

# Algorithms and Data Structures

Degree in Bioinformatics, UPF

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With help from Ramon Ferrer i Cancho, Jordi Delgado,  
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Dept. CS, UPC

Winter 2023–24

# We start with halfgroups

Hence, course presentation deferred to Monday.

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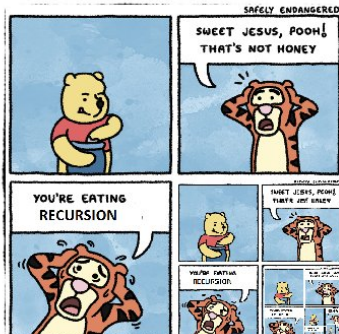
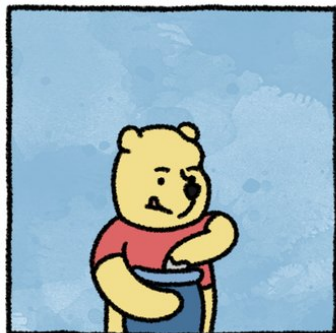
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- ▶ And we start programming.
- ▶ There is a key programming notion behind every course on Algorithms and Data Structures:

**recursion!**

SAFELY ENDANGERED



# Recursion, I

A must

Half or more of every course like this one is based on recursive programs and recursive structuring of data.

## A recursive function

includes necessarily, among whatever else is necessary,

- Base** cases: solved without recursion.

- Recursive** cases: solved by calling the function itself, either directly or indirectly.

- Test** to distinguish between them (most likely an alternative instruction).

It is **crucial** that the recursive call(s) send parameters that are “in some sense smaller” than the value received:

- they must **progress** towards the base cases.

# Recursion, II

How to think and conceive recursive structures

Recall the **induction principle**.

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## How to think and conceive recursive structures

Recall the **induction principle**.

You must

- ▶ Reach an **extremely clear** notion of what the program achieves,
- ▶ **write it down** in as much formality as you are capable to,
- ▶ and solve the problem while relying on **that** notion to reason **inductively** about the recursive calls.

**Never** let your thinking slip down through what happens at the recursive calls themselves.

The Python tutor may be helpful to reach further understanding.

# Recursion, III

## Indirect recursion

There is recursion whenever there is a cycle of function calls.

- ▶ Function  $f$  calls itself, or
- ▶ function  $f$  calls function  $g$  and, in turn,  $g$  calls  $f$ ,
- ▶ function  $f$  calls  $g$ , which calls  $h$ , which calls  $f$ ...

**Today:** We refresh and introduce a few notions of graphs and trees, and practice recursive programming on trees.

[https://en.wikipedia.org/wiki/Gallery\\_of\\_named\\_graphs](https://en.wikipedia.org/wiki/Gallery_of_named_graphs)



# Trees as Graphs

A couple of important adjectives

## Easy to see a tree as a graph

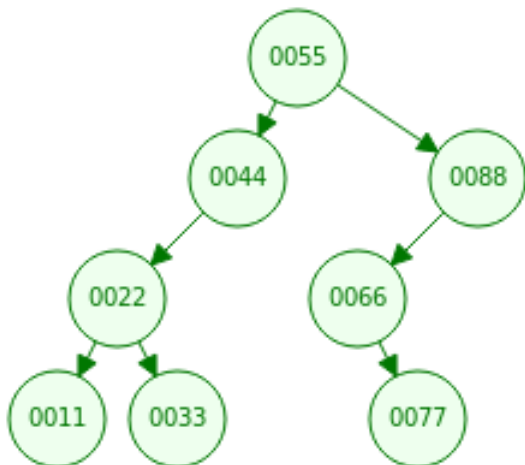
but one needs to pay a bit of attention to a couple of things.

- ▶ Rooted trees versus free trees:
  - ▶ in a **rooted tree**, there is a distinguished node that we call **root**;
  - ▶ if we do not distinguish a root, then we call it a **free tree**.
  - ▶ In a rooted tree, there is a unique path from each node to the root.
  - ▶ Then, **subtrees** (or **children**) of a node are those appearing in the direction opposite to the root.
- ▶ Ordered or unordered trees:
  - ▶ in a rooted tree, the subtrees can form a *set* (**unordered** trees) or a *sequence* (**ordered** trees).
- ▶ Very important variant: **binary trees**.

Careful: very often, you find written “tree” and must figure out the adjectives on your own, from the context.

# A Binary Tree

Actually, a BST as we will study in due course



# Tree Traversals

Example traversals on the example tree

**Traversal** (a.k.a. Full scan, cat. “recoregut”, cast. “recoredo”):  
passing through all the elements in a data structure.

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Several traversal schemes possible:

- ▶ Preorder: traverse root, then (**recursively**) the left subtree, then (**recursively**) the right subtree;

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- ▶ levelwise (we will return to this in due time).

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- ▶ levelwise (we will return to this in due time).

## On multiway trees

Preorder and postorder have natural generalizations.

# Logistics, I

- ▶ José Luis Balcázar  
jose.luis.balcazar@upc.edu  
Please do not employ jose.balcazar@prof.esci.upf.edu
- ▶ Meeting according to the general schedule:  
Theory and (*compulsory!*) Lab sessions.
- ▶ Additional personal conversations as needed:
  - ▶ Normally, I can be available around our room before and after the theory session.
  - ▶ Alternative slots for longer appointments, by email if necessary.
- ▶ Slides available from  
[https://www.cs.upc.edu/~balqui/slides\\_ADS\\_24.pdf](https://www.cs.upc.edu/~balqui/slides_ADS_24.pdf)  
(link also available through <http://aula.esci.upf.edu>).
- ▶ The slide deck is “live”; update often your copy!
- ▶ Mandatory Jutge course (for exams) and optional additional ones.

# Course Contents

- ▶ Recalling **recursion** and related topics.
- ▶ Combinatorial Search Schemes:
  - ▶ Backtracking algorithms,
  - ▶ **Dynamic Programming**.
- ▶ Linear data structures.
- ▶ Tree traversals and graph traversals revisited.
- ▶ Fundamental notions of **heaps**, balanced trees, and hashing.
- ▶ Dynamic memory: basics of pointer programming.
- ▶ Optional: C++ programming — mostly on your own.
- ▶ Optional: STL, the standard template library of C++ — mostly on your own.

# Evaluation, I

Part individual, part in small teams

**Deliverable:** Documented programming project in pairs, on assigned topics.

**Lab tasks:** individual, unless negotiated differently with me.

**All exams:** individual.

# Evaluation, II

**Deliverable:** 25% of the grade.

**Lab tasks:** 25% of the grade, taken jointly.

**Midterm:** 25% of the grade, Monday February 12th.

**Final exam:** 25% of the grade; as of today, March 18th 15h seems likely.

**Recovery:** date and time TBD.

# Evaluation, III

## Topics for programming projects

Topic is rather free but the project **must** include algorithmic or data structures content beyond what is covered in the course, such as:

- ▶ Applications of alternative or more sophisticated algorithm schemes.
- ▶ Pointer-based list and tree implementations in C++.
- ▶ Balanced search trees: AVL BSTs, B+ trees.
- ▶ Hashing.
- ▶ Advanced usage of graph libraries.
- ▶ Graph drawing software.
- ▶ ...

# Index

## Combinatorial Search

- Structure of Subproblems

- Set-Based Backtracking

- Backtracking with Non-Binary Decisions

- Backtracking for Optimization

- Exponential Growth

- Dynamic Programming

- Greedy Schemes and Other Approaches

## Data Structures

## Dynamic Memory

# Framework for Algorithmic Schemes, I

An intuitive framework for developing algorithms and comparisons among them:  
**combinatorial search**

There are many strategies for designing algorithms; several of them exhibit a particularly successful record.

## Intuitive context to explain them

and discuss their similarities and differences:

- ▶ Notion of “instance” of a computational problem,
- ▶ notion of “candidate solutions” for each instance,
- ▶ notion of “solutions aimed at”, in two possible ways:
  - (a) mere existence (one solution? or all of them?),
  - (b) optimality (maximization? minimization?).

Of course, not all computing problems fit this framework; but many do, quite closely, and many more do if we relax the interpretations a bit.



# Spanning Trees, I

Review and algorithmic ideas

Also called “minimal connectors”

Given a connected graph with edge weights, find a subgraph that is still connected and has weight as small as possible. (Variants. . .)

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Properties:

1. The answer is always a (free, unordered) tree. **Why?**
2. The edge of least cost, if unique, must belong to the answer.

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2. The edge of least cost, if unique, must belong to the answer.

Algorithmic approaches:

**Kruskal:** keep adding the lowest-cost edge, unless it creates a cycle, in which case it can be discarded.

**Prim:** keep expanding the current tree by the lowest-cost edge that keeps it a tree; if it does not, can be discarded.

