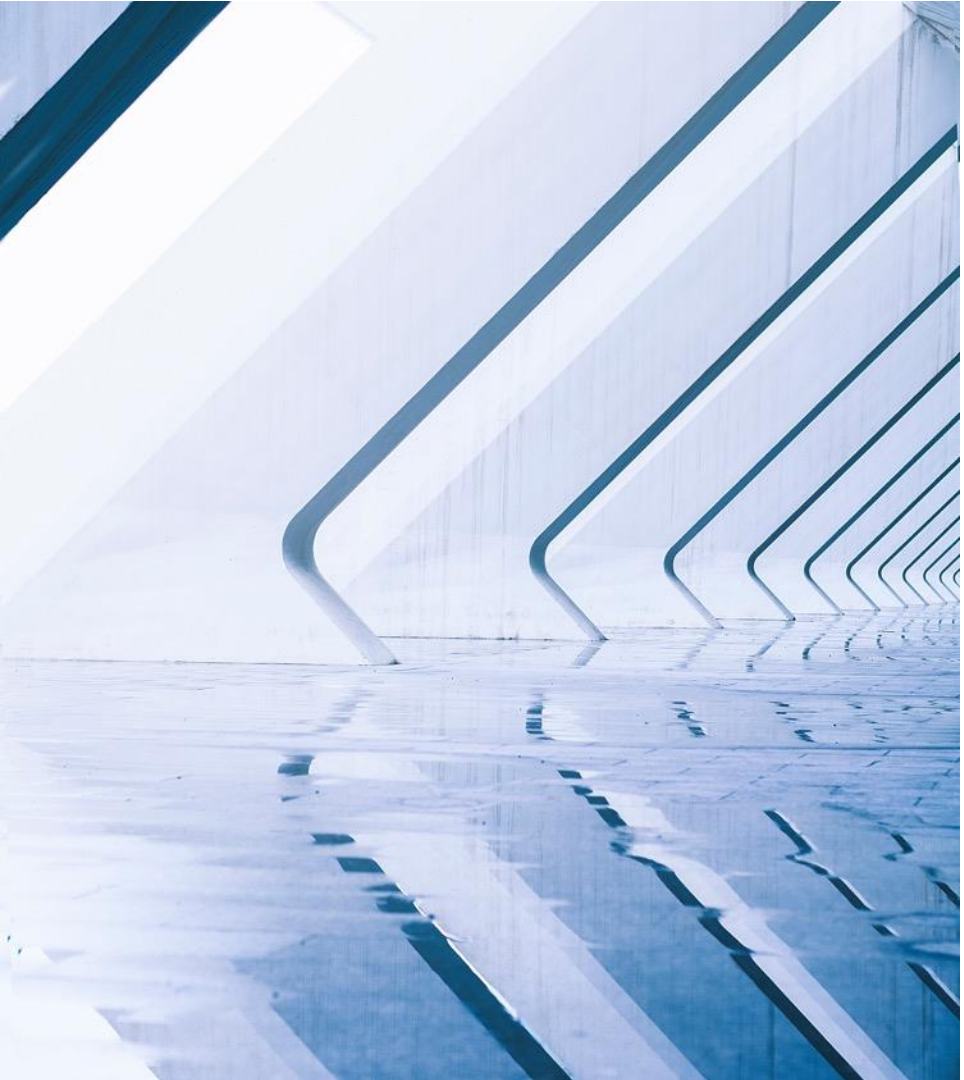


FICO

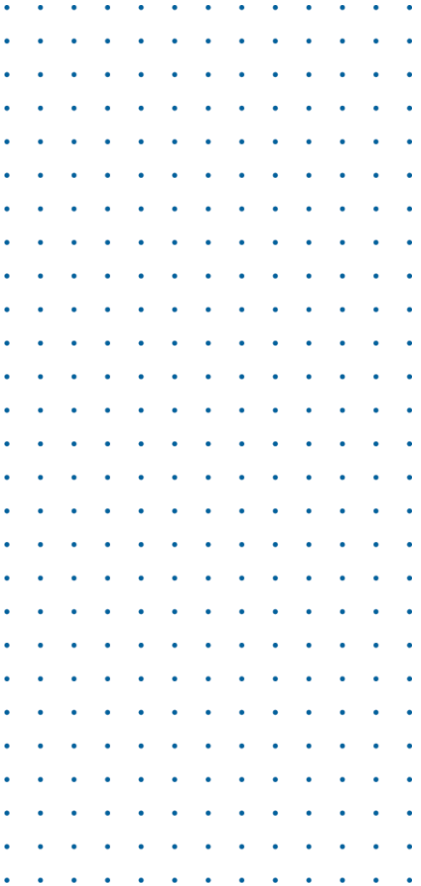
Modelling Aspects

Special constructs, numerics, etc

Timo Berthold

Agenda

- Model building process
- Examples
- 0/1 vs general integer, assignment formulations
- Combinatorial Constraints
- Indicator Constraints
- How not to do it
- Concluding remarks



Building a model

What is modeling?

