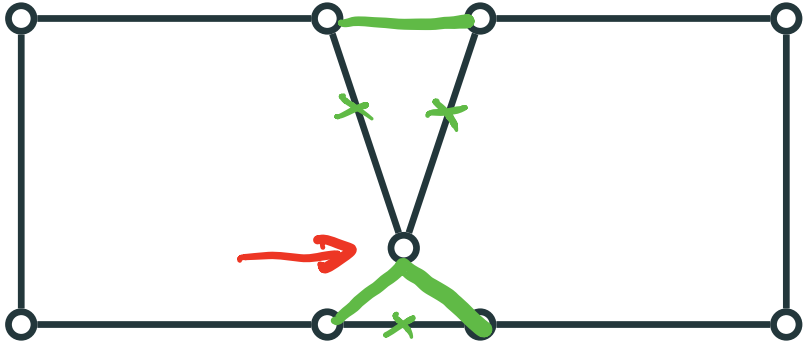
Example

Changing two edges in a suboptimal solution:



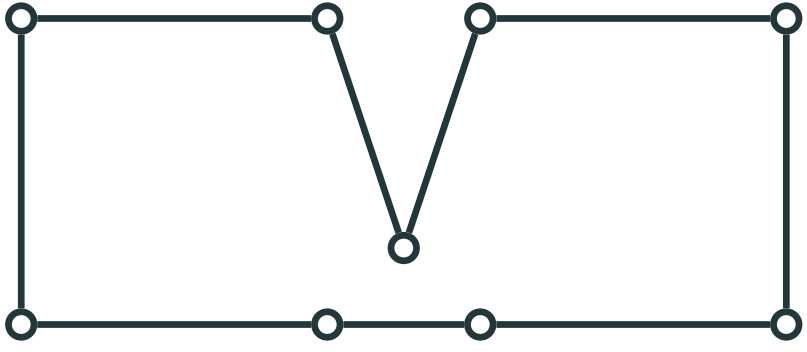
Example

A suboptimal solution that cannot be improved by changing two edges:



Example

A suboptimal solution that cannot be improved by changing two edges:



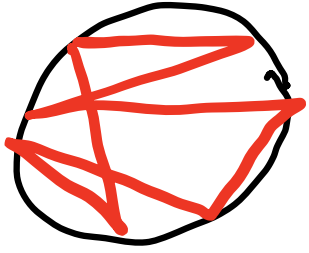
Need to allow changing three edges to improve this solution

Local Search

Local Search with parameter d: $= 2, 3, 4, 10$

- $s \leftarrow$ some initial solution
- while it is possible to change d edges in s to get a better cycle s':
  - $s \leftarrow s'$
- return s

Properties



- Computes a local optimum instead of a global optimum

Properties

- Computes a local optimum instead of a global optimum
- The larger d, the better the resulting solution and the higher is the running time

$d=2$ pairs of edges $O(n^2)$

$d=10$ 10-tuples of edges $O(n^{10})$

Performance

- Trade-off between quality and running time of a single iteration

Performance

- Trade-off between quality and running time of a single iteration
- Still, the number of iterations may be exponential and the quality of the found cycle may be poor

Performance

- Trade-off between quality and running time of a single iteration
- Still, the number of iterations may be exponential and the quality of the found cycle may be poor
- But works well in practice

doesn't always run fast
doesn't always return opt solution

Satisfiability

SAT

$$(x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee \neg x_2) \wedge (\neg x_1 \vee x_3) \wedge (x_2 \vee \neg x_3)$$

SAT

1. $x_1 = x_2 = x_3 = 1$

$$(x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee \neg x_2) \wedge (\neg x_1 \vee x_3) \wedge (x_2 \vee \neg x_3)$$

2. UNSAT

$$(x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee \neg x_2) \wedge (\neg x_1 \vee x_3) \wedge (x_2 \vee \neg x_3) \wedge (\neg x_1 \vee \neg x_2 \vee \neg x_3)$$

We've seen exp-time algs

We'll heuristic algs

Backtracking

2^n - trivial algs

$x_1 \quad x_2 \ldots \quad x_n$

- Construct a solution piece by piece

Backtracking

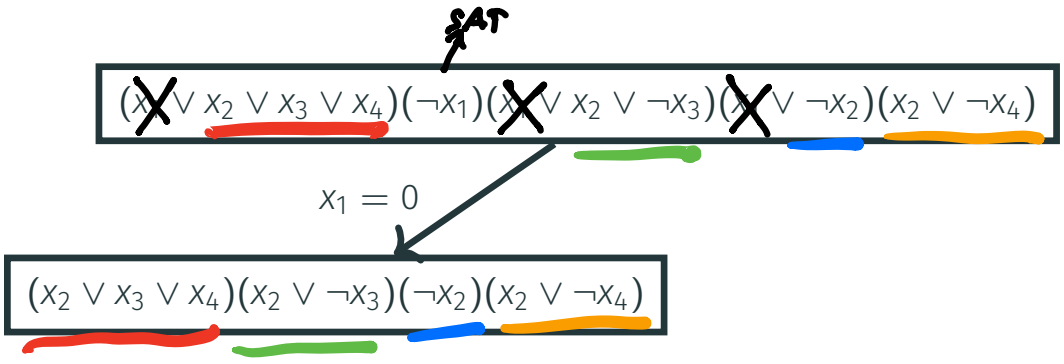
- Construct a solution piece by piece
- Backtrack if the current partial solution cannot be extended to a valid solution