# Examples of the Framework, I

Or: Spanning Trees, II

Two examples on spanning trees:

Given a connected graph with edge weights, find a connected subgraph

(a) that connects all the vertices without creating cycles;

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Spanning tree:

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“given a connected graph with weights in the edges...”
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# Examples of the Framework, II

Or: Knapsack, I

Often, there is **more than one** way to set up the scheme.

Three examples on knapsacks:

Given numbers  $V$  and  $W$  and a set of objects, each with a weight and a value, find a subset of these objects

- (a) that reaches total value at least  $V$  but weighs at most  $W$ ;
- (b) that reaches the highest possible value but weighs at most  $W$ ;
- (c) that reaches total value at least  $V$  but weighs as little as possible.



# Examples of the Framework, III

Or: Knapsack, II

## Knapsack:

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“reaches the highest possible value but weighs at most  $W$ ”,  
or:  
“reaches total value at least  $V$  but weighs as little as possible”.

We study optimization cases later, and decisional versions first.

# Knapsack, III

## Decisional version

### Given:

- ▶ objects  $i \in \{0, \dots, N-1\}$
- ▶ with weights  $w[i]$  and values  $v[i]$ ,
- ▶ maximum capacity of knapsack  $W$ ,
- ▶ desired total value  $V$ :

find a set of objects to take for the knapsack:

- ▶ total weight does not exceed the maximum capacity,
- ▶ total value is at least the desired total value.

### Example:

Maximum weight  $W = 26$ , desired value  $V = 45$  with objects of:

Weight:	9	8	12	11	7
Value:	16	15	24	23	13

# Knapsack, IV

Why not, simply, scan the whole powerset? “Brute force” (perebor)

```
def slow_knapsack(objects, W, V):  
    for candidate in powerset(objects):  
        if (totalweight(candidate) <= W  
            and totalvalue(candidate) >= V):  
            return candidate
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You have a choice of options for the powerset iterable:

- ▶ Start by trying your hand without any other inspiration: P18957.
- ▶ Maybe you saw it as a basic recursion example of previous quarter.
- ▶ Recipe in the Python documentation, chapter on itertools, section “itertools recipes” (provides subsets ordered by size).
- ▶ My favorite: a recursive generator (learn on yourself about generators and come up with it, ask me if necessary).

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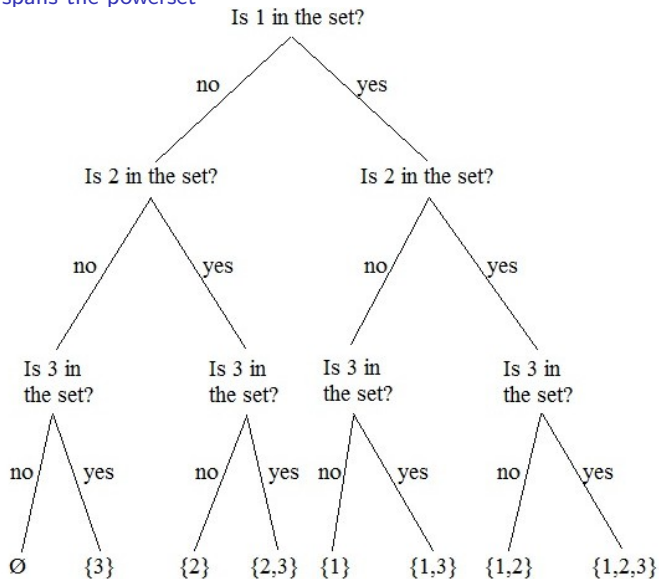
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- ▶ My favorite: a recursive generator (learn on yourself about generators and come up with it, ask me if necessary).
- ▶ **Too slow** for all practical purposes.

# Knapsack, V

Implicit tree that spans the powerset



By: Brian M. Scott at [math.stackexchange.com](https://math.stackexchange.com)

# Knapsack, VI

Tree-based traversal of the powerset, also “brute force”

```
def knapsack(weights, values, current_item,
             max_w, min_v, cand, ...):
    if current_item == -1:
        if ("candidate value" >= min_v and
            "candidate weight" <= max_w): return cand
        else: return list()
    else:
        "current_item >= 0"
        sol = knapsack(weights, values, current_item - 1,
                       max_w, min_v, cand, ...)
        if sol: return sol
    else:
        return knapsack(weights, values, current_item - 1,
                        max_w, min_v,
                        cand + [ current_item ], ...)
```

# Knapsack, VII

Tree-based traversal of the powerset, also “brute force” – extra details

```
def knapsack(weights, values, current_item,
             max_w, min_v, cand, cand_w, cand_v):
    if current_item == -1:
        if cand_v >= min_v and cand_w <= max_w:
            return cand
        else: return list()
    else:
        sol = knapsack(weights, values, current_item - 1,
                       max_w, min_v, cand, cand_w, cand_v)
        if sol: return sol
        else:
            return knapsack( weights, values, current_item - 1,
                             max_w, min_v,
                             cand + [ current_item ],
                             cand_w + weights[current_item],
                             cand_v + values[current_item] )
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# Framework for Algorithmic Schemes, II

We still need a bit more conceptualization

## Additionally:

The solution candidates are structured into

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(the subproblem might be solvable, we must go on) or
  - (c) a “complete” candidate solution  
(that is, a solved subproblem that actually provides a solution to the original instance).

# Examples of the Framework, IV

Or: Spanning Trees, III

Spanning tree (with or without connectivity?)

Subproblem:

- ▶ complete a single spanning tree of the graph given
  - ▶ one partial tree already constructed, or, alternatively,

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  - ▶ one partial tree already constructed, or, alternatively,
  - ▶ a set of partial trees already constructed (spanning forest)...

Sequence of decisions: grow a current tree by one further edge.

- (a) already unacceptable: the new edge creates a cycle;
- (b) complete candidate solution: connects all vertices;
- (c) acceptable but still incomplete: rest of cases.

# Examples of the Framework, V

Or: Knapsack, VIII

## Knapsack:

Objects with weights and values.

Subproblem: given a set of objects already selected, add further objects to it.

# Examples of the Framework, V

Or: Knapsack, VIII

## Knapsack:

Objects with weights and values.

Subproblem: given a set of objects already selected, add further objects to it.

Sequence of decisions: consider one further object; either **pick** it or **discard** it.

- (a) already unacceptable: the new total weight is over  $W$ ;
- (b) complete candidate solution: no further undecided objects remain;
- (c) acceptable but still incomplete: rest of cases.

Often there is **more than one** way to set up the scheme. This is but one.

# Backtracking, I

## Traversal of the implicit tree

### What is it?

Related to tree preorder traversal, except that the tree remains **implicit**.

- ▶ Imagine each subproblem as a **vertex** in a (very large) tree.
- ▶ **Edges** correspond to decisions that change a subproblem into another one.

The main idea is:

If we identify that a subproblem is not feasible, we spare ourselves traversing all the solutions that include attempts to solve that subproblem (**dead ends**).

# Backtracking, II

The optimization case will come later

## Three options:

1. Search-like scheme: stop the exploration if we are satisfied with only one solution.
2. Full traversal: we want all solutions and must complete the traversal.
3. Optimization: want to see all solutions to pick the “best” one according to some criterion.

## Implicit tree:

- ▶ Binary tree in **set-based** backtracking where we construct a set through binary membership decisions.
- ▶ General tree when decisions are not binary (to be studied soon too).



# Knapsack, IX

## Set-based backtracking

**Subproblem:** What do we consider as a subproblem?

Knapsack restricted to the first  $k$  objects.

**Infeasibility:** When do we backtrack from a subproblem?

Insufficient value? Adding objects might solve it.

Excess weight?

Adding objects will **not** make it feasible!

**Alternative:** Work it out “the other way around”!

Start by taking everything,

keep discarding objects until fitting the weight,

declare infeasibility when value drops below threshold.

