PG4200: Algorithms And Data Structures

Lesson 10:
Decision and Optimization
Problems

Runtime Of Algorithms

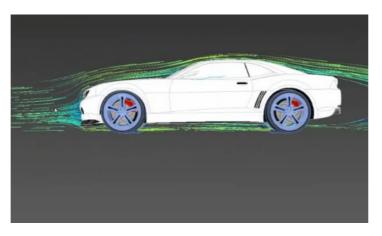
- Depending on input size N of the addressed problem
- Polynomial $O(N^k)$: usually fine, for small k
- Exponential O(10^N): hopeless, unless tiny N
 - Eg, number of atoms in the whole universe is estimated to be no more than $10^{82}\,$

Complex Problems

- There are a lot of problems in science and engineering for which we do not know any algorithm that can solve them in *polynomial* time
 - Such algorithms might exist, but we do not know them yet
- Brute Force: try all possible combinations, until find valid solution... but that is exponential!!!
- We need some heuristics to address these problems
 - But no guarantee that we can find a solution in reasonable time

Vehicle Design

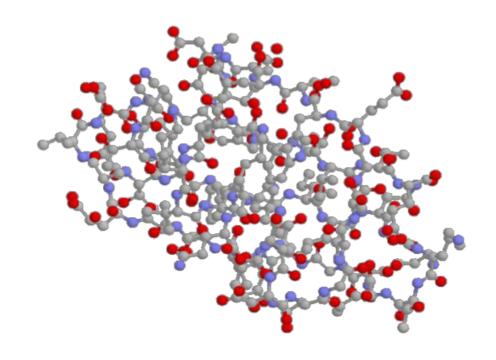


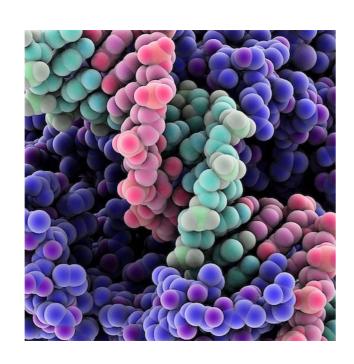


- How to find best shape to reduce air resistance?
- Can have different designs, and then test them in a wind tunnel



Protein Design





 How to find the right sequence of amino acids which will result in a protein with some sought properties?

Stock Market



 How to find best investment portfolio to maximize profit?



