Day 4 - Optimization in real life

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Outline

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6 rules of optimization code

1. The code is structured as depicted on the right
2. Every index set is its own object
3. Variables are written as dictionaries with indices as keys and variable objects as values.
4. Each constraint and callback is a separate functions
5. All the individual components as well as the entire optimization problem have to be unit tested.

Tools and techniques for optimization code

Model document: A document that details how the model looks like. I like to use LaTeX, since it is the cleanest and most flexible.

Version control: A code repository that you `commit` your incremental changes to the code to. I like to use git and github.com

Continuous integration: A setup such that every time you commit your code, all the unit tests are run. It shows you as soon as things are broken.

Test-driven development: A strategy where you write the unit tests *first*, and then the method that satisfies it.

Work flow for optimization problems

1. Identify what you are trying to solve
2. Formulate a model
3. Implement the model, including unit tests
4. Test whether the problem satisfies the needs. If yes, done. If no, return to Step 2.

Outline

1. Structuring optimization code
   - The 6 rules of writing beautiful optimization code

Performance tuning

Premature optimization is the root of all evil. (Donald Knuth)

- Optimization is a computationally very heavy operation.
- So the most frequent question for optimization problems, "how fast can you solve it?", is the wrong question. The right question is: "how fast do you need it to be solved?".
- We have different leavers we can pull, depending on the specific problem at hand.

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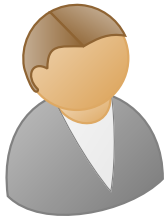
How does it actually work?



Andrew

Result visualization

I need an Excel spreadsheet that uses the result to predict our overall CAPEX. Can you do that?

Anne

Data collection

The data is available on this website. Can't we use that directly?

James

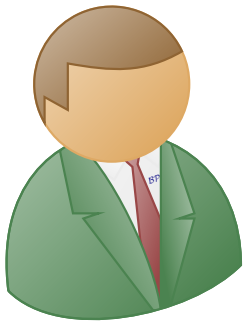
Performance

Currently, the program needs 2 hours to run! We need it in 15 minutes tops! What can we do?

Where does optimization fit in your world?

Outline

How to solve a performance problem



James

Engineer

Currently, the program needs 2 hours to run! We need it in 15 minutes tops! What can we do?

Outline

1. Structuring optimization code
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What does it take to build something useful?

There are mainly four main components to this:

Solution design: Where does the optimization problem fit?

Process design: How do you arrive at the model/optimization strategy you are going to use?

Software development: How am I going to make the computer do what I want?

The human factor: How do people impact the tool?

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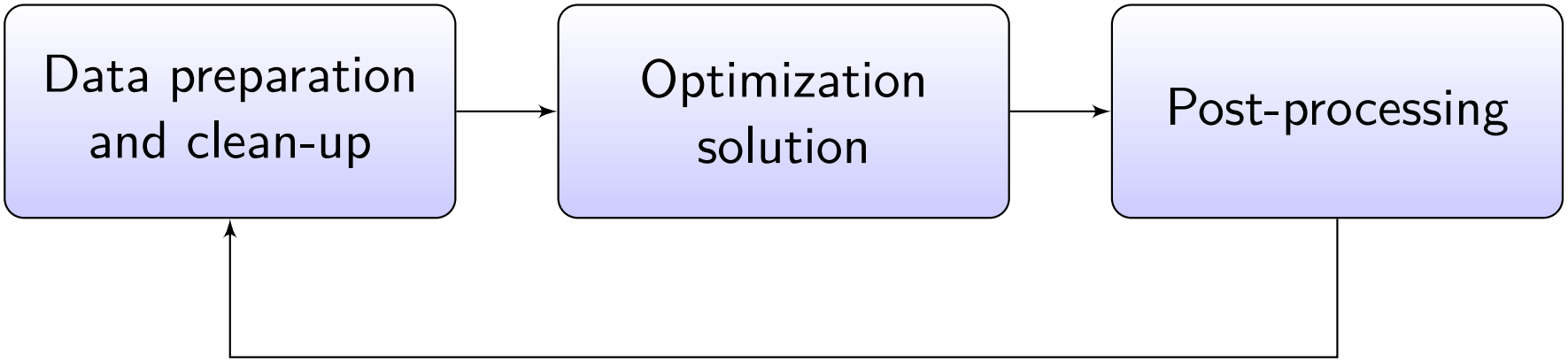
Where does optimization fit?