- Describing a particular situation using a collection of logical and mathematical relationships.
  - An objective function is used to evaluate alternative solutions.
  - Constraints define the alternative solutions that are feasible for the situation under consideration.
- Why do we build models?
  - Too many possibilities to enumerate
  - What-if scenarios might be difficult to evaluate
  - Experimentation might not be possible

The model building process

- Think about what is important to the situation and the problem considered
- An abstraction of the complete problem
- Simplification of the problem can yield tractable problems and interpretable solutions

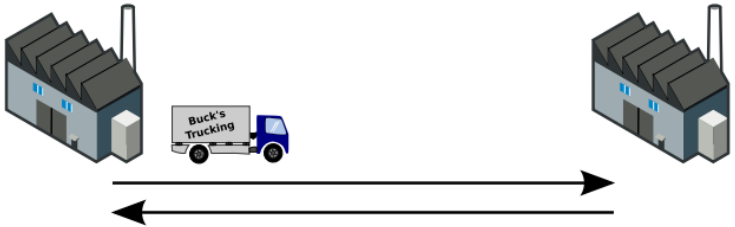
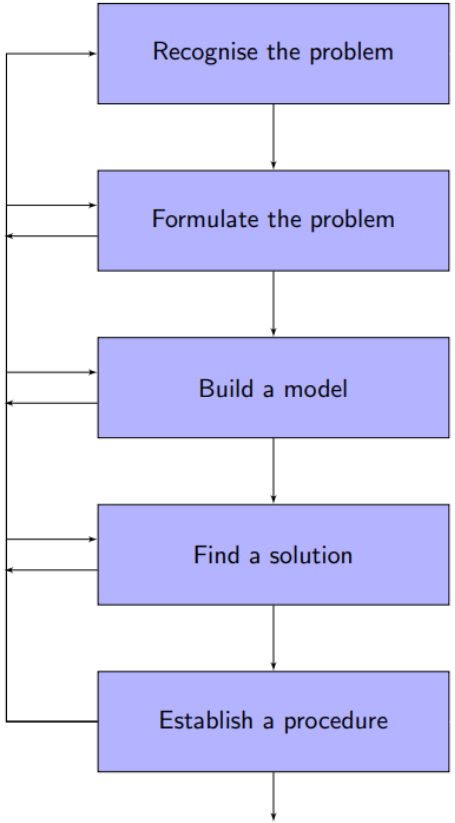
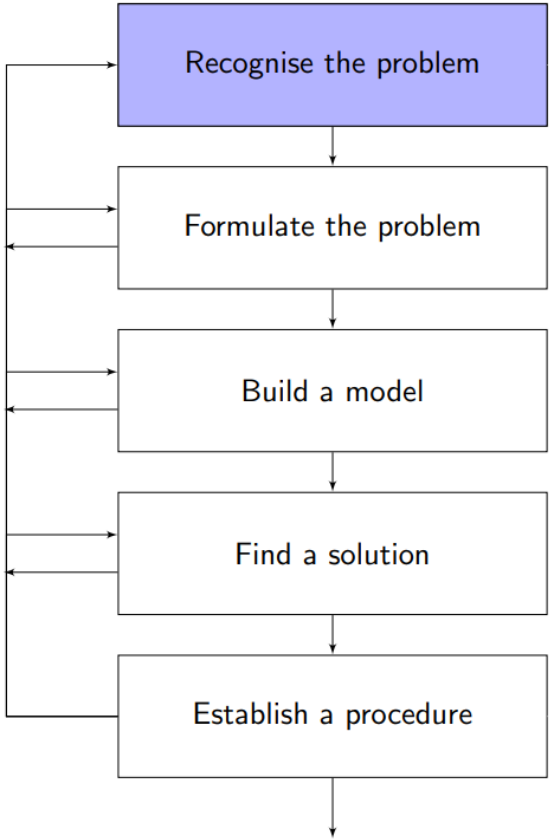


image source: Steve Maher



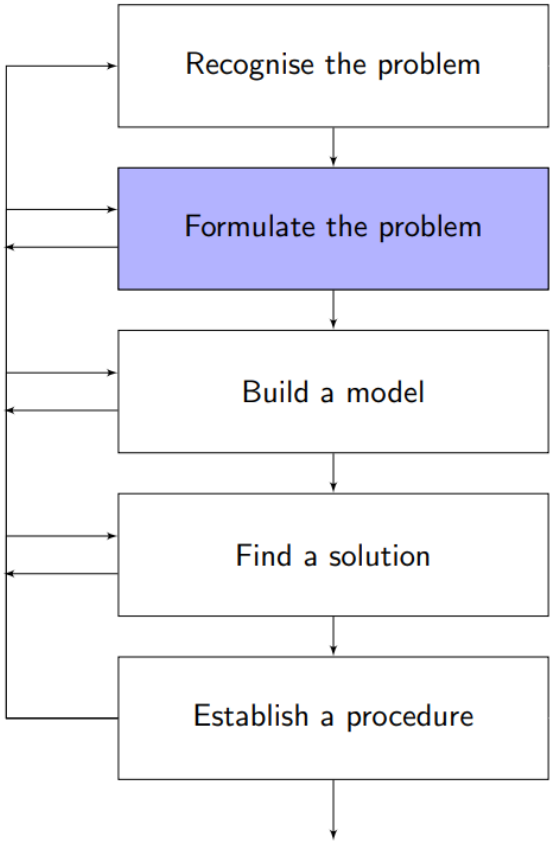
The model building process

- Identify the problem
  - Can be abstract or real world
  - Single out a concrete question