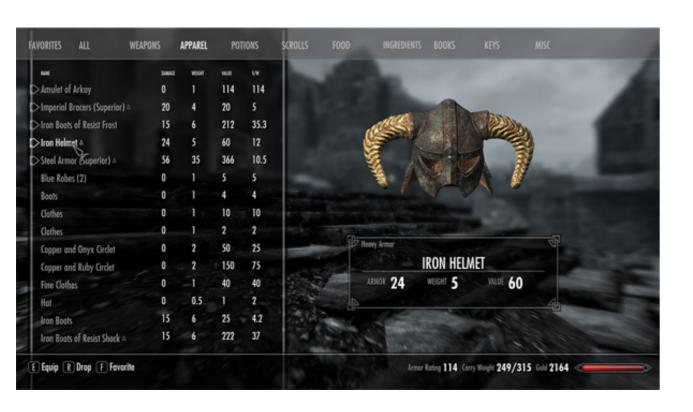
Class Schedule



I DAG C NT NA - 22.12.2017 SENDRE SØK Algoritmer og datastrukturer (PG4200-17), Enterpriseprogrammering 2 (PG6100-17)						
	TID	EMNE	KLASSE, STUDENTGRUPPE, STUDENT	AKTIVITET, PROSJEKT	LÆRER	ROM
u 40	TI 03.10.2017					
	13:00 - 15:00		Margrethe Øra Thorsen	Øving		Stillerom FU110
	FR 06.10.2017					
	09:15 - 12:00	Enterpriseprogrammering 2 (PG6100-17)	Programmering 15	Forelesning	Andrea Arcuri	Undervisningsrom F205
u 41	TI 10.10.2017					
	08:15 - 12:00	Algoritmer og datastrukturer (PG4200-17)	Intelligente systemer 16, Programmering 16, Spillprogrammering 16			Auditorium VU06
	FR 13.10.2017					
	09:15 - 12:00	Enterpriseprogrammering 2 (PG6100-17)	Programmering 15	Forelesning	Andrea Arcuri	Undervisningsrom F206
ı 42	TI 17.10.2017					
	08:15 - 12:00	Algoritmer og datastrukturer (PG4200-17)	Intelligente systemer 16, Programmering 16, Spillprogrammering 16			Auditorium VU06

- How to find best class schedule for which:
 - There is time for all classes
 - Classes in same year are not in parallel (ie conflicting)
 - Preferences of lectures are taken into account
 - Etc.
 - ?

RPG Equipment



 In RPGs, how find best combination of wearable items to maximize attack and defense under the constraints of maximum weight and item slots available?

Optimization Problem

- 2 main components: Search Space and Fitness Function
- Goal: find the best solution from the search space such that the fitness function is minimized/maximized

Search Space

- Set X of all possible solutions for the problem
- If a solution can be represented with 0/1 bit sequence of length N, then search space is all possible bit strings of size N
- Search space is usually huge, eg 2^N
 - Otherwise use brute force, and so would not be a problem

Fitness Function

- f(x)=h
- Given a solution x in X, calculate an heuristic h that specifies how good the solution is
- Problem dependent, to minimize or maximize:
 - Minimize air resistance
 - Maximize protein structure properties
 - Maximize Return Of Investment
 - etc.

Optimization Algorithms

- Algorithm that explores the search space X
- Only a tiny sample of X can be evaluated
- Use fitness f(x) to guide the exploration to fitter areas of the search space with better solutions
- Stopping criterion: after evaluating K solutions (or K amount of time is passed), return best x among the evaluated solutions
- Many different kinds of optimization algorithms...
 - But as a user, still need to provide the representation and f(x)

Search Operator

- S(X) = X'
- An operator that, from a solution x, gives a new one x'
- Still need to evaluate its fitness, ie f(x')
- The optimization algorithm will use the search operators to choose which new x'in X to evaluate
- The search operator will depend on the problem representation
- Example: flip a bit in a bit-sequence representation

Example: Knapsack Problem (KP)

- Insert N items to a knapsack
- Each item has a weight w and a value v

- \$2 1kg \$2 1kg \$10 4kg
- The knapsack has a maximum load of weight L
- Goal: find the selection of items that can be inserted within limit L, and for which the total value is maximized
- Note: many real-world problems are instances of the knapsack problem

Details

- Each unique item has an index from 0 to N-1
- A solution can be represented as an array x of 0s (item not present) and 1s (item present)
- Maximize: $f(x) = \sum_{i=0}^{N-1} v[i] * x[i]$
- Constraint: $\sum_{i=0}^{N-1} w[i] * x[i] \leq L$
- Can have f(x)=0 if constraint is not satisfied