Backtracking

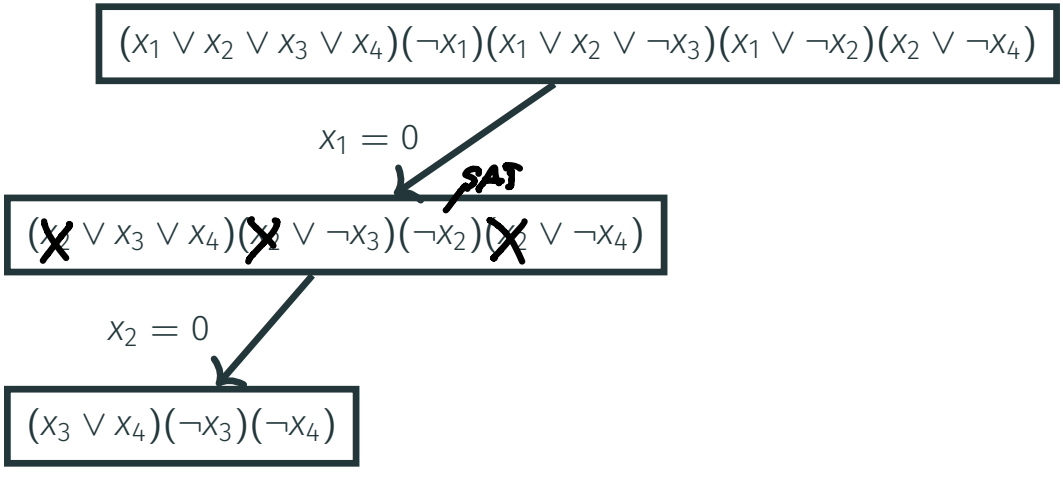
Example

$$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$$

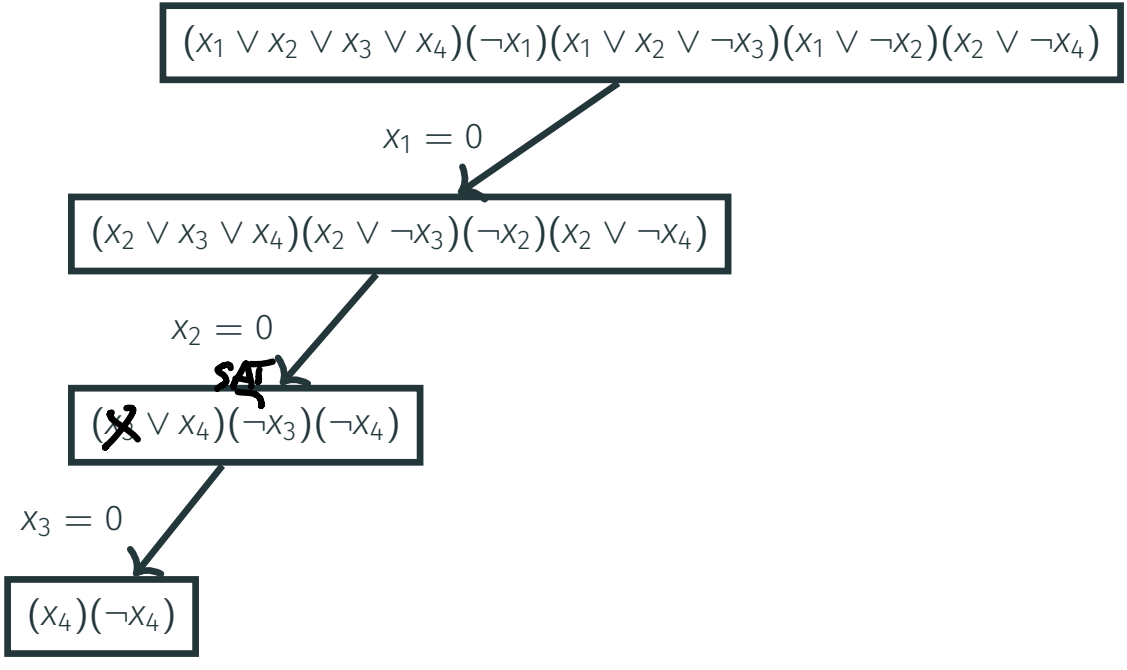
Example


SAT
$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$

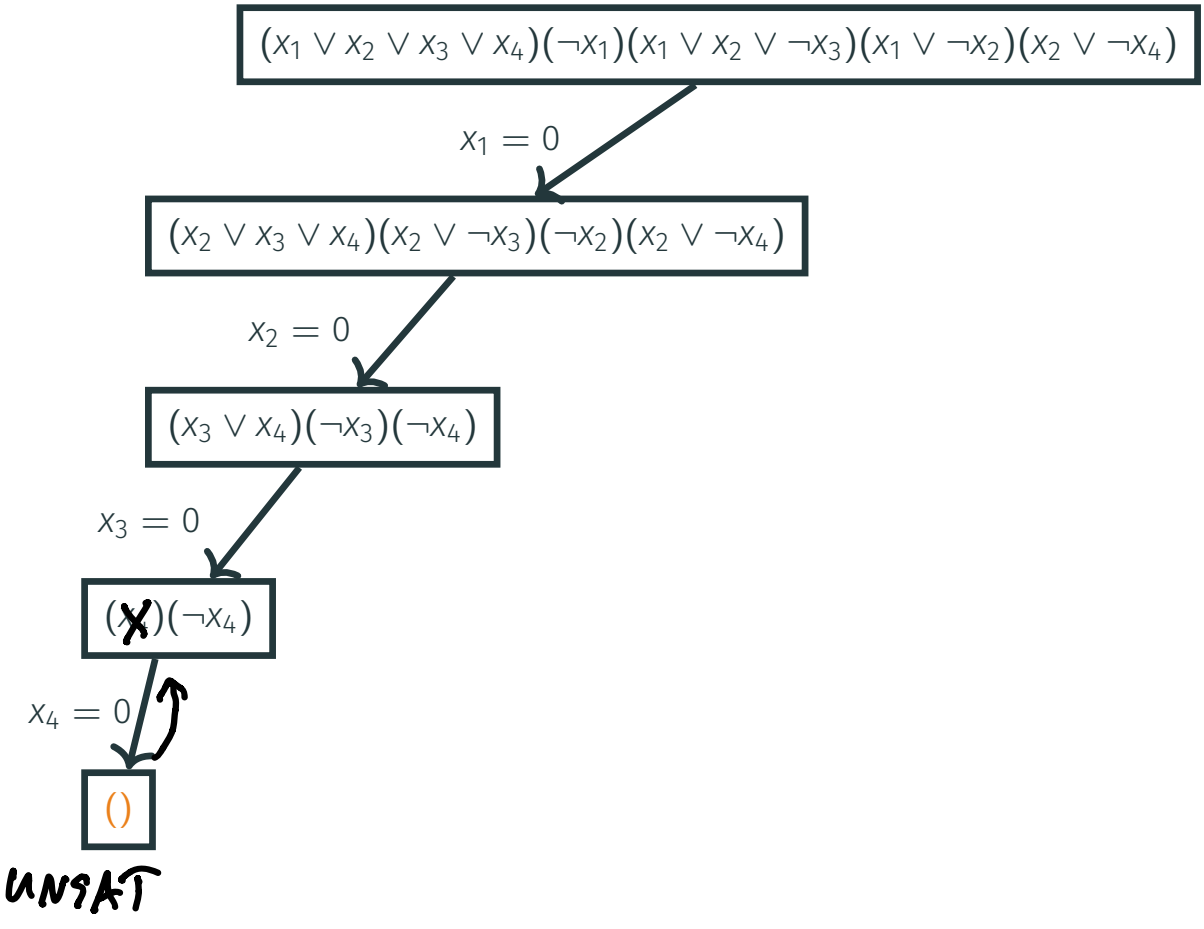
Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
SAT
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$