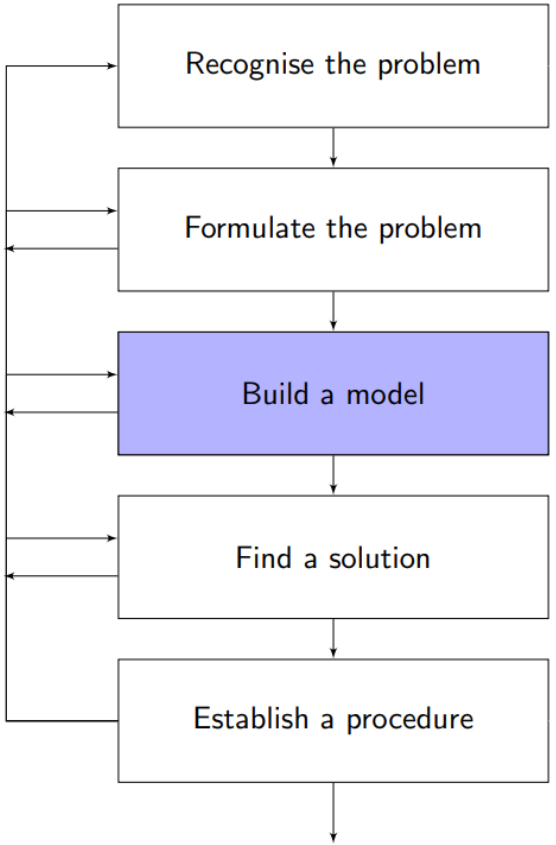
The model building process

- Identify the important features
  - Define this problem in mathematical and logical notation
  - Never forget that your model is an abstraction of reality



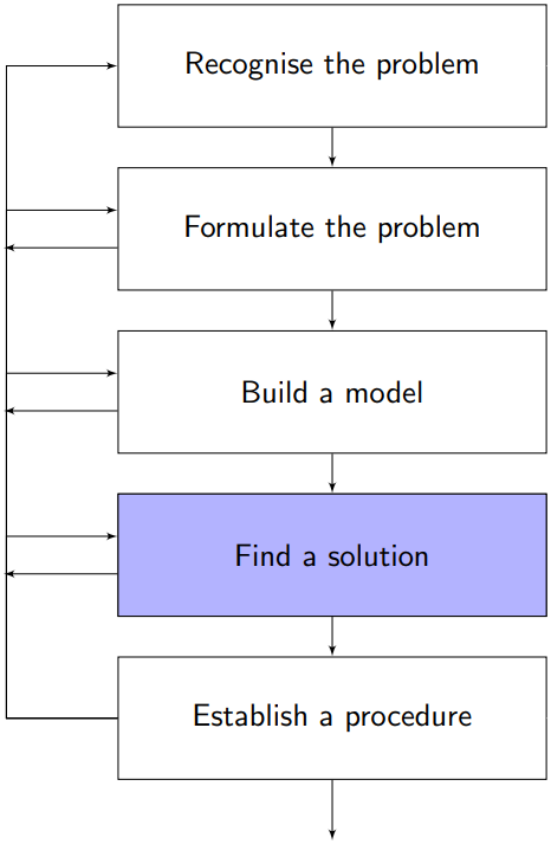
The model building process

- Transfer the mathematical problem formulation to a model
  - Make use of available modelling tools
    - direct coding via API or modeling language
  - Think about alternative formulations

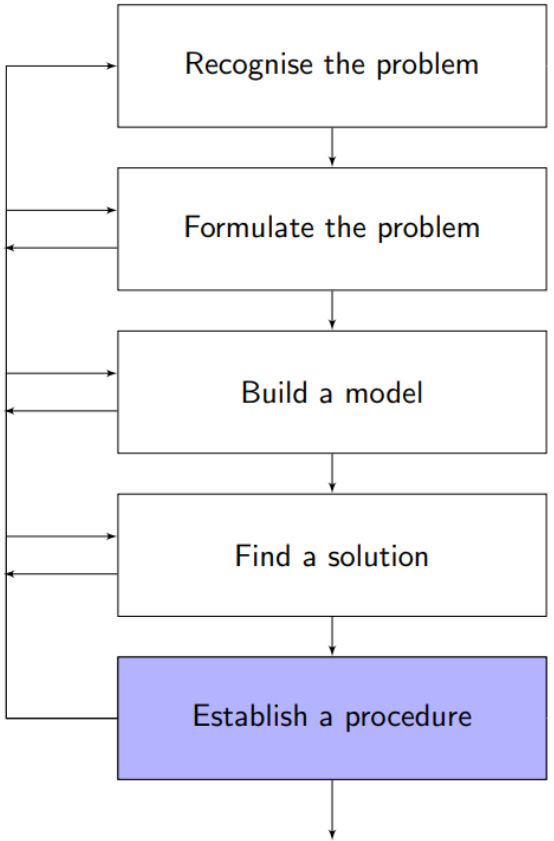


The model building process

- Employ tools to solve the mathematical model
  - In our case, typically a MIP solver
  - Check validity of solution in practice