## Knapsack, X

```
def knapsack(weights, values, current_item, max_w, min_v,
             cand, cand_w, cand_v):
    if current_item == -1:
        if cand_v >= min_v:
            return cand
        else:
            return list()
    else:
        "current_item >= 0"
        sol = knapsack(weights, values, current_item - 1,
                       max_w, min_v, cand, cand_w, cand_v)
        if not sol and weights[current_item] <= max_w:
            sol = knapsack(weights, values, current_item - 1,
                           max_w - weights[current_item], min_v,
                           cand + [ current_item ],
                           cand_w + weights[current_item],
                           cand_v + values[current_item])
    return sol
```

## Knapsack, XI (closer to the tree-based exploration)

```
def knapsack(weights, values, current_item, max_w, min_v,
             cand, cand_w, cand_v):
    if current_item == -1:
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            sol = knapsack(weights, values, current_item - 1,
                           max_w, min_v,
                           cand + [ current_item ],
                           cand_w + weights[current_item],
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    return sol
```

# Knapsack, XII

Avoid making copies! Example on “all solutions”

```
def knapsack(weights, values, current_item, max_w, min_v,
             cand, cand_w, cand_v):
    if current_item == -1:
        if cand_v >= min_v and cand_w <= max_w:
            return [ cand ]
        ...
    else:
        ...
        if weights[current_item] <= max_w:
            cand.append(current_item)
            ... knapsack(weights, values, current_item - 1,
                          max_w, min_v,
                          cand,
                          cand_w + weights[current_item],
                          cand_v + values[current_item])
            ...
    return sol
```

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            ... knapsack(weights, values, current_item - 1,
                          max_w, min_v,
                          cand,
                          cand_w + weights[current_item],
                          cand_v + values[current_item])
            cand.pop() # backtrack!
    return sol
```

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```
def knapsack(weights, values, current_item, max_w, min_v,
             cand, cand_w, cand_v):
    if current_item == -1:
        if cand_v >= min_v and cand_w <= max_w:
            return [ cand.copy() ]
        ...
    else:
        ...
        if weights[current_item] <= max_w:
            cand.append(current_item)
            ... knapsack(weights, values, current_item - 1,
                          max_w, min_v,
                          cand,
                          cand_w + weights[current_item],
                          cand_v + values[current_item])
            cand.pop() # backtrack!
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```

# Knapsack, XIII

## Yet another option

Instead of carrying around the candidates as we proceed down the tree. . .

Can we just obtain the existing solutions below each successor and combine them?

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## Yet another option

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Can we just obtain the existing solutions below each successor and combine them?

**Yes**, of course. The program is even a bit faster but (in my humble opinion) harder to understand.

We will apply that strategy later on today for **optimization**.



# Graph Colorability

Beyond the binary decisions of set-based backtracking

## Vertex coloring:

Given a graph, assign a color to each vertex in such a way that no edge connects two vertices of the same color.

[http://mathworld.wolfram.com/images/eps-gif/  
VertexColoring\\_750.gif](http://mathworld.wolfram.com/images/eps-gif/VertexColoring_750.gif)

## Edge coloring:

Given a graph, assign a color to each edge in such a way that no vertex shows two meeting edges of the same color.

[http://mathworld.wolfram.com/images/eps-gif/  
EdgeColoring\\_850.gif](http://mathworld.wolfram.com/images/eps-gif/EdgeColoring_850.gif)

We focus on **edge coloring** today, see Wikipedia link.

# Example: Edge Colorability, I

The implicit tree: graph with more and more colored edges

Given a graph  $G$  and a natural number  $k$  of different colors, assign colors to the edges so that all colors are different at every vertex.

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To keep the implicit graph a tree, we must be a bit careful.



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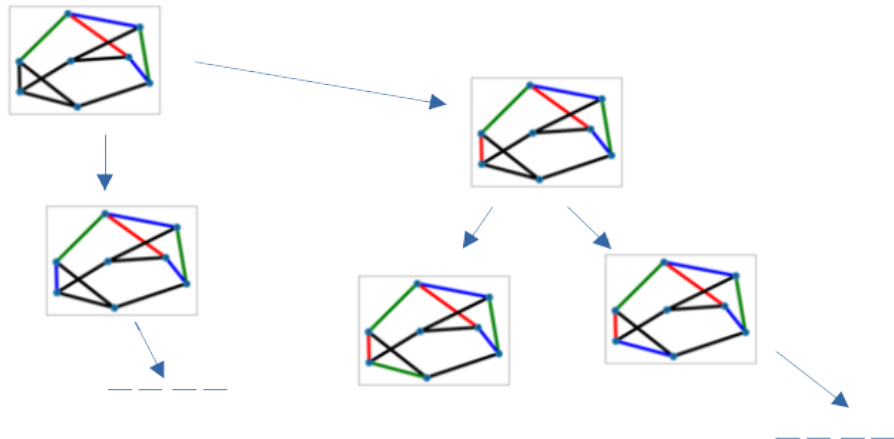
To keep the implicit graph a tree, we must be a bit careful.

Examples and demos:

mostly on 3-regular graphs (all vertices of degree 3) and  $k = 3$ .

# Example: Edge Colorability, II

The implicit tree (a fragment)



# Example: Edge Colorability, III

Finding one solution

Force an order on the edges

and maintain it strictly, so that if a path in the implicit graph colors first edge  $e_1$  and later edge  $e_2$ , then the same happens to all paths.

# Example: Edge Colorability, III

## Finding one solution

### Force an order on the edges

and maintain it strictly, so that if a path in the implicit graph colors first edge  $e_1$  and later edge  $e_2$ , then the same happens to all paths.

Then, the implicit graph is effectively a tree.

### Demo

based on NetworkX and GraphViz:

- ▶ we fix an order of the edges (as given by the NetworkX `graph.edges()` method);
- ▶ we keep a list of available colors at each vertex;
- ▶ we try using in turn each available color for the current edge and launch the recursive call, stop the loop and finish the recursions if successful.

Additional paraphernalia to keep reporting and to draw the graph (e. g. the dict `gd` with the GraphViz layout).

## Example: Edge Colorability, IV

### Finding one solution

```
def edgecolor(g, edgelist):
    if not edgelist: return True
    else:
        u, v = edgelist.pop()
        possib = g.nodes[u]['free'] & g.nodes[v]['free']
        for c in possib:
            g.edges[u, v]['color'] = c
            g.nodes[u]['free'].remove(c)
            g.nodes[v]['free'].remove(c)
            success = edgecolor(g, edgelist)
            if success: return True
            # else, free again the colors, try next possib
            g.edges[u, v]['color'] = noncolor
            g.nodes[u]['free'].add(c)
            g.nodes[v]['free'].add(c)
        edgelist.append((u, v)) # backtrack!
    return False
```

# Example: Edge Colorability, V

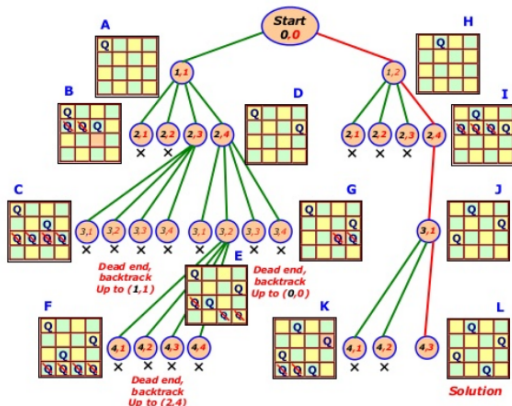
Can we do better?

## Ideas to follow up:

- ▶ Fix the names of the three colors of some particular vertex so as to avoid exploring subtrees that only differ in the names of the colors.
- ▶ Design carefully the edge ordering.
  - ▶ For instance, a depth-first search strategy may be a good idea.
  - ▶ Indeed, this ensures that, at each edge, at least one of the endpoints has already lost at least one color.
- ▶ ...

# Example: N-queens, I

The implicit tree: generated and explored part up to the first solution



Source: <https://www.slideshare.net/praveenkumar33449138/02-problem-solvingsearchcontrol>



## Example: N-queens, II

Finding all solutions

```
def attempt(row, board, size):  
    if row == size:  
        board.draw()  
    else:  
        for column in range(size):  
            if board.free(row, column):  
                board.put_q(row, column)  
                attempt(row + 1, board, size)  
                board.remove_q(row, column)
```

Initial call:

```
board = Board()  
size = int(input("How many queens? "))  
attempt(0, board, size)
```

# Example: N-queens, III

## Finding one solution

```
def attempt(row, board, size):
    if row == size:
        return True
    else:
        for column in range(size):
            if board.free(row, column):
                board.put_q(row, column)
                s = attempt(row + 1, board, size)
                if s:
                    return True
                else:
                    board.remove_q(row, column)
        return False
```

# Example: N-queens, III

## Finding one solution

```
def attempt(row, board, size):  
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        for column in range(size):  
            if board.free(row, column):  
                board.put_q(row, column)  
                s = attempt(row + 1, board, size)  
                if s:  
                    return True  
                else:  
                    board.remove_q(row, column)  
        return False
```

Initial call: declare board, get size, and call thus:

```
if attempt(0, board, size):  
    board.draw()
```

# Example: N-queens, IV

Can we **do better**?

## Ideas to follow up:

- ▶ Find ways to avoid exploring a partial solution that is symmetrical to one already explored and failed.
- ▶ Explore each row in a different order:
  - ▶ for every square in the current row, compute how many squares in subsequent rows would be lost from there,
  - ▶ then explore squares that leave as much freedom as possible before those that are more restrictive (“best-first search”).
- ▶ ...

# Framework for Algorithmic Schemes, III

## Existence versus optimization

### In the case of optimization problems

(either maximization or minimization) we need as well:

an **objective function** to optimize,

- ▶ defined on candidate solutions but
- ▶ in such a way that it naturally extends to local subproblems (sequences of decisions).

Objective function on spanning trees:

- ▶ weight of the current partial tree?
- ▶ best possible weight for a complete spanning tree that extends the given one?

Objective function on graph coloring:

- ▶ Color the edges of the given graph with as few colors as possible.

# Knapsack, XIV

## Towards backtracking for optimization

### Given:

- ▶ objects  $i \in \{0, \dots, N - 1\}$
- ▶ with values  $v[i]$  and weights  $w[i]$ ,
- ▶ maximum capacity of knapsack  $W$ :

report the best set of objects to take for the knapsack:

- ▶ total weight does not exceed the maximum capacity,
- ▶ total value is as large as possible.

# Examples of the Framework, VI

Or: Knapsack, XV

## Alternative:

Reach the lowest possible weight with a value of at least  $V$ .

Objective function:

- ▶ current value?
- ▶ best possible value attainable by expanding the current choice?

# Examples of the Framework, VI

Or: Knapsack, XV

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Reach the lowest possible weight with a value of at least  $V$ .

Objective function:

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Subproblem: given a set of objects not yet discarded, discard further objects from it.

(Complete the scheme on your own.)



# Knapsack, XVI

Scan the whole powerset again?