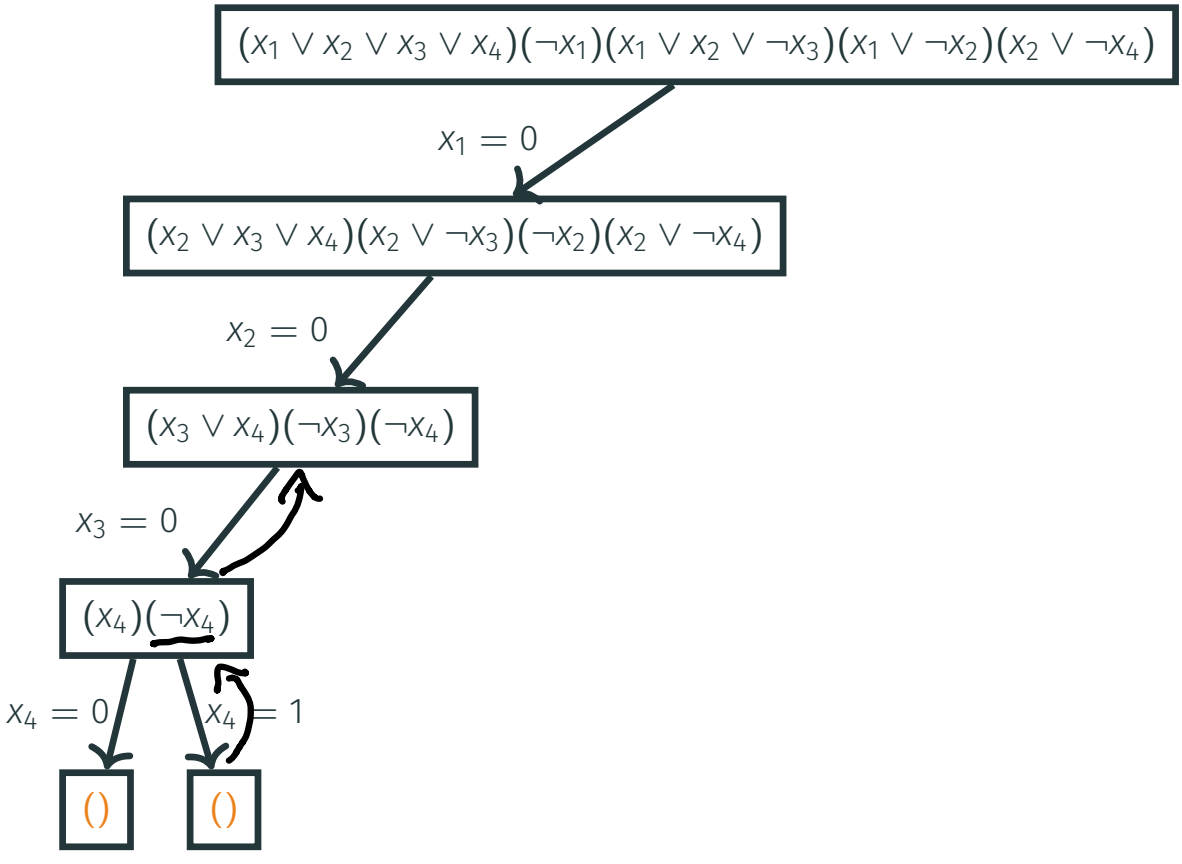
Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
SAT
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
$x_3 = 0$
$(x_4)(\neg x_4)$

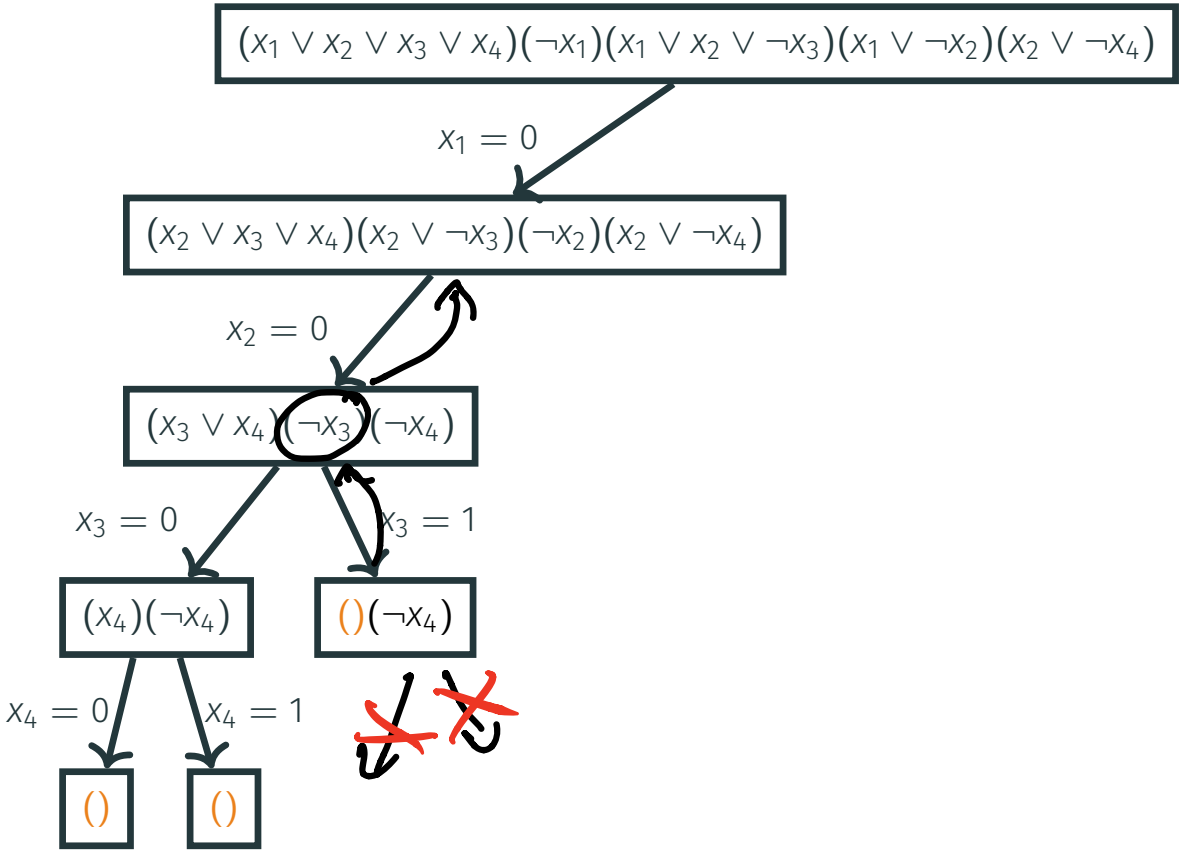
Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
$x_3 = 0$
$(\not{x}_4)(\neg x_4)$
$x_4 = 0$
()
UNSAT