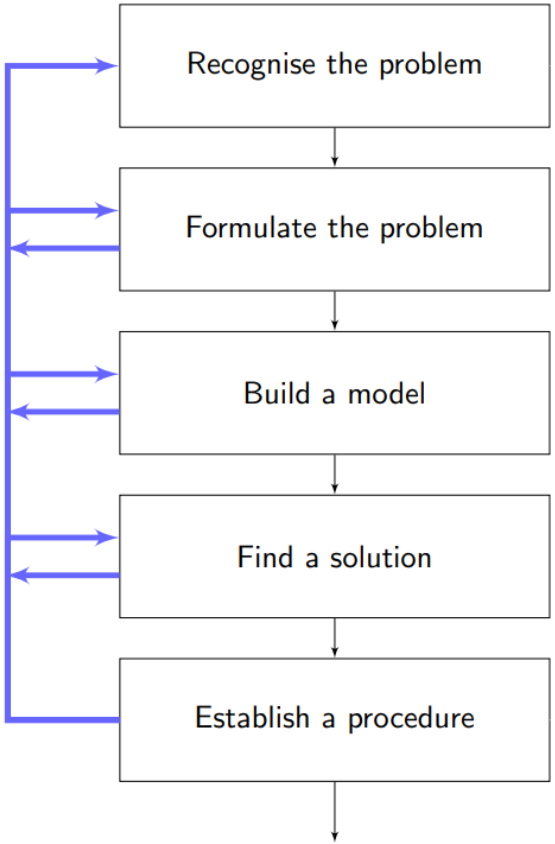
The model building process



- Deployment:
  - Design a procedure to implement the solution
  - This is where a lot of OR projects fail!

The model building CYCLE

- FEEDBACK
  - Each stage helps refine the previous stages
  - The modelling process aids the understanding of the problem.
  - The problem understanding develops and the solution approach becomes clearer.



Example: Knapsack

- A burglar has a knapsack with 15kg capacity
- The burglar breaks into a house with the following items:
  1kg worth 2000€, 1kg worth 1000€, 2kg worth 2000 €, 4kg worth 10000€, 12kg worth 4000 €
- What are the variables? What are the constraints? What is the objective?
  - Variables: $x_i \in \{0,1\}$: Do I take item i?
  - Constraint: Must not exceed capacity: $x_1 + x_2 + 2x_3 + 4x_4 + 12x_5 \leq 15$
  - Objective: Maximize revenue: $\max 2x_1 + x_2 + 2x_3 + 10x_4 + 4x_5$
- $\max 2x_1 + x_2 + 2x_3 + 10x_4 + 4x_5$
  s.t. $x_1 + x_2 + 2x_3 + 4x_4 + 12x_5 \leq 15$
  $x_i \in \{0,1\}$

General integers and other variable types

Binaries or integer variables?

- Rule of thumb
  - Use general integers whenever they represent actual quantities and ordering is important
  - Whenever integers represent just „some different values“, use binaries instead
- Example: Sudoku

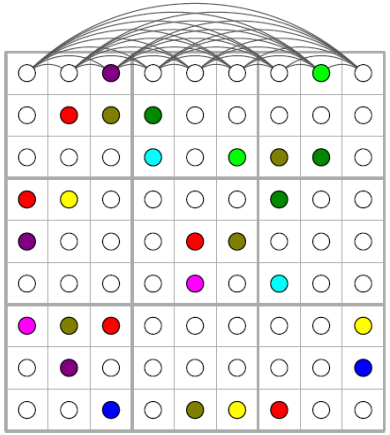
8			6			9		5
				2		3	1	
		7	3	1	8		6	
2	4						7	3
		2	7	9		1		
5				8			3	6
		3						

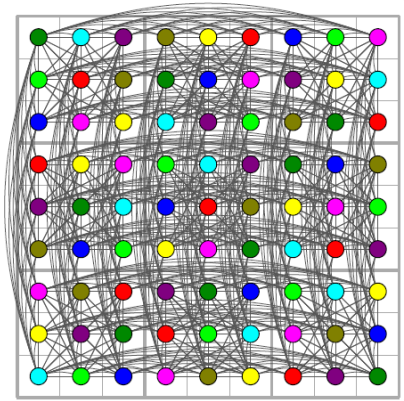
Naive approach:
Use 81 integer variables $1 \leq y_i \leq 9$
And then...?

Sudoku → graph coloring

- Each number corresponds to a color, each cell to a vertex.
  - 9 binaries per cell: x_{ijk}
  - Exactly one color: $\sum_k x_{ijk} = 1 \ \forall i,j$
- Edges when two cells must not have the same color/number, e.g., $x_{1,1,1} + x_{1,2,1} \leq 1$
  - Can do better and add clique equations: $\sum_j x_{ijk} = 1 \ \forall i,k$
- Sudoku corresponds to the question: Is there a feasible 9-coloring of a partially colored graph with 27 9-cliques?