- Typically, an optimization solution lives in a broader sea of applications.
- The arrows in the picture above may represent APIs (Application Programming Interfaces), i.e. ways to communicate with other programs and programming languages.
- Each box in the picture above typically has a front-end/user interface and a back-end, where the actual work happens.
- As a developer/data scientist, you will have to work with all three of these boxes regularly.

4 rules for data preparation and clean-up

Rule 1: Test

When importing data, it is insanely easy to make mistakes (e.g. units and rounding errors). Always **test** that your data import is correct.

Rule 2: Document data clean-up

Your actual data is most likely going to be messy, i.e. it needs clean-up. You **will** take some random decisions there (cut-off values, clustering etc.). Make sure to document that as well as you can:

- Collect all your "magic numbers" in one place.
- Comment your code
- Ideally, write a separate document to keep all of this clean.

4 rules for data preparation and clean-up

Rule 3: Know where your data lives

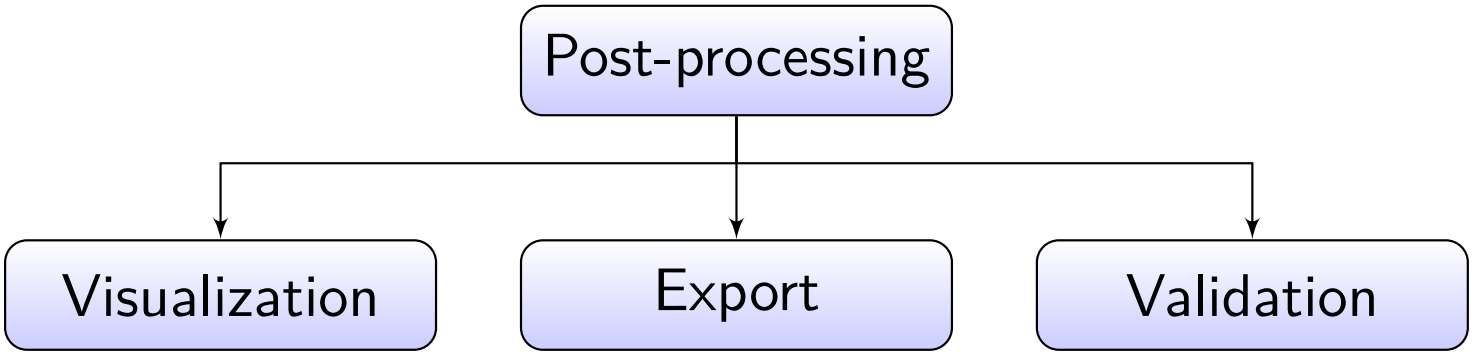
Are you taking some stock market prices from somewhere? Or the pressure measurement from somewhere else?

- Do you have access?
- What happens when the data is unavailable?
- Who is responsible?

Rule 4: Keep data preparation separate

Never mix data import and data preparation with other parts of your code.

Post-processing 101



Visualization: One figure says more than 1000 data points. Tip: draw something on paper. However, this is a bottomless pit, i.e. know when it is good enough.

Export: What format do you need? If possible, use a consistent (and automated) naming strategy! Also, databases can make your life a whole lot easier!

Validation: If the validation happens outside of your program (e.g. high-fidelity modelling system), make sure to respect the data preparation and clean-up rules.

3 tips for visualization

Tip 1: It's worth it

Even if it takes long, writing a good data visualization is **always** worth it. Everybody will ask for the visualization, nobody will ask for the data points.