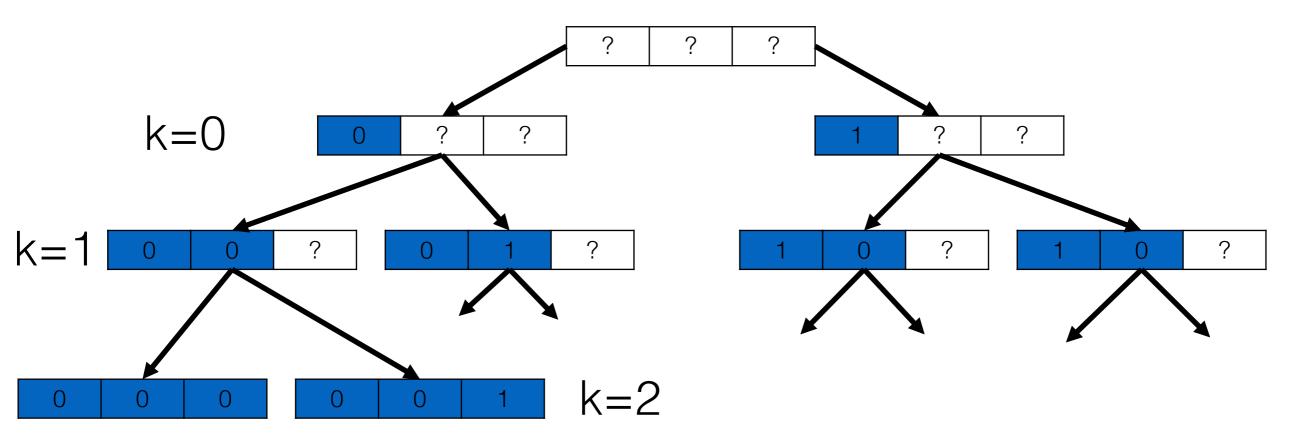
Brute Force

- Given size N, enumerate all possible bit arrays
- Return the one with maximum f(x)
- Astronomically expensive, but for tiny N
 - $2^{10} = 1024$
 - $2^{20} = 1,048,576$
 - $2^{50} \cong 1,120,000,000,000,000$
 - etc

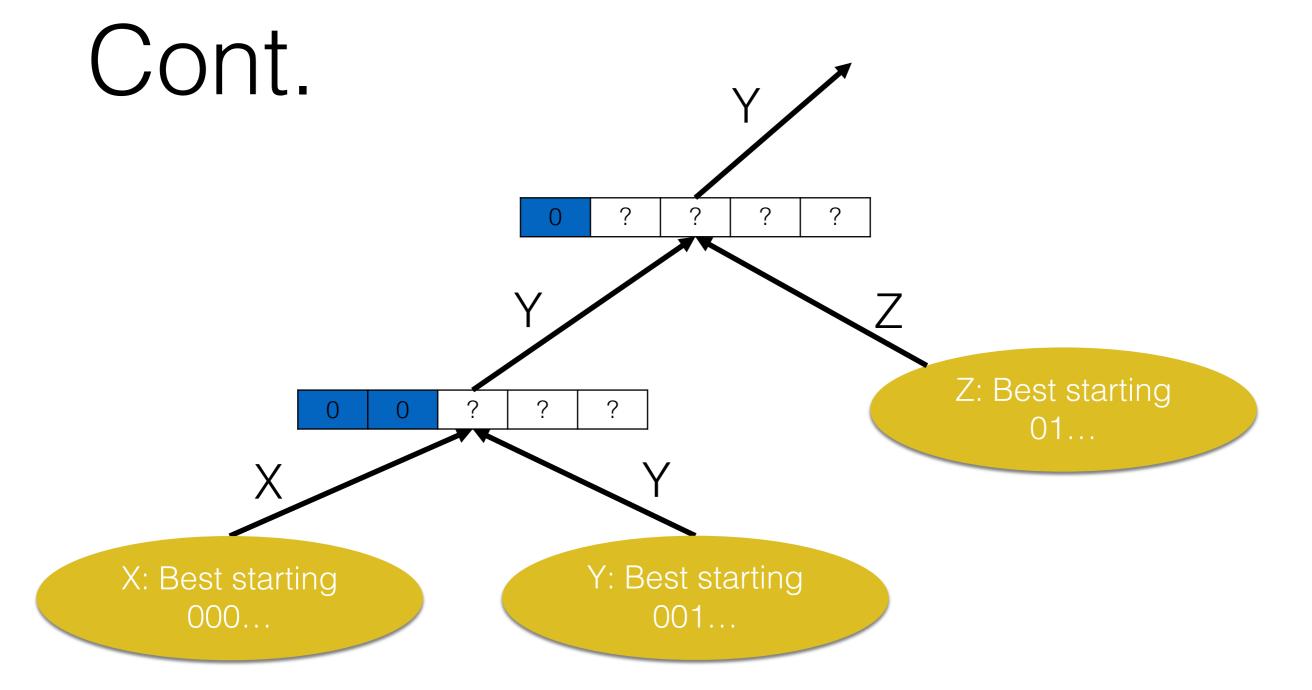
How To Brute Force?