		7					9	
	3	8	2					
			4		9	8	2	
3	6					2		
7				3	8			
				5		4		
5	8	3						6
	7							1
		1		8	6	3		





2	4	7	8	6	3	1	9	5
9	3	8	2	1	5	7	6	4
1	5	6	4	7	9	8	2	3
3	6	5	9	4	7	2	1	8
7	2	4	1	3	8	6	5	9
8	1	9	6	5	2	4	3	7
5	8	3	7	2	1	9	4	6
6	7	2	3	9	4	5	8	1
4	9	1	5	8	6	3	7	2

Assignment structure

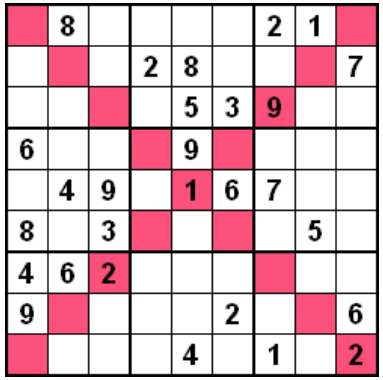
$$
\begin{aligned}
&\text{maximize} && 0 \\
&\text{subject to} && \sum_{v=1}^{9} x_{vrc} = 1 \text{ for } r, c \in [1,9] \\
& && \sum_{r=1}^{9} x_{vrc} = 1 \text{ for } v, c \in [1,9] \\
& && \sum_{c=1}^{9} x_{vrc} = 1 \text{ for } v, r \in [1,9] \\
& && \sum_{r=3p-2}^{3p} \sum_{c=3q-2}^{3q} x_{vrc} = 1 \text{ for } v \in [1,9] \text{ and } p, q \in [1,3]
\end{aligned}
$$

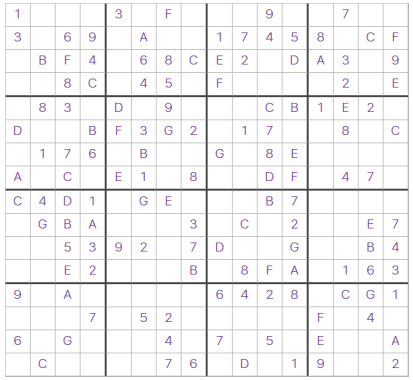
8			6			9		5
				2		3	1	
		7	3	1	8		6	
2	4						7	3
		2	7	9		1		
5				8			3	6
		3						

- Important concept: Assignment structure
  - Assignment problem: Given costs c_{ij} for assigning object i to person j
  - $\min \sum_{i,j} c_{ij} x_{ij}$
    s.t. $\sum_i x_{ij} = 1$
    $\sum_j x_{ij} = 1$
  - Easy, but a common substructure in other problems

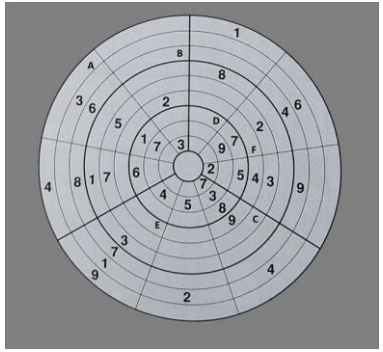
Many variants, similar models

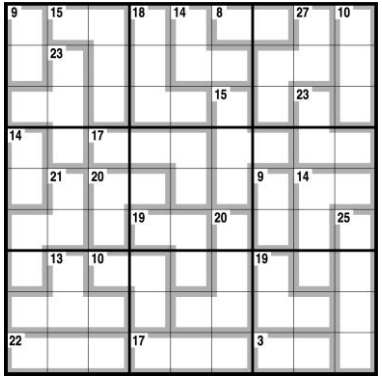
- X-Sudoku
- 16x16-Sudoku
- 3D-Sudoku





- Ensaimada
- Killer-Sudoku
- Comparison-Sudoku





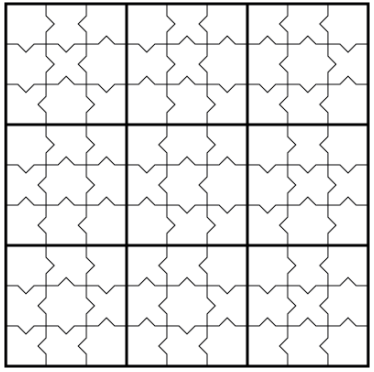


image sources: Wikipedia, derstandard.at, sudoku-cube.de.aptoide.com

Many choices in modeling

TSP – the most famous optimization problem?