```
def slow_knapsack(objects, W):  
    mx = 0  
    for candidate in powerset(objects):  
        if (totalweight(candidate) <= W  
            and totalvalue(candidate) > mx):  
            best = candidate  
            mx = totalvalue(best)  
    return best, mx
```

Too slow for all practical purposes.

# Knapsack, XVII

## Backtracking for optimization

```
def best_knapsack(values, weights, itm, limw):
    "best knapsack under limw weight w/ items in range(itm)"
    if itm == 0 or limw == 0:
        "no items or weight available, emptyset only solution"
        return set(), 0
    else:
        "solve first excluding current item, itm-1"
        k0, v0 = best_knapsack(values, weights, itm-1, limw)
        if weights[itm-1] <= limw:
            "current item fits, so solve now including it"
            k1, v1 = best_knapsack(values, weights, itm-1,
                                    limw-weights[itm-1])
            if v0 < v1 + values[itm-1]:
                "second solution is better"
                k1.add(itm-1)
                return k1, v1 + values[itm-1]
        return k0, v0
```

# Knapsack, XVIII

If we want to go beyond, it may be worthwhile to embrace OO

A number of additional ideas can be implemented:

- ▶ Can we report the successive updates to the “best-so-far” solution?
- ▶ Should we explore the items in some specific order? (Careful with the way the recursive calls handle that!)
  - ▶ Weight?
  - ▶ Value?

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  - ▶ Ratio value/weight?
  - ▶ Increasing or decreasing?
- ▶ ...

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- ▶ ...

Adding functionality to the simple scheme is the wrong approach!

- ▶ Code gets complicated and sloppy very soon.
- ▶ At some early point the quantity of rig-like decisions makes the program go wrong with very little control for correcting it.
- ▶ Reach up to **object orientation**.

# Factorial Function Growth, I

Exhaustive search (“try all possible solutions”) is unlikely to be acceptable

When a new (to us) problem comes:

How do we proceed?

1. Formalize it following the combinatorial search scheme.
2. Maybe explore alternative ways to cast the problem into the scheme, until finding some very smart ad-hoc algorithm that works (e.g. so-called “greedy schemes”)...

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or giving up.
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Shall we explore all possibilities?

- ▶ All subsets (the whole powerset). . .  $2^N$  cases.
- ▶ All permutations. . .  $N!$  cases.



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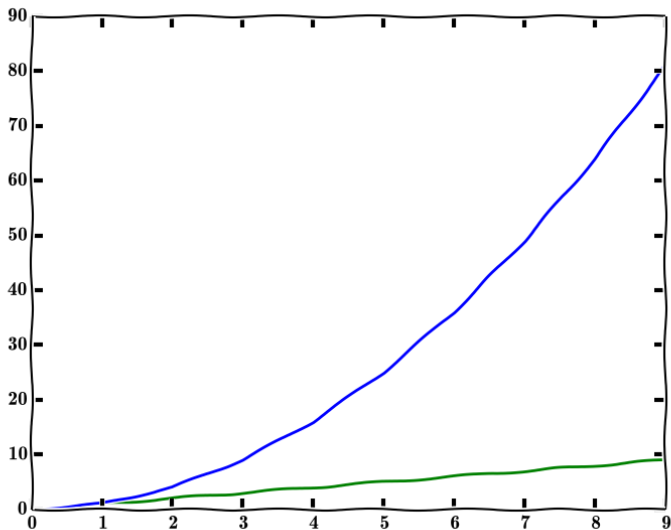
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Risk of **combinatorial explosion**, see Wikipedia link.

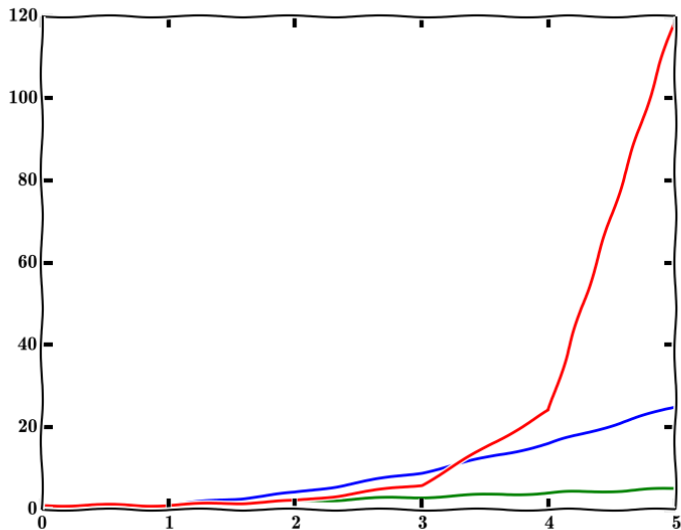
# Factorial Function Growth, II

Thou shalt not take the name of the Exponential in vain



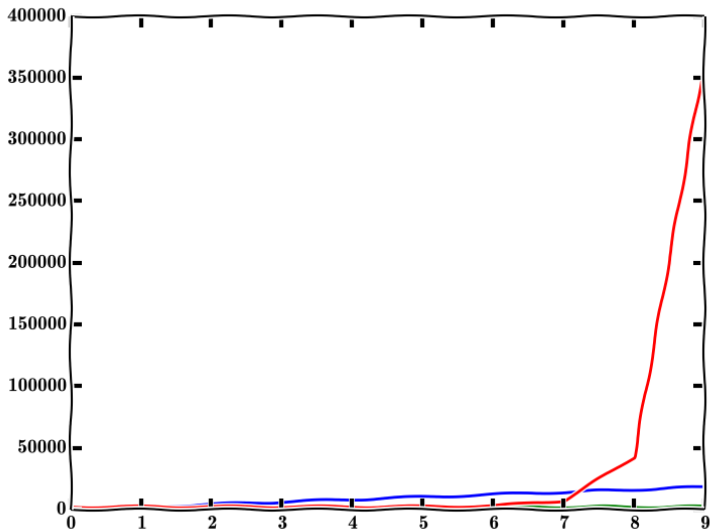
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# Factorial Function Growth, III

$N!$  grows exponentially, Stirling dicit

Suppose:

- ▶ we only need one elementary operation for each of  $N!$  configurations, and
- ▶ we could do 13000 trillion operations per second ( $13 \times 10^{15}$ ).

Then we would spend

for  $N = 12$ : billionths of a second ( $10^{-9}$ );

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for  $N = 18$ : half a second;

for  $N = 21$ : one hour;

for  $N = 24$ : one and a half years;

for  $N = 27$ : over 250 centuries. . .

# Factorial Function Growth, IV

Try all possible solutions **only** if you must — and, then, do it well

Confronted with a case that seems to need exhaustive search  
(Don't forget to ask around whether anybody has proved  
**NP-hardness!**, see Wikipedia link.)

1. Focus on **existence** first, leave optimization for the subsequent stage;
2. throw in a quick-and-dirty, **exponentially slow** but fast-to-program algorithm to make sure that you need to do better, and to get some counts on quantities of different subproblems involved;
3. go for a **backtracking** solution;
4. frequent repeated subproblems?, consider trying a **dynamic programming** approach (maybe after backtracking, or maybe directly head-on).

# Dynamic Programming, I

Recommended reading: [nice](#) account of the origins by Richard Bellman himself

For a given combinatorial search problem, is the following true?

**Bellman's Principle of Optimality:**

the part of the optimal global solution that corresponds to any subproblem is itself a locally optimal solution.

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This condition **does not hold always**.

But... **does it hold often enough!**

Rather good and instructive article on Wikipedia:

[https://en.wikipedia.org/wiki/Dynamic\\_programming](https://en.wikipedia.org/wiki/Dynamic_programming)

# Dynamic Programming, II

Tabulating partial solutions to local subproblems

Organize subproblems and partial solutions into a **table** form  
and devise a rule for **filling in each cell** of the table,  
on the basis of cells that you know you can fill before it.



# Dynamic Programming, II

## Tabulating partial solutions to local subproblems

Organize subproblems and partial solutions into a **table** form and devise a rule for **filling in each cell** of the table, on the basis of cells that you know you can fill before it.

- ▶ Once the table is conceived, be careful in implementing it efficiently.
- ▶ For instance, you may need only one row in order to construct the next, or...
- ▶ Dynamic Programming is particularly efficient when many repeated subproblems keep appearing while solving the original problem.
- ▶ May look like inefficient... until one finds out how many (possibly repeated) subproblems are solved by a backtracking scheme.

“The gold ones are Galleons. Seventeen silver Sickles to a Galleon and twenty-nine Knuts to a Sickle, it's easy enough.”

J. K. Rowling  
*Harry Potter and the Philosopher's Stone*  
(1997)

# Giving change, I

<https://jutge.org/problems/P81009>

Given goal and available coin denominations:

- ▶ goal quantity  $M$  to reach by adding up coins
- ▶ of denominations  $d_1, \dots, d_n$ .

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Related both to Knapsack and to Subset Sum.

- ▶ Similar to Subset Sum more than to Knapsack: the goal is to be reached **exactly**.
- ▶ Difference with Subset Sum: “unboundedly available” coins/objects, we can take several of each, repeated as necessary.

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(Some coin denominations allow for substantially faster solutions.  
Back to that after the midterm.)

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Dynamic Programming: tabulate partial solutions

Entry  $T[i, h]$  of table  $T$  tells how many coins are used to get quantity  $h$  with only the first  $i$  denominations, so that. . .

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The Principle of Optimality holds:

A fragment of an optimal solution is itself an optimal solution.

# Giving change, III

“The details are the jungle in which the devil hides.” [N. Wirth]

- ▶ Do we need an indexing of the denominations?

Consider using only positions 1 on of a list, `denoms`, for  $d_1, \dots, d_n$ , avoiding  $d_0$ .

“Placeholder” value in `denoms[0]`.

- ▶ (We simplify that indexing in a more efficient subsequent version.)
- ▶ Precise meaning of each of the rows?
- ▶  $T[0, h]$ ? Particularly  $T[0, 0]$ ...

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- ▶  $T[0, h]$  for  $h > 0$  must say somehow: “impossible”.  
 $T[0, h] = \text{float}(\text{"inf"})$  — why?

## Giving change, IV