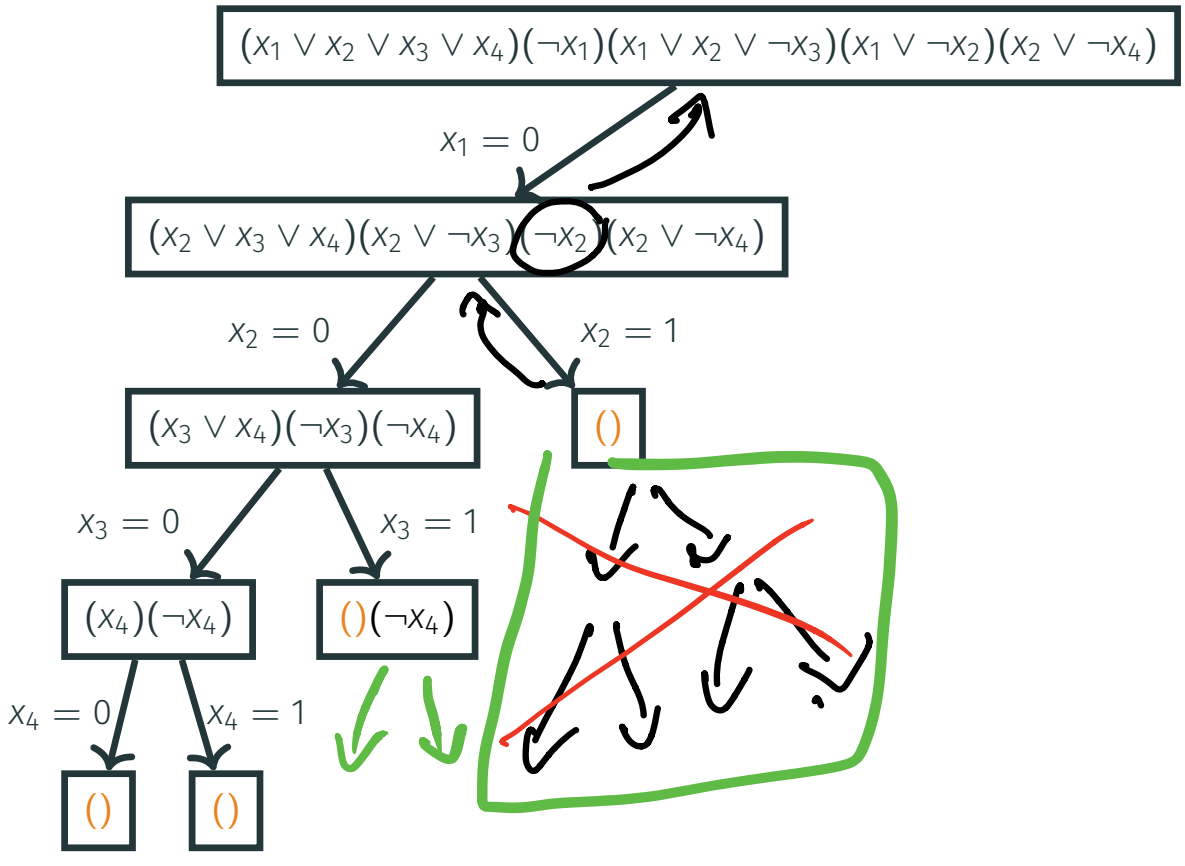
Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
$x_3 = 0$
$(x_4)(\neg x_4)$
$x_4 = 0$
$x_4 = 1$
()
()