- TSP: Given a complete graph $G = (V, E)$ and distances c_{ij} for all $(i, j) \in E$:
  - Find a Hamiltonian cycle (tour) of minimum length.
- Classical MIP formulation:
  - $\min \sum c_e y_e$
    s.t. $\sum_{e \in \delta(v)} y_e = 2$ for all $v \in V$
    $\sum_{e \in \delta(S)} y_e \geq 2$ for all $S \subseteq V, S \neq \emptyset$
    $y_e \in \{0,1\}$
- Highly efficient special-purpose codes
  - Concorde

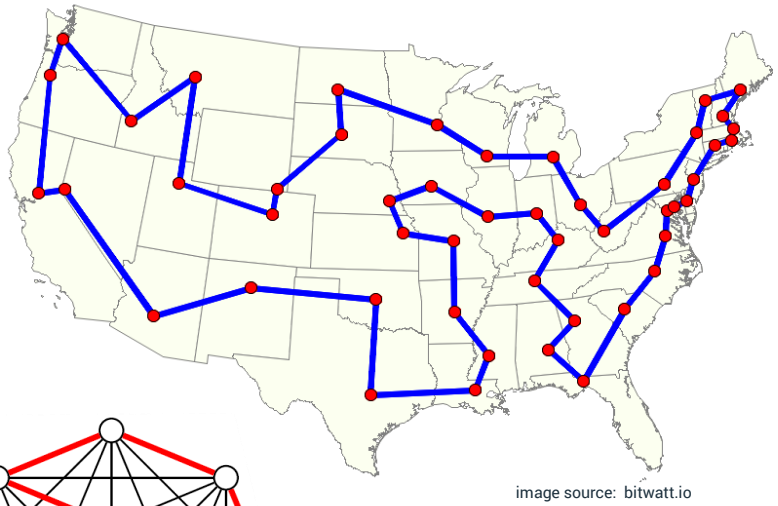
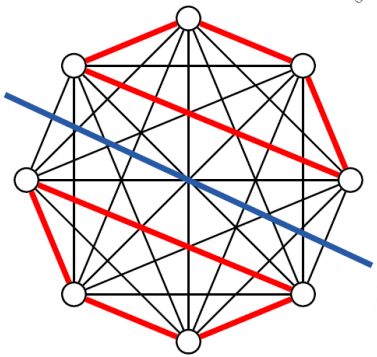


image source: bitwatt.io



TSP – Miller Tucker Zemlin formulation (1960)

- Consider G as directed graph with arcs (ij) and (ji) between all $i, j \in V$. Use variables y_{ij} (whether (ij) is part of the tour), u_i (for the number of nodes visited before i)
  - $\min \sum c_{ij} y_{ij}$

    s.t. $\sum_{(i,j)\in\delta^-(j)} y_{ij} = 1$ for all $j \in V$

    $\sum_{(i,j)\in\delta^+(i)} y_{ij} = 1$ for all i $\in V$

    $u_1 = 0$

    $u_i - u_j + (n-1)y_{ij} \leq n-2$ for all $(i,j) \in A, j \neq 1$

    $1 \leq u_i \leq n-1$ for all $i \in \tilde{V} := V \backslash \{1\}$

    $y_{ij} \in \{0,1\}$

    $u_i \in \mathbb{Z}_{\geq 0}$

TSP – Vyve Wolsey formulation (2006)

- Now, interpret TSP as fixed charge network design problem
  - delivering one unit of flow from source node to each other node
  - For each city $l \in V$, define neighborhood $l \in V_l \subseteq V$ (typically k nearest nodes)
  - Introduce variables w_{ij}^l for flow to city l on arc (i,j)

$$\min \sum c_{ij} y_{ij}$$

s.t. $\sum_{(i,j)\in\delta^-(j)} y_{ij} = 1$ for all $j \in V$

$\sum_{(i,j)\in\delta^+(i)} y_{ij} = 1$ for all i $\in V$

$u_1 = 0$

$u_i - u_j + (n-1)y_{ij} \leq n-2$ for all $(i,j) \in A, j \neq 1$

$1 \leq u_i \leq n-1$ for all $i \in \tilde{V}$

$y_{ij} \in \{0,1\}$, $u_i \in \mathbb{Z}_{\geq 0}$

$\sum_{(i,l)\in\delta^-(l)} w_{il}^l - \sum_{(i,l)\in\delta^+(l)} w_{li}^l = 1$ for all $l \in \tilde{V}$

$\sum_{(i,j)\in\delta^-(j)} w_{ij}^l - \sum_{(i,j)\in\delta^+(j)} w_{ji}^l = 0$ for all $l \in \tilde{V}, j \in V_l, j \neq l$

$0 \leq w_{ij}^l \leq y_{ij}$ for all $l \in \tilde{V}, (i,j) \in A(V_l) \cup \delta^-(V_l)$

Many different variations (Achterberg et al 2008)

- Vyve-Wolsey strengthens Miller-Tucker-Zemlin: It gives a better LP bound
- In the following, we consider redundant changes, that do not change the LP bound (or the set of integer optimal solutions)
- Yet, they can have a huge effect on solver performance

- Relaxations (that remove redundant constraints):
  - Remove upper bounds on u_i
  - Equality in the flow conservation constraints can be ommited:
    $\sum_{(i,l)\in\delta^-(l)} w_{il}^l - \sum_{(i,l)\in\delta^+(l)} w_{li}^l \geq 1$
    $\sum_{(i,j)\in\delta^-(j)} w_{ij}^l - \sum_{(i,j)\in\delta^+(j)} w_{ji}^l \geq 0$