```
def minchange(goal, denoms):  
    dptable = {}  
    for quantity in range(goal + 1):  
        dptable[0, quantity] = float("inf")  
    for coin in range(len(denoms)):  
        dptable[coin, 0] = 0  
    for quantity in range(1, goal + 1):  
        for coin in range(1, len(denoms)):  
            if denoms[coin] <= quantity:  
                dptable[coin, quantity] = min(  
                    dptable[coin - 1, quantity],  
                    1 + dptable[coin, quantity - denoms[coin]])  
            else:  
                dptable[coin, quantity] = dptable[coin - 1, quantity]  
    return (-1 if dptable[len(denoms) - 1, goal] > goal  
            else dptable[len(denoms) - 1, goal])
```

# Dynamic Programming, III

But... we want to know how to achieve the quantity!

In the table of this specific problem we can read whether each denomination was actually employed: keep testing whether

```
dptable[coin, quantity] != dptable[coin - 1, quantity]
```

and keep updating downwards quantity accordingly and collecting the used coins.



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**In general:** The basic Dynamic Programming scheme leads often only to the **cost** of the best solution, and needs a bit of extra work to find out the **best solution** itself.

Namely: at the time of updating a cell on the main table, record in a **secondary table** the key information that motivated the update.

## Giving change, V

```
def minchange(goal, denoms):  
    dptable = {}  
    best = {}  
    ...  
    if (denoms[coin] <= quantity and  
        1 + dptable[coin, quantity - denoms[coin]] <  
            dptable[coin - 1, quantity]):  
        dptable[coin, quantity] = (1 +  
                                    dptable[coin, quantity - denoms[coin]])  
        best[quantity] = denoms[coin]  
    ...
```

## Giving change, V

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def minchange(goal, denoms):
    dptable = {}
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            dptable[coin - 1, quantity]):
        dptable[coin, quantity] = (1 +
                                    dptable[coin, quantity - denoms[coin]])
        best[quantity] = denoms[coin]
    ...

def trace(best, goal):
    coins = []
    while goal:
        use = best[goal]
        coins.append(use)
        goal -= use
    return coins
```

# Giving change, VI

Do we need the whole table?

Once we have that solution in place:

- ▶ Can we simplify the data structures?
- ▶ Often, simplifying the data structures helps simplifying the code.

We maintain only one row of the table and initialize it as if with a coin of “denomination zero”.

## Giving change, VII

```
dptable = [ float("inf") ] * (goal + 1)
dptable[0] = 0
for quant in range(1, goal + 1):
    "dptable[quant]: how many coins needed to add up to it"
    for coin in denoms:
        "try using it - actual value, not just an index"
        if coin <= quant:
            dptable[quant] = min(
                dptable[quant],
                1 + dptable[quant - coin])
```

At the end, `dptable[goal] > goal` means again that it is not possible.

# Shortest Paths, I

Are there costs? Can they be negative?

## Shortest path problems in graphs

They are extremely common: many practical problems boil down to finding shortest paths.

We consider first the “single-source” case: find paths that start at a given vertex.

- ▶ Do edges have various associated costs?
- ▶ Are there edges with a negative cost?
- ▶ If yes... is there a cycle of total negative weight?
- ▶ Then the problem is pretty complicated and only recently solved.

# Shortest Paths, II

## Algorithmic options

- ▶ When the cost of traversing edges is constant:

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sophistications like A\* and beyond (more on this after the  
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- ▶ Observe that this only makes sense for **directed** graphs.

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- ▶ And observe that... a fragment of a shortest path **is** a  
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there is no cycle of total negative weight.
- ▶ Observe that this only makes sense for **directed** graphs.
- ▶ And observe that... a fragment of a shortest path **is** a  
shortest path!,
- ▶ **even** in the presence of negative weights!

# Shortest Paths, III

## Dynamic Programming to the rescue

Let  $u$  be the fixed source vertex: tabulate the distance to vertex  $v$  in a maximum of  $i$  steps.

The solution is when  $i$  is at most 1 less than the number of vertices.

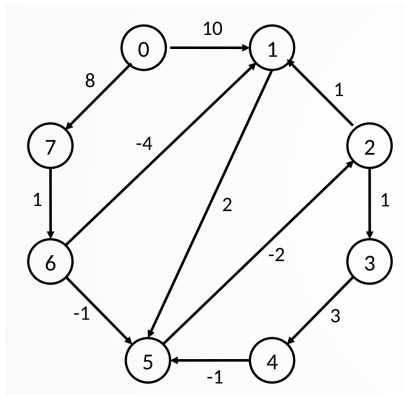


Image source: Jordi Delgado, UPC

# Shortest Paths, IV

## Identifying a notion of “subproblem”

Graph of  $n$  vertices; source is vertex  $s$ ;  $\text{dist}[v, i]$  is the distance from  $s$  to  $v$  in at most  $i$  steps.

If  $\text{dist}[v, i]$  is optimal and the last edge is  $(u, v)$ , then  $\text{dist}[u, i-1]$  must be optimal.



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```
for all  $v$  in  $V$ :
```

```
     $\text{dist}[v, 0] = \text{'infinity'}$  # discussed in a minute
```

```
     $\text{dist}[s, 0] = 0$ 
```

```
for  $i$  in range(1,  $n$ ):
```

```
    for all the edges  $(u, v)$ :
```

```
         $\text{dist}[v, i] = \min($ 
```

```
             $\text{dist}[v, i-1],$ 
```

```
             $\text{dist}[u, i-1] + \text{cost}[u, v] )$ 
```

# Shortest Paths, V

## Bellman-Ford algorithm

```
for all v in V:
    dist[v] = float('inf') # or any other 'big' value

dist[s] = 0

for i in range(1, n):
    for all the edges (u, v):
        if dist[v] > dist[u] + cost[u,v]:
            dist[v] = dist[u] + cost[u, v]
```

# Shortest Paths, VI

How to reconstruct the shortest paths?