- Use recursion
- 2 recursive calls, considering a bit for each level/index K
 with either 0 or 1
- At each recursion call, increase K by 1, until K=N
- Going to have 2^N leaves, each one representing a different bit-string of 0/1

Example: N=3



- Can use a single buffer array
- When reaching a leaf, clone array, and return it
 - ie, stopping criterion for the recursion is K=N-1
- When a call is finished, the best returned cloned array between the 2 recursive calls is given back
- Note: above tree is not completed, due to space...



- Assume Y better than X and Z
- When reached a leaf, and we go up the call tree, only the best between the 2 subtrees is returned to the caller... all the way up to the root
- Note: the behavior here is very similar to a depth-first search
- Here, not only Y is the best solution starting with 001, but also the best starting with 00 (as better than X), and also the best starting with 0 (as better than Z)

Greedy Algorithm

- Build a solution as quickly as possible
- Don't explore the search space, but rather focus on the most promising path in it
- Actual implementation is problem dependent
- For example on KP:
 - Start from empty selection x
 - Add 1 item at a time to x (but how to choose???)
 - Stop when not possible to add any item

KP Example

- L = 26
- W = [12, 7, 11, 8, 9]
- V = [24, 13, 23, 15, 16]
- From

https://people.sc.fsu.edu/~jburkardt/datasets/knapsack_01/knapsack_01.html

Greedy: Heaviest First

Χ	1	0	1	0	0
W	12	7	11	8	9
V	24	13	23	15	16

- First choose (12,24)
- Then choose (11,13)
- Weight becomes 12 + 11 = 23
- Cannot add any other element without exceeding L=26
- f(x) = 24 + 23 = 47
- Is 47 the best score we can achieve???

Greedy: Lightest First

Χ	0	1	0	1	1
W	12	7	11	8	9
V	24	13	23	15	16

- Choosing (7,13), (8,15) and (9,16)
- Weight becomes 7 + 8 + 9 = 24 < 26
- Cannot add any other element without exceeding L=26
- f(x) = 13 + 15 + 16 = 44
- Worse solution 44 than previous 47

Greedy: Best Ratio

Χ	1	0	1	0	0
W	12	7	11	8	9
V	24	13	23	15	16
Ratio	2.00	1.85	2.09	1.87	1.77

- Consider first the best ratio v/w, ie which item gives best return for unit of weight
- Choose (11,23) and then (12,24)
- Cannot add any other element without exceeding L=26
- f(x) = 24 + 23 = 47
- Different order of insertion, but still 47

Best Solution

Χ	0	1	1	1	0
W	12	7	11	8	9
V	24	13	23	15	16

- Weight is 7 + 11 + 8 = 26
- f(x) = 13 + 23 + 15 = 51
- Better than the previous 47
- Greedy algorithms can be fast, but can give poor results
- Need something more general, with better results

General Optimization Algorithms

- Random Search (in this class)
- Hill Climbing (in this class)
- Simulated Annealing
- Genetic Algorithms (next class)
- Ant Colony Algorithms
- Particle Swarm Algorithms
- Etc. etc. (there are many)

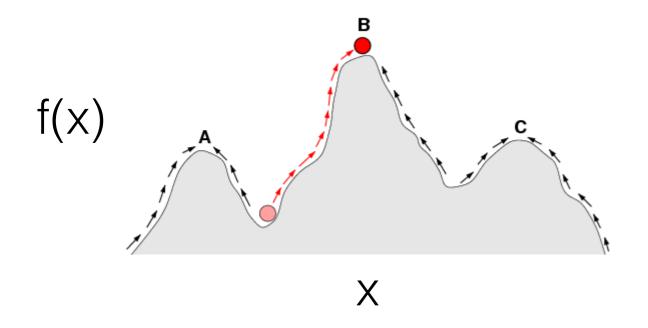
Random Search (RS)