Many different variations II

- Additional restrictions:
  - Ordering variables have to be integer: $u_i \in \mathbb{Z}$
  - Explicit bounds on flow variables: $w_{ij}^l \leq 1$
  - Flow variables have to be integer: $w_{ij}^l \in \mathbb{Z}$
  - Fix variables w_{ij}^l with $(i,j) \in \delta^+(V_l)$ to zero
- Some of those restrictions, the solver can figure out itself (E.g., fixing w_{ij}^l with $(i,j) \in \delta^+(V_l)$ to zero)
- Others lead to huge reductions (e.g., changing flow constraints to inequality)
- 64 cases, which fall into three clusters w.r.t. problem size (minor variations still occur)
  - Some solve in seconds, others not in a day

Quiz time

- Modelling a 9x9 Sudoku as integer programs ist best done with
  a) 81 general integer variables
  b) 81 binary variables
  c) 729 binary variables
- Where do most OR projects fail?
  a) Model formulation
  b) Deployment
  c) Solution finding
- Adding redundant information to a model:
  a) Will not change the performance
  b) Will always slow down the solver
  c) Might change performance dramactically, in either direction

Quiz time

- Modelling a Sudoku as integer programs ist best done with
  a) 81 general integer variables
  b) 81 binary variables
  c) 729 binary variables
- Where do most OR projects fail?
  a) Model formulation
  b) Deployment
  c) Solution finding
- Adding redundant information to a model:
  a) Will not change the performance
  b) Will always slow down the solver
  c) Might change performance dramactically, in either direction

Logical constraints

Logical Constraints

- For binary resultant r and operators x_i
  - $r = \mathrm{AND}(x_1, \ldots, x_n) : r = 1 \Leftrightarrow x_1 = \cdots = x_n = 1$
  - $r = \mathrm{OR}(x_1, \ldots, x_n) \quad : r = 1 \Leftrightarrow \exists i : x_i = 1$
  - $r = \mathrm{XOR}(x_1, \ldots, x_n) : r = 1 \Leftrightarrow |i : x_i = 1|$ is odd

- Relatively common constructs in modelling
- Easy to linearize
  - Or are they?

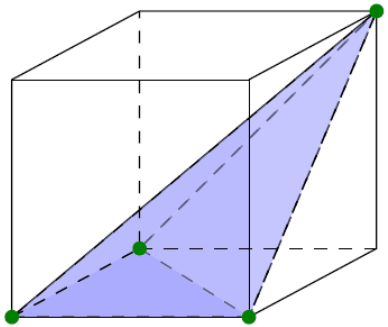
Advantages

- Convenient for modelling
  - Supported by many languages and solver interfaces
  - Together with MIN, MAX, ABS constraints
- Solver might decide dynamically how to linearize them
- Solver might use constraint specific presolving techniques
  - $r = \mathrm{AND}(x, y, z),\ z = \mathrm{AND}(a, b) \Rightarrow r = \mathrm{AND}(x, y, a, b)$
- Higher-level formulation might give additional structural insights that can be exploited

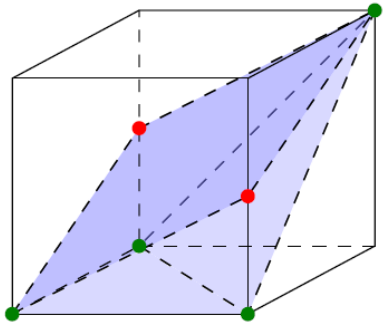
Domain propagation

- Procedure of iterating over constraints, for given (local) bounds of variables and deducing new bounds
  - Typically (at least for finite domain) until some form of consistency is reached
- Four rules for an AND constraint $r = \text{AND}(x_1, \dots, x_n)$
  1. $r = 1 \rightarrow x_i = 1$ for all i
  2. $x_i = 1$ for all $i \rightarrow r = 1$
  3. $\exists i\colon x_i = 0 \rightarrow r = 0$
  4. $r = 0$ and $x_i = 1 \forall i \in \{1, \dots, n\} \backslash \{j\} \rightarrow x_j = 0$

Domain propagation



- $\sum_{i=1}^{n} x_i - r \leq n - 1$
- $x_i - r \geq 0$ for all $i \in \{1, \ldots, n\}$
- Strong relaxation
  - n+1 linear constraints
  - Only integral vertices (green)



- $\sum_{i=1}^{n} x_i - r \leq n - 1$
- $\sum_{i=1}^{n} x_i - nr \geq 0$
- Weak relaxation
  - 2 linear constraints
  - Contains fractional vertices (red)