```
for all v in V:
    dist[v] = float('inf') # or any other 'big' value
    prev[v] = None

dist[s] = 0

for i in range(1, n):
    for all the edges (u, v):
        if dist[v] > dist[u] + cost[u,v]:
            dist[v] = dist[u] + cost[u, v]
            prev[v] = u
```

# Shortest Paths, VII

Key step: invent the right notion of subproblem

## All-pairs shortest paths

Given a directed or undirected graph, find the shortest distances between all pairs of vertices:

the Floyd(-Warshall(-Roy)) algorithm.

## Dynamic Programming strategy:

- ▶ Subproblems defined by: up to which vertices are allowed as intermediate steps?
- ▶ Initiation means using no vertices as intermediate steps: only direct, single-edge reachability.
- ▶ Assuming tabulated all shortest distances that only use intermediate vertices less than  $k$ , how do we find out shortest distances when vertex  $k$  is allowed as well?

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$$\text{dist}(i, j, k) = \min( \text{dist}(i, j, k-1), \\ \text{dist}(i, k, k-1) + \text{dist}(k, j, k-1) )$$

# Knapsack, XIX

Just a couple of words

How do we approach Knapsack by Dynamic Programming?

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...provided that...

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Complete it by thinking carefully about the boundary conditions.

# Knapsack, XX

## Implementation options

- ▶ Indexing: start at zero? reserve zero for bookkeeping? ...
- ▶ “Spelled out” 2-dimensional table?
  - ▶ Easier to connect visually the code with the Bellman equation.
  - ▶ Simpler reconstruction of the solution:
    - ▶ 2-dimensional table storing reasons for changes;
    - ▶ simple alternative (shared by some similar problems):  
`test dptab[obj, weight] != dptab[obj - 1, weight]` to  
see whether obj is used for weight.

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`test dptab[obj, weight] != dptab[obj - 1, weight]` to see whether obj is used for weight.
- ▶ Flatten it instead into a 1-dimensional list?
  - ▶ More efficient in memory and (slightly) in time.
  - ▶ Crisper code, less error-prone.
  - ▶ Still two dimensions in the secondary table.

# Supersequences, I

Connection to Bioinformatics not that far away

Given two strings, find (one of) the shortest string(s) that is a supersequence of both.

(Invent your examples with the letters A, T, G, C.)

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Again: we start by just computing how long it is, then add later code to trace an actual solution.

If  $x$  is one shortest common supersequence of  $s$  and  $t$ , what can we find out about it?



# Supersequences, II

## Some considerations

1. Case of empty input sequences?

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3. Case that the initial letters of the input sequences are different?
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3. Case that the initial letters of the input sequences are different?
  - ▶ Outcome must start with one of them.
  - ▶ Rest of result is . . . a subproblem with one string kept and the other **shorter**.

# Supersequences, III

How do we set up our table

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**Careful!** This time, entries in the table depend on other entries with **larger** indices!

# Supersequences, IV

Hint at code