Tip 2: Use other people

Try to use the community of your programming language as much as possible: data/information visualization is a very common thing to do.

Tip 3: Make it easy

Make visualization easy to use, e.g. something like:

ShowResults(optimizationResult)

and package all the "nasty" details away, since visualization code tends to be very long.

APIs - your best friends in programming

Application Programming Interface (API)

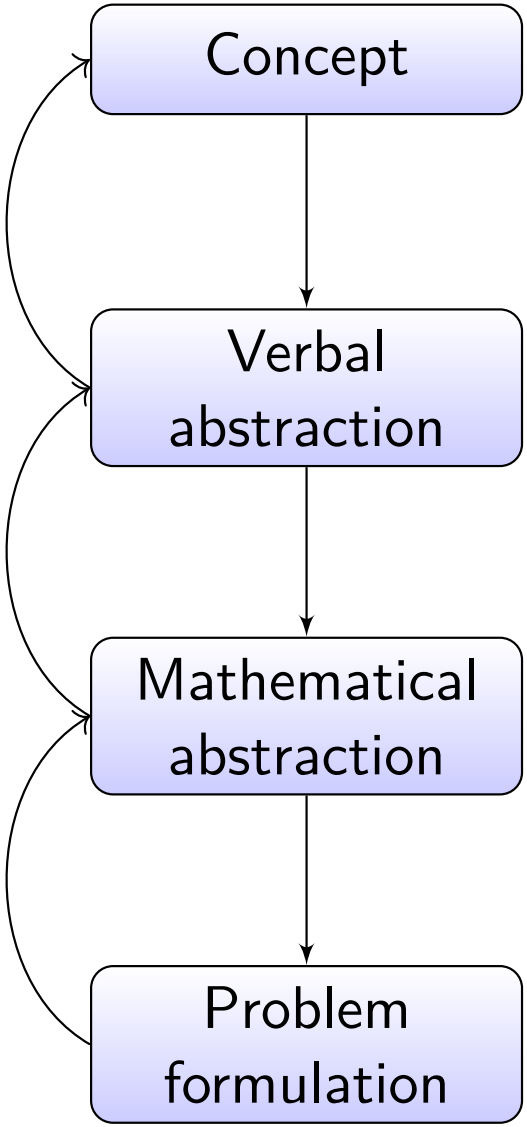
An API allows **application** A to use a line of **programming** to **interface** with application B.

- There APIs for all major programming languages and tools (e.g. MATLAB).
- They allow you to use the strengths of language A and language B together!
- Also: if you want to migrate (say from MATLAB to Python), then you can use a "MATLAB for Python" API as an intermediary step.

```
import matlab.engine
eng = matlab.engine.start_matlab()
t = eng.gcd(100.0,80.0,nargout=3)
print(t)
(20.0, 1.0, -1.0)
```

Outline

The process of modelling



"Let's optimize our batch schedule!"

minimize cost

subject to Physical constraints

...

$x_{i,j}$: flow variables; ...

$$\underset{x}{\text{minimize}} \quad \sum_{i,j} c_{i,j} x_{i,j}$$

$$\text{subject to} \quad \sum_{i,j} x_{i,j} - \sum_{j,k} x_{j,k} = 0$$

...

- This may take many iterations.
- Be ready to discard ideas if something better comes.
- Validate each step separately with the relevant people.

Modelling FAQs

When is my model "good enough"?

A model is always an approximation, and you have to decide when you are happy with it. Oftentimes, performance is the key bottleneck in making a more accurate model.