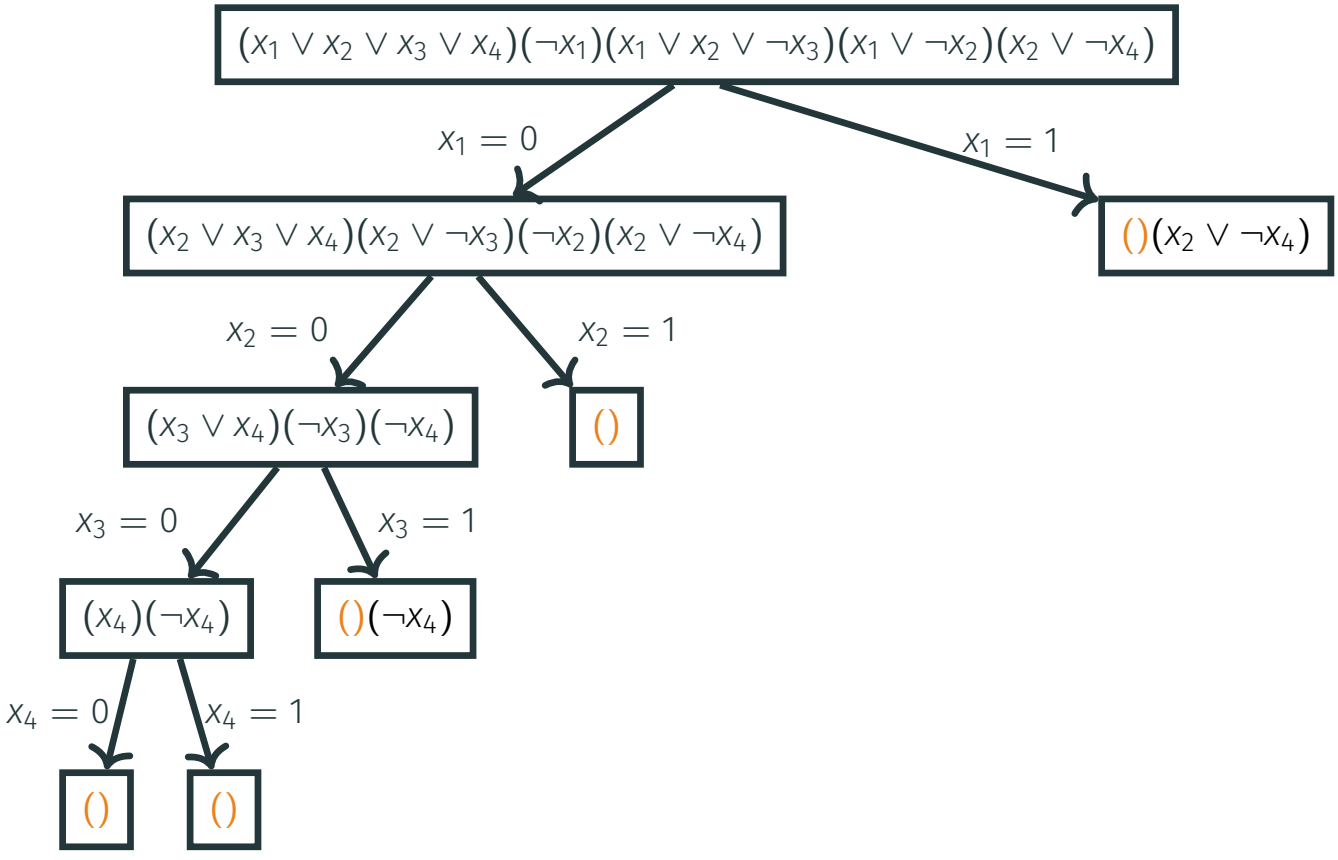
Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
$x_3 = 0$
$x_3 = 1$
$(x_4)(\neg x_4)$
$()(\neg x_4)$
$x_4 = 0$
$x_4 = 1$
()
()

Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$x_2 = 0$
$x_2 = 1$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
()
$x_3 = 0$
$x_3 = 1$
$(x_4)(\neg x_4)$
$()(\neg x_4)$
$x_4 = 0$
$x_4 = 1$
()
()

Example


$(x_1 \vee x_2 \vee x_3 \vee x_4)(\neg x_1)(x_1 \vee x_2 \vee \neg x_3)(x_1 \vee \neg x_2)(x_2 \vee \neg x_4)$
$x_1 = 0$
$x_1 = 1$
$(x_2 \vee x_3 \vee x_4)(x_2 \vee \neg x_3)(\neg x_2)(x_2 \vee \neg x_4)$
$()(x_2 \vee \neg x_4)$
$x_2 = 0$
$x_2 = 1$
$(x_3 \vee x_4)(\neg x_3)(\neg x_4)$
$()$
$x_3 = 0$
$x_3 = 1$
$(x_4)(\neg x_4)$
$()(\neg x_4)$
$x_4 = 0$
$x_4 = 1$
$()$
$()$

Backtracking Algorithm

- SolveSAT(F):
  - if F has no clauses:
    return "sat"
  - if F contains an empty clause:
    return "unsat"

unsatisfied clause with no vars

Backtracking Algorithm

- SolveSAT(F):
  - if F has no clauses:
    return “sat”
  - if F contains an empty clause:
    return “unsat”
  - $x \leftarrow$ unassigned variable of F

Backtracking Algorithm

- SolveSAT(F):
  - if F has no clauses:
    return “sat”
  - if F contains an empty clause:
    return “unsat”
  - $x \leftarrow$ unassigned variable of F
  - if SolveSAT($F[x \leftarrow 0]$) $=$ “sat”:
    return “sat”