```
initialize
for i in reversed(range(len(s))):
    for j in reversed(range(len(t))):
        if s[i] == t[j]:
            S[i, j] = 1 + S[i+1, j+1]
        else:
            S[i, j] = 1 + min(S[i+1, j], S[i, j+1])
return S[0,0]
```

# Supersequences, V

## Tracing back the solution

Usual method: secondary table that says, for each  $i$  and  $j$ , what letter do we take for the result.

If  $s[i] == t[j]$ , the same letter.

If  $s[i] != t[j]$ , implement an inequality test instead of the `min` operation and store the letter that corresponds to the better value.

# K-Means: Goal

Minimize the squared error

## Geometry (working hypothesis):

Euclidean distance on the reals.

- ▶ Data:  $n$  real vectors  $x_i$ , positive integer  $k$ ;
- ▶ want: to split them into  $k$  clusters  $C_j$ ;
- ▶ we will pick a real vector  $c_j$  representing each cluster  $C_j$  (its centroid);
- ▶ we want to minimize the average squared error:

$$\frac{1}{n} \sum_j \sum_{x_i \in C_j} d(x_i, c_j)^2$$

Note:

We do **not** require the  $c_j$  to be among the  $x_i$ .

# K-Means: Goal

Minimize the squared error

## Geometry (working hypothesis):

Euclidean distance on the reals.

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Note:

We do **not** require the  $c_j$  to be among the  $x_i$ .

**Bad news:** Utterly infeasible at dimension 2 and beyond;  
complexity theorists say: *NP-hard*.

# K-Means: Partial Approach

Let's think a bit more about it

If heavens would give us the centroids:

Then, constructing the clusters is **easy**: each point to its closest centroid, as otherwise the error increases.

# K-Means: Partial Approach

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If heavens would give us the clusters:

Then, finding the centroids is **easy**: minimize  $\sum_{x_i \in C} d(x_i, c)^2$ , by forcing the derivative to zero; and that tells us that each centroid must be set at the mass center of its cluster, as otherwise the error increases.



# K-Means: HowTo

## Stage-wise approximation

### We alternate

among the two things we know how to do, starting from  $k$  initial centroid candidates:

- ▶ recompute the **clusters**,
- ▶ recompute the **centroids**,
- ▶ repeat.

**Often advisable:** try several runs!

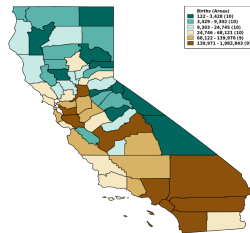
# Unsupervised Discretization

Or: one-dimensional clustering

Given list of floats, organize them into just a few “bins” (or “buckets”, or “clusters”...)

Separate case of “supervised discretization”, not covered here.

Parallel research in so-called choropleth maps, a branch of Cartography, where the solution we describe here goes by the name of Jenks’ natural breaks.



(Source: Expert Health Data Programming, Inc (EHDP): Vitalnet)

# One-Dimensional, Global-Optimum K-Means, I

Clustering floats with DP: the Wang and Song strategy, a.k.a. Jenks' Natural Breaks

**Input:** desired number of clusters  $k$ , and  $n \geq k$  floats,  $x_1$  to  $x_n$ , assumed given in increasing order (otherwise, do a sort first).

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**Tabulate:**  $C[i, m]$ , cost of a clustering of  $x_1$  to  $x_i$  into  $m$  clusters, for  $m \leq k$  and  $m \leq i$ ; solution given by  $C[n, k]$ .

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**Initialization:**  $C[i, m] = 0$  if  $m = 0$ .

Relate to “one cluster less” by identifying  $x_j$ , the smallest point in the last ( $m$ -th) cluster.

# One-dimensional, Global-Optimum K-Means, II

Demo available

A visual demo of the process for each new point considered has been set up at:

<https://www.cs.upc.edu/~balqui/demoWSJ/>

Alpha stage!

- ▶ aesthetics fully postponed to later versions,
- ▶ usability at minimal levels...

Needs:

- ▶ the number of clusters,
- ▶ the points handled so far up to one specific pass,
- ▶ and the newcomer point,

Then, shows the computations made in order to account for the new point.

# One-dimensional, Global-Optimum K-Means, III

Difference between  $m$  clusters and  $m - 1$  clusters

$$C[i, m] = \min_{m \leq j \leq i} (C[j - 1, m - 1] + \sum_{j \leq \ell \leq i} d(x_\ell, c_{j,i})^2)$$

where the

$$c_{j,i} = \frac{1}{i-j+1} \sum_{j \leq \ell \leq i} x_\ell$$

are the corresponding candidates to the role of centroid of the  $m$ -th cluster.



# One-dimensional, Global-Optimum K-Means, IV

We can do it faster

Strategy leads to an  $O(n^3)$  algorithm.

**Acceleration:** don't compute every  $c_{j,i}$  individually but, instead, update  $c_{j,i-1}$  to find it.

This spares a linear computation and reduces the cost to  $O(n^2)$ .

(Jenks' alternative: in Cartography you only need the cutpoints, not the centroids; work out an alternative formula by replacing the centroid by its definition in the minimization scheme.)

# Greedy Algorithms in Graphs, I

## Minimal spanning trees

Consider the edge of minimal weight: if unique, it must belong to every minimal spanning tree.

# Greedy Algorithms in Graphs, I

## Minimal spanning trees

Consider the edge of minimal weight: if unique, it must belong to every minimal spanning tree.

- ▶ Similarly, midway through, for the remaining edge of minimal weight, provided it does not create a cycle.
- ▶ What if there are several edges left with minimal weight?
- ▶ Any one of them is a valid choice.

## Kruskal Algorithm:

Check out every edge in order of growing weight:

- ▶ Creates a cycle? Discard it.
- ▶ Otherwise, add it to a spanning forest.
- ▶ How to organize the edges in the appropriate order?
- ▶ How do we find out fast whether the edge creates a cycle?

Applets by David Galles

# Giving change, VIII

## The greedy scheme

### Greedy approach:

- ▶ Keep adding coins of as large a denomination as feasible.
- ▶ For some denomination sets, this greedy approach works: **canonical coin systems**, like the typical cases of many countries:
  - ▶ 1, 2, 5, 10, 20, 50;
  - ▶ 1, 5, 10, 25, 50, 100, 200;
  - ▶ ...
- ▶ For others, it does not; for instance:  
get 15 units out of 1-unit, 5-units, and 8-units elements!

[https://en.wikipedia.org/wiki/Change-making\\_problem](https://en.wikipedia.org/wiki/Change-making_problem).

# The Greedy Algorithmic Schema

What is common between that solution to giving change and Kruskal?

## Characteristics:

- ▶ Notion of “current optimality”;
- ▶ next choice is always the one that “looks best” given the current situation:
  - every locally optimal choice is globally optimal  
(greedy-choice property);
- ▶ need to argue separately that it is a good idea to go for the best choice, given that the full picture is unknown.

[https://en.wikipedia.org/wiki/Greedy\\_algorithm](https://en.wikipedia.org/wiki/Greedy_algorithm).

# Greedy Algorithms in Graphs, II

## Further minimal spanning trees

Suppose instead that what we have is a partial spanning tree (connects a subgraph).

We must connect it to the rest: can we do it using an edge of nonminimal weight?

### Prim Algorithm:

As long as we don't yet connect the whole graph,

- ▶ consider the vertices that are only one edge away from the partial tree,
- ▶ add to the partial tree (any of) the corresponding edge(s) of minimum weight.

# Greedy Algorithms in Graphs, III

## Single-source shortest paths

Assumption: no negative weights.

The single-source shortest paths form a spanning tree, but it may not be minimal.

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## Single-source shortest paths

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### Dijkstra Algorithm:

As long as we don't yet connect the whole graph,

- ▶ consider the vertices that are only one edge away from the partial tree,
- ▶ add to the partial tree (any of) the one(s) that is (are) closest to the source.



# Greedy Knapsack

With extra uses

What does it mean to “look best” for the next decision?

- ▶ Two options to consider:
  - ▶ with **divisible** objects?
  - ▶ with **indivisible** objects?
- ▶ If we work with indivisible objects, we may get from the greedy solution a too optimistic value.
- ▶ Can be used to prune subtrees of a backtracking:
  - ▶ Solve the current subproblem with greedy.
  - ▶ Compare the value with the best so far.
  - ▶ If lower, backtrack: no better solution possible from there.

# A Comparison

Two subtly different properties might look alike

- ▶ The **greedy-choice property**:  
every locally optimal choice is globally optimal.
- ▶ The **principle of optimality**:  
the part of the optimal global solution that corresponds to any subproblem is itself a locally optimal solution.

# Complexity of Some Graph Algorithms

Some can be accelerated with smart data structures

On graphs of  $n$  vertices and  $m$  edges (note that  $m \leq n^2$ ).

- ▶ **Minimal Spanning trees** via Prim or Kruskal:  $\Theta(m \log m)$ ;  
Prim can be refined further with very sophisticated data structures.
- ▶ **Shortest Paths:**
  - ▶ Via Dijkstra, single source, requires positive weights:  $\Theta(\max(m, n) \log n)$ .
  - ▶ Via Bellman-Ford, single source, arbitrary weights:  $\Theta(m \times n)$ .
  - ▶ Via Floyd, all pairs:  $\Theta(n^3)$ .

# Beyond Basic Algorithmics

Pending: to return to DFS and BFS, after a bit of data structures

- ▶ Best-first search?  
(That is,  $A^*$  and cousins like Iterative Deepening, essentially, sophistications on top of Dijkstra, [https://en.wikipedia.org/wiki/Best-first\\_search](https://en.wikipedia.org/wiki/Best-first_search).)
- ▶ Branch-and-bound?
- ▶ Extra sophistications? (branch-and-cut,  $AO^*$ , alpha-beta pruning. . . )

All the time, paying attention to learn more about algorithmics and checking whether they can be put to work on your specific problem (greedy schemes, divide-and-conquer, linear programming, quadratic/semidefinite programming. . . )

# Index

Combinatorial Search

Data Structures

- Linear Data Structures

- Search Trees

- Hashing

Dynamic Memory

# Linear Data Structures

Conceive them in a 1D arrangement

## Balance:

- ▶ **Many operations available**: high usefulness and flexibility.
- ▶ **Few operations available**: can concentrate on offering a very efficient implementation for them.
  - ▶ Stacks: **LIFO** (Last In, First Out) principle, both efficient growth (push) and efficient consultation (pop) at one end.
  - ▶ Queues: **FIFO** (First in, First Out) principle, efficient growth at one end and efficient consultation at the other.
  - ▶ Deques, “double-ended queues”: efficient access at both ends both for growth and consultation.

Generic, **very ambiguous** term: “lists”.

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Generic, **very ambiguous** term: “lists”.

For instance: Python lists “are **not** lists” but so-called flexible arrays — more about this later on.

Applets by David Galles

# The Deque

A curious balance between queues, stacks, and lists

Pronounced as “*deck*”.

A double-ended queue

Can operate as a stack or as a queue at both sides of the sequence. . .



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- ▶ For contrast: Python lists offer constant time `append` and default-argument `pop`: very good as stacks.
- ▶ But: both `lst.pop(0)` and `lst[1:]` take linear time, as does adding elements at the “low indices” end.

In fact, due to internal memory reallocations, even *append* on large lists might take long sometimes — the constant-time `append` is only in the “amortized” sense; but slowness cases happen hardly ever enough.

# Python Lists

Construction and destruction: memory usage and time

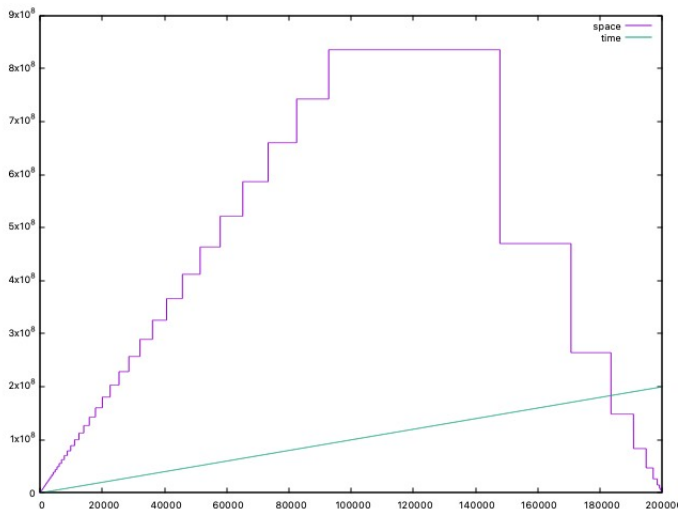


Image source: Jordi Petit, UPC

# Binary Search Trees, I

## The treesort tool

BSTs are ordered in **inorder**.

Representing a set with a **BST**: at each node,

- ▶ items in the left subtree are smaller than the item at the root,
- ▶ items in the right subtree are larger than the item at the root;
- ▶ if repeated items are authorized (**bags** instead of sets), one must choose exactly one of
  - ▶ “smaller than or equal to” for the left subtree or
  - ▶ “larger than or equal to” for the right subtree

and **always** apply the same choice.

Applets by David Galles

# Balanced Trees

## Two very relevant options

Search and insertion complexities in BSTs are linear in the height of the tree.

- ▶ Degenerate cases of low branching factor lead to slow searches,
- ▶ it would be best to keep some balance:
  - ▶ AVL trees are binary trees that keep a height balance: the height of siblings never differs by more than one.
  - ▶ This suffices to guarantee logarithmic time search.
  - ▶ B trees and B+ trees are multiway trees (that is, many subtrees per root, very appropriate for disk-based memory) that keep a strict height balance: all leaves at the same depth.



# Intuitions About Balanced Trees

With the help of visualizations of the algorithms

How do they work?

- ▶ AVL trees keep a height balance by means of **rotations**.
- ▶ B-trees and B+ trees instead keep balance by allowing a varying number of data items in each node.
  - ▶ The most elementary case of B-trees is 2-3-trees;
  - ▶ general B-trees are not common, but the B+ tree variant is heavily used by many DBMS's for index creation.

# Hashing

With a couple of Python-based checks

To “hash”:

To obtain a relatively short integer out of the bits that configure the internal representation of an object.

Often,

1. the bits are cut into chunks of a fixed size,
2. the chunks are interpreted as integers,
3. and some arithmetic is applied to combine them all into a single final number.

In Python: “hashable” objects already furnish their own “hash” function. Mutable types are **not** hashable.

# Hashing At Work

For sets, dictionaries, maps, or a database index

Useful for implementing sets and partial functions.

- ▶ Sets in Python apply hash to their elements so as to check for their existence in constant time.
- ▶ Partial functions can be implemented using hash on their domains:
  - ▶ **dictionaries** in Python,
  - ▶ **maps** in C++.

`https://en.wikipedia.org/wiki/File:  
Hash\_table\_4\_1\_1\_0\_0\_1\_0\_LL.svg`

# Collisions

## Lack of injectivity

Collisions appear when two or more entries (elements of a set, keys of a map/dictionary) happen to give rise to the **same** hash value.

## Handling collisions:

Several possibilities.

- ▶ Open addressing: in case of collision, a second hash function is applied, then a third...  
Naïve schemes don't work too well; somewhat sophisticated ones are necessary.
- ▶ **Linked hashing**: each hash value is associated to the **list** of values leading to that hash that appeared so far (the **bucket**).

Visualization is again very helpful.

# Hashing Variants

Many additional related ideas

If the whole set of potential values is known in advance, it might be possible to create **perfect hashing** without collisions, but this is uncommon in practice.

External memory (=disk) variants require some specific considerations.

Do we want similar keys to hash to similar values? Both answers are possible (“locality-sensitive hashing”).

Different from, but closely related to: checksums, fingerprints... (see [https://en.wikipedia.org/wiki/Hash\\_function](https://en.wikipedia.org/wiki/Hash_function)).

# Warning

## On homonyms

Hitting with the right meaning of a word requires to take into account the context.

Example: **object**.

Example: **key**.

The most prominent case in our course: **heap**.

# Index

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# Dynamic Memory

## Internal memory handling

The main (**core**) memory of the computer consists of many “cells” called **words**:

- ▶ each able to contain a fixed number of bits  
(always 64 in modern general-purpose computers), and
- ▶ each being identifiable through its **address**.

Dynamic memory means giving our programs the capacity of employing **explicitly**, somehow, the addresses of the words that store the program's internal values, or similar ways of retrieving them.

We explore a bit on Python to see the addresses in action and learn why we used `is` to compare with `None`, `True`, or `False`.



# Heap and Stack

## Two ways of handling internal memory

The core memory of each computer consists of words.  
In most current machines each word stores 64 bits.  
Each word has its corresponding **address** that identifies it.

**All are alike.**

But it is convenient to handle them in two different ways, as if two regions were different:

- ▶ The **stack** and
- ▶ the **heap**.

# The Stack

For successive function calls and local information

A good portion of the information necessary to run a program is quite **well-structured**:

- ▶ Program counter,
- ▶ pending, incomplete function calls,
- ▶ return points for each incomplete function call,
- ▶ local variables within each of them. . .

Well-structured in the sense that only the **current** one is going through modifications at a particular moment, and the others wait in a well-defined line.

[https://en.wikipedia.org/wiki/Call\\_stack](https://en.wikipedia.org/wiki/Call_stack)

(Give now meaning to the expression **stack overflow**!)

# The Heap

## Memory allocated on demand

In a different region of the memory, that will be maintained **separate** from the stack, the system marks chunks of memory to provide to the programs for their memory requests.

It is **necessary** to:

- ▶ keep track of the size of each chunk,
- ▶ keep track of the chunks given to the programs to ensure that no conflict happens,
- ▶ decide what chunk to provide to each request coming in, and
- ▶ every now and then, it would be nice if a “garbage collector” would run around and recover chunks not used anymore (bytecode-based languages like Java and Python can –and do– have it but native-code-targeted compilers like C and C++ do not).

# Pointers, I

In C++

For each type  $T$  you can come up with,  
there is the type **pointer to  $T$** , denoted  $T^*$ .

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But, from the program, you don't get to see them as such: you must obey the rules of the type.

Of course, all operations on type  $T$  are available on **the thing pointed to by** a pointer to  $T$ ...

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# Pointers, II

## Pointer and reference syntax in C++

For a type `T`, and assuming that value `v` is of type `T`:

`T* p` declares variable `p` to be of type “pointer to `T`”  
(often written `T *p` as if you were declaring `*p` to be  
of type `T` — in fact, to declare two of them one  
writes: `T *p, *q`),

`*p` is something of type `T` referenced by (or: “pointed to  
by”) `p`,

`&v` is of type `T*`, namely, the actual way to reference  
specifically `v`.

Thus, we can create several “names” (**aliases**) for the same value!

- ▶ That is, several ways to reference the same value.
- ▶ Very powerful but **very risky**!
- ▶ May create “nameless” values, and they may become inaccessible if we lose all references.

# Example with Variations

Just the key fragment

Particularly important: the assignments to `p` and to `*p`!