- Easiest of the optimization algorithms
- Sample a random solution from search space X
- Keep sampling until run out of time
- Keep track of best solution found so far

Hill Climbing (HC)

- Start from a random solution
- Keep track of / store one solution
- Use search operator to do small modifications
- If better solution, move to it, and repeat
- If no better solution in the neighborhood, restart from a random solution

Very Simplified Example



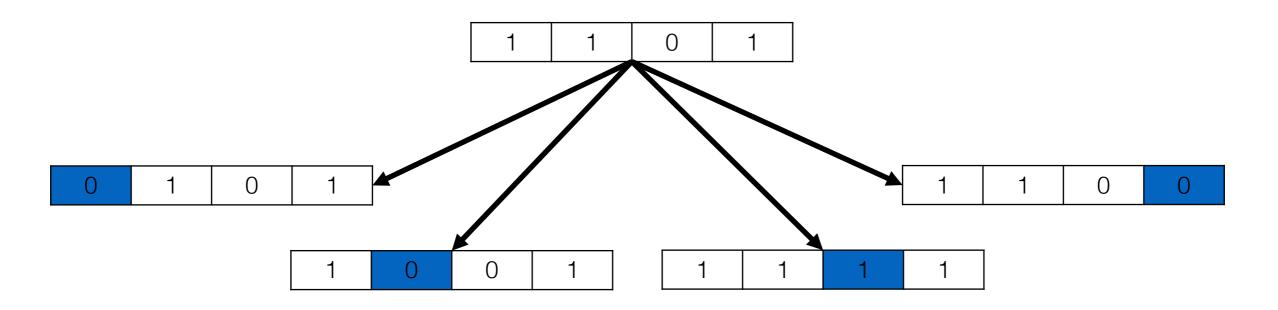
Fitness Landscape

- Consider problem in which x is a number
- Search operator is +- 1 on such x
- "Climb" up to maximize f(x)
- B is global optimum
- A and C are local optima
- Final result depends from starting point

HC for KP

- HC is a general algorithm
- But still need to define a proper search operator for each problem domain
- Example:
 - add/remove 1 item (small neighborhood)
 - remove K items, add J different items (larger neighborhood)
- The larger the neighborhood, the slower the ascent, so the less restart we can do within same time
 - le, it is not necessarily better

Neighborhood Example

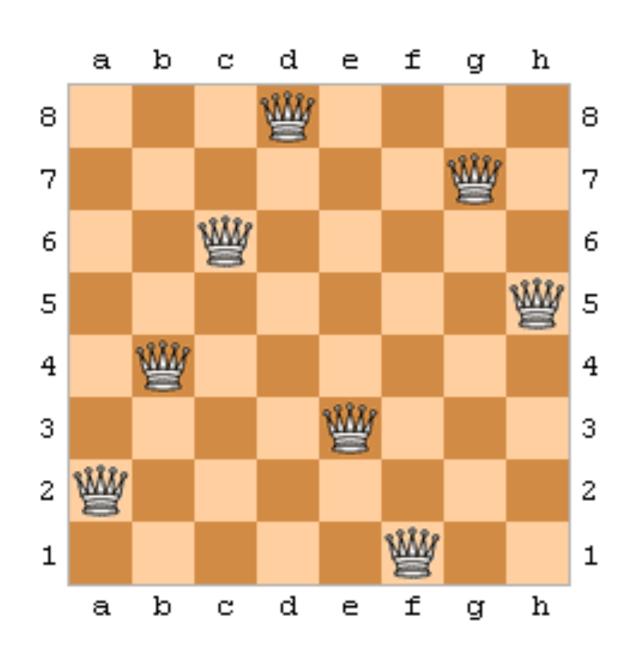


- Eg, flip 1 bit in a bit-string
- Given N bits, search space is 2^N , and each neighborhood is composed of N different solutions
- Note: could consider larger neighborhoods (eg, flip K bits), but then the neighborhood size would increase significantly
 - this could make each step of HC slower