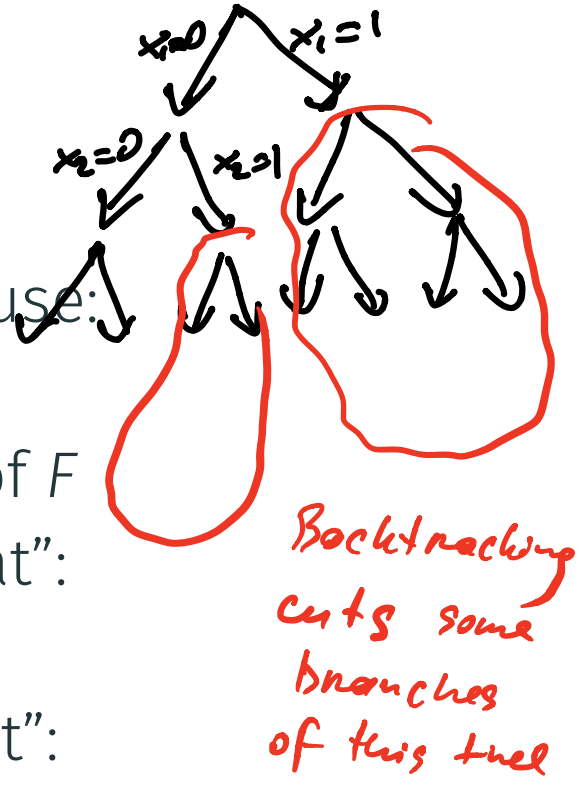
Backtracking Algorithm

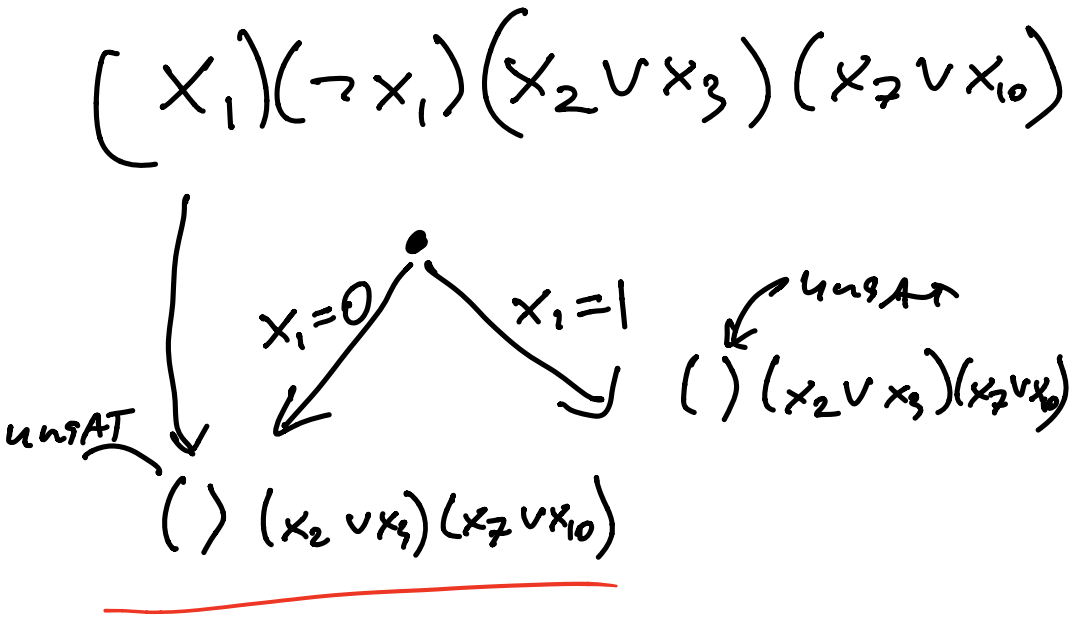
- SolveSAT(F):
  - if F has no clauses:
    return "sat"
  - if F contains an empty clause:
    return "unsat"
  - $x \leftarrow$ unassigned variable of F
  - if SolveSAT($F[x \leftarrow 0]$) = "sat":
    return "sat"
  - if SolveSAT($F[x \leftarrow 1]$) = "sat":
    return "sat"

if no solutions with $x=0$ or $x=1$, then there are no solutions $\Rightarrow$ fla is UNSAT

Backtracking Algorithm

- SolveSAT(F):
  - if F has no clauses:
    return “sat”
  - if F contains an empty clause:
    return “unsat”
  - $x \leftarrow$ unassigned variable of F
  - if SolveSAT($F[x \leftarrow 0]$) $=$ “sat”:
    return “sat”
  - if SolveSAT($F[x \leftarrow 1]$) $=$ “sat”:
    return “sat”
  - return “unsat”




$(x_1)(\neg x_1)(x_2 \vee x_3)(x_7 \vee x_{10})$
$x_1 = 0$
$x_1 = 1$
unsAT
unsAT
$(\ )(x_2 \vee x_3)(x_7 \vee x_{10})$
$(\ )(x_2 \vee x_3)(x_7 \vee x_{10})$

Backtracking

- Thus, instead of considering all 2^n branches of the recursion tree, we track carefully each branch

Backtracking

- Thus, instead of considering all 2^n branches of the recursion tree, we track carefully each branch
- When we realize that a branch is dead (cannot be extended to a solution), we immediately cut it

SAT Solvers

- Backtracking is used in many state-of-the-art SAT-solvers

SAT Solvers

- Backtracking is used in many state-of-the-art SAT-solvers
- SAT-solvers use tricky heuristics to choose a variable to branch on, simplify a formula before branching, and use efficient data structures

Example: choose a var that appears more often

Example: $x=0$ or $x=1$ first?

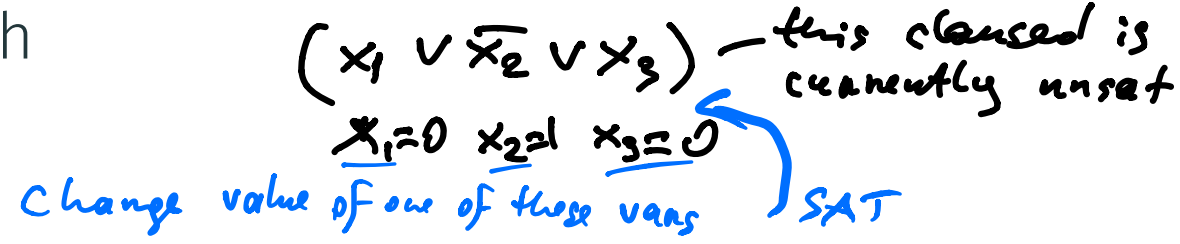
x	x	x	$\bar{x}$
1	1	1	0

Simplify: $(x_1 \vee \bar{x}_2)(x_3)(x_4 \vee \bar{x}_3)$

$x_3 = 1$

SAT Solvers

- Backtracking is used in many state-of-the-art SAT-solvers
- SAT-solvers use tricky heuristics to choose a variable to branch on, simplify a formula before branching, and use efficient data structures
- Another commonly used technique is local search



Applications

THE ART OF COMPUTER PROGRAMMING

VOLUME 4 PRE-FASCICLE 6A

A DRAFT OF SECTION 7.2.2.2: SATISFIABILITY

DONALD E. KNUTH *Stanford University*

The Art of Computer Programming

Wow! — Section 7.2.2.2 has turned out to be the longest section, by far, in The Art of Computer Programming. The SAT problem is evidently a "killer app," because it is key to the solution of so many problems. Consequently I can only hope that my lengthy treatment does not also kill off my faithful readers!