```
int x;  
int* p;  
p = &x;  
x = 5;  
cout << *p << endl;    // writes 5  
*p = 3;  
cout << x << endl;     // writes 3
```



# Wrong Pointer Usages

Run variations on the example

The “**Segmentation fault** (core dumped)” message – popularly transformed into the infinitive “to segfault”:

what is `*p` when `p == nullptr`?

# Wrong Pointer Usages

Run variations on the example

The “**Segmentation fault** (core dumped)” message – popularly transformed into the infinitive “to segfault”:

what is `*p` when `p == nullptr`?

Still we get a warning that something was wrong! Not always the case:

what is `*p` when `p` has just been declared?

If you forget to initialize a pointer, you may run into trouble!

**Suggestion:** Ask the compiler for help, and compile always with `-Wall`.

Learn more:

[https://en.wikipedia.org/wiki/Segmentation\\_fault](https://en.wikipedia.org/wiki/Segmentation_fault)

# Pointer to struct

A common shorthand in the syntax

We need to name the type in order to mention it at the `new` call:

```
typedef struct {  
    int code;  
    string name;  
} st;  
st *p = new st;
```

Then we have **two options**:

```
(*p).code = 9;  
(*p).name = "aeiou";  
cout << (*p).code << endl;
```

Or, **much** more common for better readability:

```
p->code = 9;  
p->name = "aeiou";  
cout << p->code << endl;
```

# Pointers, III

## What can be a pointer?

If `p` is a pointer to `T`, then it is either:

- ▶ a **reference** (most likely a memory address, but this will be irrelevant within our course) to “the thing pointed to by `p`”, which is of type `T` of course, or
- ▶ the special value `nullptr`, or
- ▶ garbage, and then it may become quite dangerous.

It can be dangerous even when it is a reference to some other variable, because it could be info that should not be accessible at that point.

# Pointer Assignment

The 3 possible things to assign to a pointer

The options are:

- ▶ A reference borrowed from some other variable,
- ▶ some free memory space in adequate quantity: `new T`, or
- ▶ `nullptr`:

```
int x = 5;
int *p, *q, *r;
p = &x;
x = 5;
q = nullptr;
q = p;
r = new int;
*r = 85;
cout << r << " " << *r << endl;
```

# Handling Memory with `new`

Utmost care to be exercised

If we require computer memory with `p = new T`, the memory area where the `T` value resides does **not** have a “proper” name: only the indirect name `*p`.

If `p` is modified, and unless it has been copied to other pointers, that memory area becomes **inaccessible** and risks getting unusable by any program (**memory leak**).

# Returning Allocated Memory

Every `new` must be matched by a `delete`

In order to avoid memory leaks, make sure to **return** all memory space requested by `new` back to the operating system when it becomes unnecessary, with the operation `delete`:

```
T* p = new T;
```

```
[...]
```

```
delete p;
```

# Linked Lists: Simplest Form

Usually we don't program them ourselves

In a sense, we see here a “recursive type”:

```
struct Node {  
    int data;  
    Node *next;  
};
```

Then the list is a Node\*.

The empty list is a nullptr Node\* pointer.

(Double links sometimes necessary: forward and backward.)



# Traversing Simple Linked Lists

Unsophisticate programming as introductory examples

```
struct Node {  
    int data;  
    Node *next;  
};
```

```
int traverse_and_sum(Node *head) {  
    if (head == nullptr) return 0;  
    else return head->data + traverse_and_sum(head->next);  
}
```

# Binary Trees: Simplest Form

The standard library does not offer trees

A more sophisticate recursive type.

```
struct Node {  
    int data;  
    Node *lft, *rft;  
};
```

The empty tree is a nullptr Node\* pointer.

# Binary Trees: Simplest Form

The standard library does not offer trees

A more sophisticate recursive type.

```
struct Node {  
    int data;  
    Node *l1st, *r1st;  
};
```

The empty tree is a nullptr Node\* pointer.

```
void inorder_traversal(Node *t) {  
    if (t != nullptr) {  
        inorder_traversal(t->l1st);  
        cout << t->data << endl;  
        // or s += t->data, or whatever we use the data for  
        inorder_traversal(t->r1st);  
    }  
}
```

# Further Reading on Data Structures

## C++ specific:

1. Operations on pointer-based lists:
  - ▶ singly-linked,
  - ▶ doubly-linked where each node has two pointers: to the next node and to the previous one.
2. **The STL** (Standard Template Library).
3. Handling various forms of trees (**not** in the STL!)

## General concepts:

- ▶ Tries,
- ▶ Fibonacci heaps,
- ▶ Additional algorithms:
  - ▶ Radix sort,
  - ▶ Topological sort of acyclic graphs.
  - ▶ Maximum flow problems and algorithms in graphs.