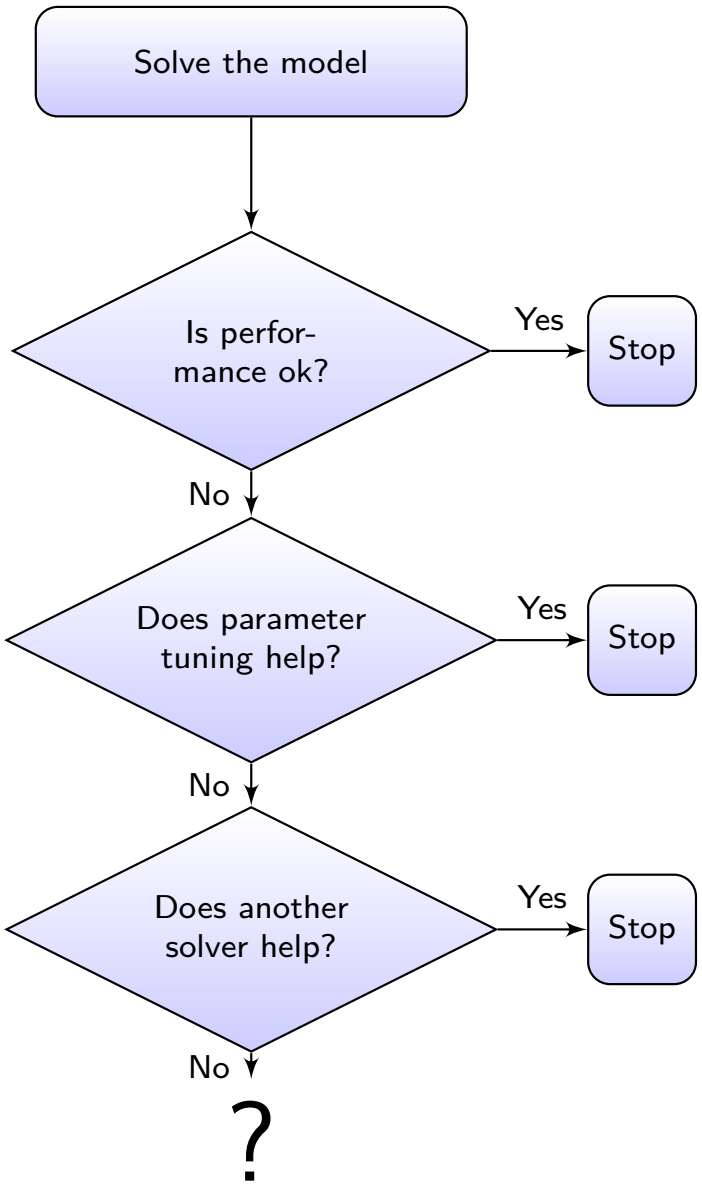
Are modelling and optimization separate?

Yes, to a good extent, since you need a model before you can optimize. However, you should know what you can optimize (LP/NLP/et.) and not be afraid to go back to the modelling if the optimization behaviour is not satisfactory.

How can I become a better modeller for optimization problems?

Learning by doing, essentially. But also reading other peoples work and approaches really helps to sharpen your skills.

Solving your model



The golden rule of performance tuning

Always set yourself a **quantifiable** performance goal.

- When you have a model, try to solve it with a minimum working example.
- If you cannot get the performance you need from a solver, you need to do your own thing. Typically, this means one or more of the following:
  - Develop simplified model
  - Get better hardware
  - Heuristics

Heuristics

Definition

"A heuristic is a technique designed for solving a problem more quickly when classic methods are too slow, or for finding an approximate solution when classic methods fail to find any exact solution" (Wikipedia)

Examples on how to tackle the development of a heuristic:

Imitate the human: Encode the decision processes of a human, e.g. "I would always pick the closest node".

Check similar problems: Check whether your problem structure is similar to a "famous" problem for which good approximate algorithms exist.

Break down into subproblems: Construct a feasible solution by decomposing the main problem and solving the subproblems.

Outline

Why software development?

How much coding do I need?

"Unless you magically find yourself endowed with limitless programming support, sooner or later (most likely sooner) you are likely to need to do some coding." (Paul Rubin)

- Producing good code is hard!
- That said: by rigorously following some simple rules you can make sure that your code stays maintainable and usable.
- However for larger software projects it may be useful to work together with a software developer.