Donald Knuth

SAT Handbook

Conference, Competition, Journal

- Annual SAT Conference (since 1996):
  `http://satisfiability.org`

Conference, Competition, Journal

- Annual SAT Conferense (since 1996):
  `http://satisfiability.org`
- Annual SAT Solving competitions (since 2002):
  `http://www.satcompetition.org/`

$n = 7000$ 2^n time will not work

Conference, Competition, Journal

- Annual SAT Conferense (since 1996): `http://satisfiability.org`
- Annual SAT Solving competitions (since 2002): `http://www.satcompetition.org/`
- Journal on Satisfiability, Boolean Modeling and Computation: `http://jsatjournal.org/`

Math Proofs

nature International weekly journal of science

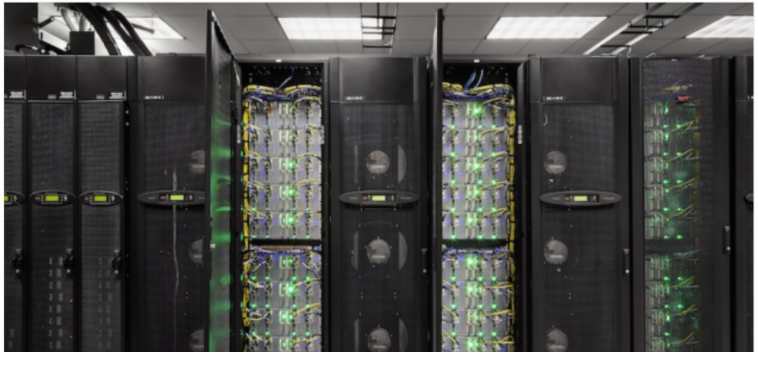
NATURE | NEWS

Two-hundred-terabyte maths proof is largest ever

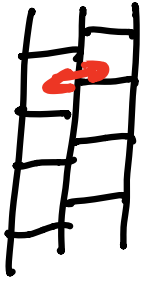
A computer cracks the Boolean Pythagorean triples problem — but is it really maths?

Evelyn Lamb

26 May 2016



Math Proofs



GEOMETRY

Computer Search Settles 90-Year-Old Math Problem

d = 7 - dim space

10

By translating Keller's conjecture into a computer-friendly search for a type of graph, researchers have finally resolved a problem about covering spaces with tiles.

SAT Solvers

python wrapper for SAT solver picosat

```
from pycosat import solve

clauses = [ [-1, -2, -3], [1, -2], [2, -3], [3,
-1], [1, 2, 3] ]

print(solve(clauses))
print(solve(clauses[1:]))
```

$(\neg x_1 \vee \neg x_2 \vee \neg x_3), (x_1 \vee \neg x_2)$ ---

python syntax for all clauses except 1st one

SAT Solvers

```
from pycosat import solve

clauses = [ [-1, -2, -3], [1, -2], [2, -3], [3,
-1], [1, 2, 3] ]

print(solve(clauses))
print(solve(clauses[1:]))
```

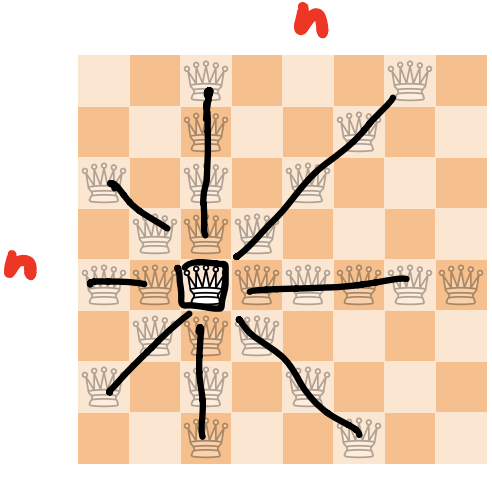
```
UNSAT
[1, 2, 3]
```

→ $x_1=1$ $x_2=1$ $x_3=1$

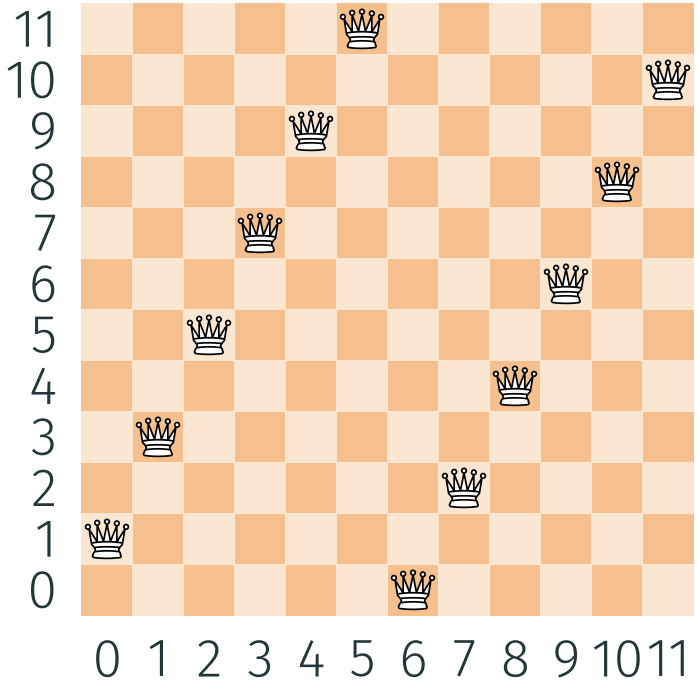
[-1, 2, -3] → $x_1=0$ $x_2=1$ $x_3=0$

N Queens

Is it possible to place n queens on an $n \times n$ board such that no two of them attack each other?