No Free Lunch (NFL) Theorem

- What is the best optimization algorithm?
 - Which best variants / choice of parameters?
- Considering all optimization problems, mathematically proved (NFL) that all optimization algorithms perform on average the same
 - Yes, it follows that, on some problems, RS is the best
- There exist no best algorithm
- But on specific problems, you can have some algorithms that are better than others, especially by exploiting domain knowledge
- It follows that a general algorithm will perform worse than a specialized variant for a specific problem

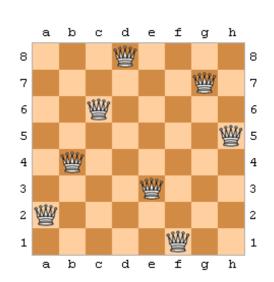
Queen Puzzle (QP)



- Position 8 queens such that no 2 queens threaten each other
- Generalization: N queens into a N*N board

QP As Optimization

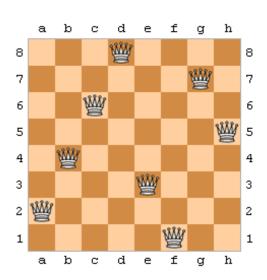
- Search Space: matrix N*N of bits
 - 1 for a queen in that position, 0 otherwise
- Search operator: flip bits in the matrix
- Fitness: need to reward having N queens, and minimize number of threatened queens



QP: Better Representation

- Binary matrix N*N would allow for any number of queens on the board (eg all 1s)
- Domain knowledge: no 2 queens on same row, no 2 queens on the same column
 - Choose representation and search operator to only explore solution for which these constraints are satisfied
- New representation: array of size N, with column indices from 0 to N-1 (position is for queen in row i)
- New operator: swap 2 column indices

QP Cont.



- Representation: [f,a,e,b,h,c,g,d]
 - Eg, queen in row 1 is in column "f", row 2 is in column "a", etc
- Search operator: swap two elements
 - Eg, swap "f" with "c", [c,a,e,b,h,f,g,d]
- By construction, I am only exploring board configurations that do not clash on columns/rows
 - But still a problem, as need to handle threating on diagonals

Decision Problem

- Technically, QP is a decision problem
- Once we find a solution with N queens no threating any other, we know we have found a global optimum
- In optimization problems, usually we cannot know if we found the best
- Decision Problem: can say "yes" or "no" about if a solution is optimal or not
- For decision problems, still doing the same as optimization, only difference is that we can know when best solution is found
- Practically all optimization problems have a decision variant for some metric K, eg "find knapsack configuration with total item values of at least K"

NP

- NP: "Nondeterministic Polynomial time"
- NP is "the set of all decision problems that can be solved in polynomial time on a theoretical non-deterministic Turing machine"
- Equivalent, easier definition: "set of all decision problems whose solutions can be verified in polynomial time"
 - le, can answer "yes" or "no" in polynomial time
- KP and QP are in NP:
 - QP: can quickly verify if N queens do not threaten each other
 - KP: can quickly verify in linear time if a solution has at least a certain value

P

- P is the set of all decision problems that can be solved in polynomial time
- P is at least a subset of NP... but is it a strict subset???
- P = NP ???
- P!= NP ???
- This is arguably the most important question in computer science for which we do not have an answer (yet)
- Consequence: there might be undiscovered, efficient algorithms to solve today's complex problems, or those might be impossible to design... we simply have no clue ⊗

Homework

- Study Book pages 910-921
 - Note: details of optimization algorithm are not in the book
- Study code in the *org.pg4200.les10* package
- Do exercises in exercises/ex10