The rules

Modularization/single responsibility

Every function should do exactly one thing. When done correctly, this also means that each function will not be very long ($<$ 100 lines of code).

Naming

Name your variables/functions such that you don't need a comment to understand what they mean. And do not be afraid of long names: "FlowIntoSubstation" is a perfectly acceptable name.

Version control

Use a version control system such as Git, SVN or VSTS. It is super-easy to implement and will save you an incredible amount of headache!

Code review

If you know somebody looks at your code, you will write better code.

From scripting to a software tool

- Oftentimes, we start by scripting ("let's just check that"), which then grows more and more if it is a good idea.
- Very rarely do we go back and look at the original code. We simply build around it.
- That can lead to grave problems, so try to do the following:
  1. Do not rush: take your time to write a clean script. The 5 minutes you save by rushing will cost you 5 hours later.
  2. Already when scripting, devise good naming rules. Names such as `test` and `temp` are **never** good.
  3. Whenever you see the opportunity, "package" something away, even if it is just one line. For example, if you often calculate the Euclidean distance, write `Euclidean(a,b)` as a function.
  4. When you decide that this will be something to work on more, start a new project and include the leanings you got from scripting.

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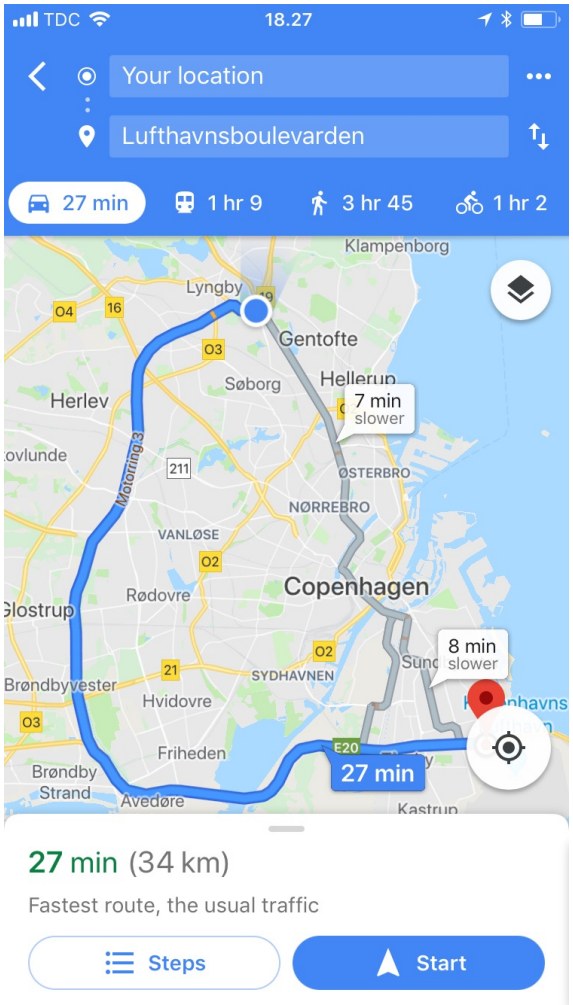
What is the human factor?



- Some applications are truly autonomous (e.g. landing of SpaceX rockets).
- However, in many cases a tool does not make a decision without a human checking (Google Maps).
- People want **decision support tools**, rather than autonomous robots (in most cases). It is key to keep this in mind when designing a tool.
- A tool which provides suggestions rather than makes decisions is typically much more accepted and used.

3 rules for considering humans

Rule 1: Keep them up-to-date

Show them very early drafts, discuss the visualization with them and **listen** to what they have to say!

Rule 2: Make them work

Ask them to provide you with what they want to see. They may just say "yes" to something because they can't be bothered to think about it.

Rule 3: Not all users are alike

Every user (group) is different, so it is not enough to talk to one person and tick the box. Really go out there and get the diverse and real feedback from everybody.