Examples

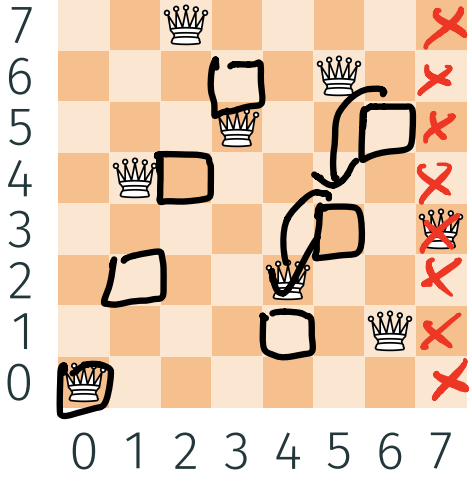


Examples

Classical solution:

Brute force : even $n=8$ $\binom{64}{8}$ way too large

Backtracking : place 1st queen $n \approx 20$



Encode/reduce to SAT

use SAT-solvers

Encoding as SAT

- n^2 0/1-variables: for $0 \leq i, j < n$, $x_{ij} = 1$ iff queen is placed into cell (i, j)

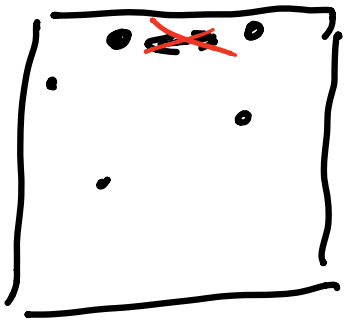
Encoding as SAT

- n^2 0/1-variables: for $0 \leq i, j < n$, $x_{ij} = 1$ iff queen is placed into cell (i, j)
- For $0 \leq i < n$, ith row contains ≥ 1 queen:

$$(x_{i1} = 1 \text{ or } x_{i2} = 1 \text{ or } \ldots \text{ or } x_{i(n-1)} = 1).$$

n queens on nxn board

$(x_{00} \vee x_{01} \vee x_{02} \vee \cdots \vee x_{0,n-1})$
$(x_{10} \vee x_{11} \vee x_{12} \vee \cdots \vee x_{1,n-1})$
$(x_{20} \vee x_{21} \vee \cdots$



Encoding as SAT

- n^2 0/1-variables: for $0 \leq i, j < n$, $x_{ij} = 1$ iff queen is placed into cell (i, j)
- For $0 \leq i < n$, ith row contains ≥ 1 queen:

$$(x_{i1} = 1 \text{ or } x_{i2} = 1 \text{ or } \ldots \text{ or } x_{i(n-1)} = 1)\,.$$

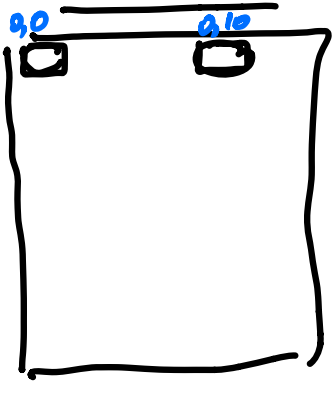
- For $0 \leq i < n$, ith row contains ≤ 1 queen:

$$\forall 0 \leq j_1 \neq j_2 < n\colon\ (x_{ij_1} = 0 \text{ or } x_{ij_2} = 0)\,.$$

$(x_{0,0}=0 \text{ OR } x_{0,10}=0)$ It's not true

$\Updownarrow$

$(\neg x_{00} \text{ OR } x_{0,10})$



Encoding as SAT

- n^2 0/1-variables: for $0 \leq i, j < n$, $x_{ij} = 1$ iff queen is placed into cell (i, j)
- For $0 \leq i < n$, ith row contains ≥ 1 queen:

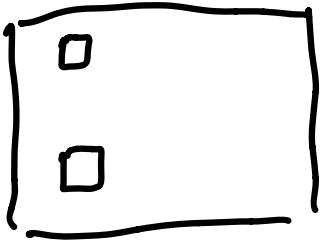
$$(x_{i1} = 1 \text{ or } x_{i2} = 1 \text{ or } \ldots \text{ or } x_{i(n-1)} = 1)\,.$$

- For $0 \leq i < n$, ith row contains ≤ 1 queen:

$$\forall 0 \leq j_1 \neq j_2 < n\colon\ (x_{ij_1} = 0 \text{ or } x_{ij_2} = 0)\,.$$

- For $0 \leq j < n$, jth column contains ≤ 1 queen:

$$\forall 0 \leq i_1 \neq i_2 < n\colon\ (x_{i_1j} = 0 \text{ or } x_{i_2j} = 0)\,.$$



Encoding as SAT

- n^2 0/1-variables: for $0 \leq i, j < n$, $x_{ij} = 1$ iff queen is placed into cell (i, j)
- For $0 \leq i < n$, ith row contains ≥ 1 queen:

$$(x_{i1} = 1 \text{ or } x_{i2} = 1 \text{ or } \ldots \text{ or } x_{i(n-1)} = 1)\,.$$

- For $0 \leq i < n$, ith row contains ≤ 1 queen:

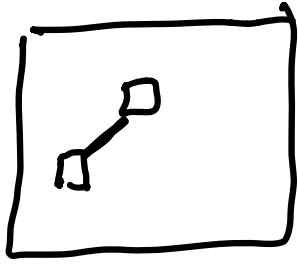
$$\forall 0 \leq j_1 \neq j_2 < n\colon\ (x_{ij_1} = 0 \text{ or } x_{ij_2} = 0)\,.$$

- For $0 \leq j < n$, jth column contains ≤ 1 queen:

$$\forall 0 \leq i_1 \neq i_2 < n\colon\ (x_{i_1 j} = 0 \text{ or } x_{i_2 j} = 0)\,.$$

- For each pair $(i_1, j_1), (i_2, j_2)$ on diagonal:

$$(x_{i_1 j_1} = 0 \text{ or } x_{i_2 j_2} = 0)\,.$$



Implementation

Descriptive programming

n = 100

```
from itertools import combinations, product
from pycosat import solve

n = 10
clauses = []


# converts a pair of integers into a unique integer
def varnum(i, j):
    assert i in range(n) and j in range(n)
    return i * n + j + 1


# each row contains at least one queen
for i in range(n):
    clauses.append([varnum(i, j) for j in range(n)])

# each row contains at most one queen
for i in range(n):
    for j1, j2 in combinations(range(n), 2):
        clauses.append([-varnum(i, j1), -varnum(i, j2)])

# each column contains at most one queen
for j in range(n):
    for i1, i2 in combinations(range(n), 2):
        clauses.append([-varnum(i1, j), -varnum(i2, j)])

# no two queens stay on the same diagonal
for i1, j1, i2, j2 in product(range(n), repeat=4):
    if i1 == i2:
        continue

    if abs(i1 - i2) == abs(j1 - j2):
        clauses.append([-varnum(i1, j1),
                        -varnum(i2, j2)])


assignment = solve(clauses)
for i, j in product(range(n), repeat=2):
    if assignment[varnum(i, j) - 1] > 0:
        print(j, end=' ')
```