Domain propagation

- There are four propagation rules for AND constraints
  1. $r = 1 \rightarrow x_i = 1$ for all i
  2. $x_i = 1$ for all $i \rightarrow r = 1$
  3. $\exists i\colon x_i = 0 \rightarrow r = 0$
  4. $r = 0 \text{ and } x_i = 1 \forall i \in \{1, \dots, n\} \backslash \{j\} \rightarrow x_j = 0$
- Do we lose information by using a linearization?
  - Rule 1 is enforced by $\sum_{i=1}^{n} x_i - nr \geq 0$ or by all $x_i - r \geq 0$
  - Rule 2 is enforced by $\sum_{i=1}^{n} x_i - r \leq n - 1$
  - Rule 3 is enforced by $\sum_{i=1}^{n} x_i - nr \geq 0$ or by $x_i - r \geq 0$
  - Rule 4 is enforced by $\sum_{i=1}^{n} x_i - r \leq n - 1$
- Problem-specific propagation might still be more efficient to implement

Indicator constraints

Indicator Constraints

- Model If-then relations
- Most simple form: If (x==1) then y==0 with x binary, y continuous
  - Often written as „x -> y=0“
  - x is called the indicator (variable)
- General form: Indicator for constraints $x \rightarrow a^T x \leq b$
  - Constraint is enforced when x=1, relaxed otherwise
- Used to model that subsets of constraints have to hold
- Or for adding penalty terms when certain constraints do not hold
- The same indicator variable can be used in different indicator constraints to model different scenarios

Indicator Constraints: big-M formulation

- Take indicator constraints $y \rightarrow a^T x \leq b$
- Linearize as $a^T x \leq b + (1 - y)\mathrm{M}$
  - Requires careful choice of M
  - E.g. $\max(a^T x - b)$, but with user knowledge, much smaller values might be feasible
  - Too small M might lead to solutions being cut off
- Propagation, theoretically the same, but numerically it might be different…
  - Big-M formulations are known to be numerically cumbersome
  - For $y \leq 1000000x,\ x \in \{0,1\}$, the solution $x = 0.0000001, y = 1$ is feasible (and integer)
- Indicator formulation often solve slower because information is not present in the LP relaxation
- Choose your big-Ms wisely!!! Try both variants, indicators and big-Ms

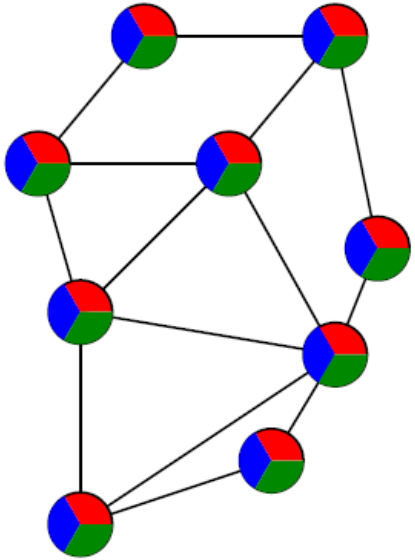
How NOT to do it

Making assumptions what structure a MIP solver can recognize

- Given a flow model with per-node flow conservation constraints
  - Capacity constraints on some subsets
  - A layered structure
  - S.t. the capacity constraints create cuts between two layers
  - And no bounds on the flow variables
  - „because this should follow from the structure“
- MIP solvers are great at making deductions from single constraints or pairs of constraints
  - Less so from a specific combinatorial structure that is implictly captured in hundreds of constraints
  - In the present case, the solver will detect that this is a network flow, but that‘s about it
- You as a modeler are the „structure“ expert, try passing information to the solver

Destroying structure that is there

- Often, hard to prove optimality for symmetric models
  - If possible, choose a non-symmetric formulation
- MIP solvers employ sophisticated methods to handle symmetries
- Breaking them by hand („I fixed a few of the decisions“) might do more harm than good
  - Also, it increases the risk of making a non-obvious error



Arbitrary big-Ms

- Model with piecewise linear functions, modelled via SOS2
  - Last point in the PWL being essentially $[\infty, \infty^2]$
  - Corresponding big-Ms also made it into the objective and other constraints
- First reaction: Oh yes, we can easily use M=1000 instead of M=1000000000
- Second thought: There was only one breakpoint, so one could model this with a SOS1
  - Even with several breakpoints, one could use the SOS2 formulation for the regular PWL and a SOS1 for „going infinity“

Concluding considerations

What does a good model look like?

- Compact is not always better
  - There are huge models (>1M variables) that solve in seconds and small (<50 variables) that do not solve in days
- Ideally, the LP optimum should be close to the integer optimum (tight formulation)
- Small number of fractionals in the LP solution is a plus
- Fixing variables should have an impact on other variables (not too many degrees of freedom)
- Keep numerics under control: not too large span of coefficients
  - Not more than six orders of magnitudes for single row/column
  - Not more than nine over the whole model
- Try to avoid big-M formulations

Things to keep in mind

- The first modelling attempt often is infeasible or unbounded
  - MIP solvers are typically super fast in detecting those „trivial“ errors
- The „second“ attempt often produces unsatisfying solutions
  - Might violate some implicit constraints that were forgotten in the model
- MIP solvers prefer extremal solutions
  - Customers often do not
  - Most often, there are alternative optima
    - Or solutions almost as good that might fulfill some robustness considerations

Things to keep in mind

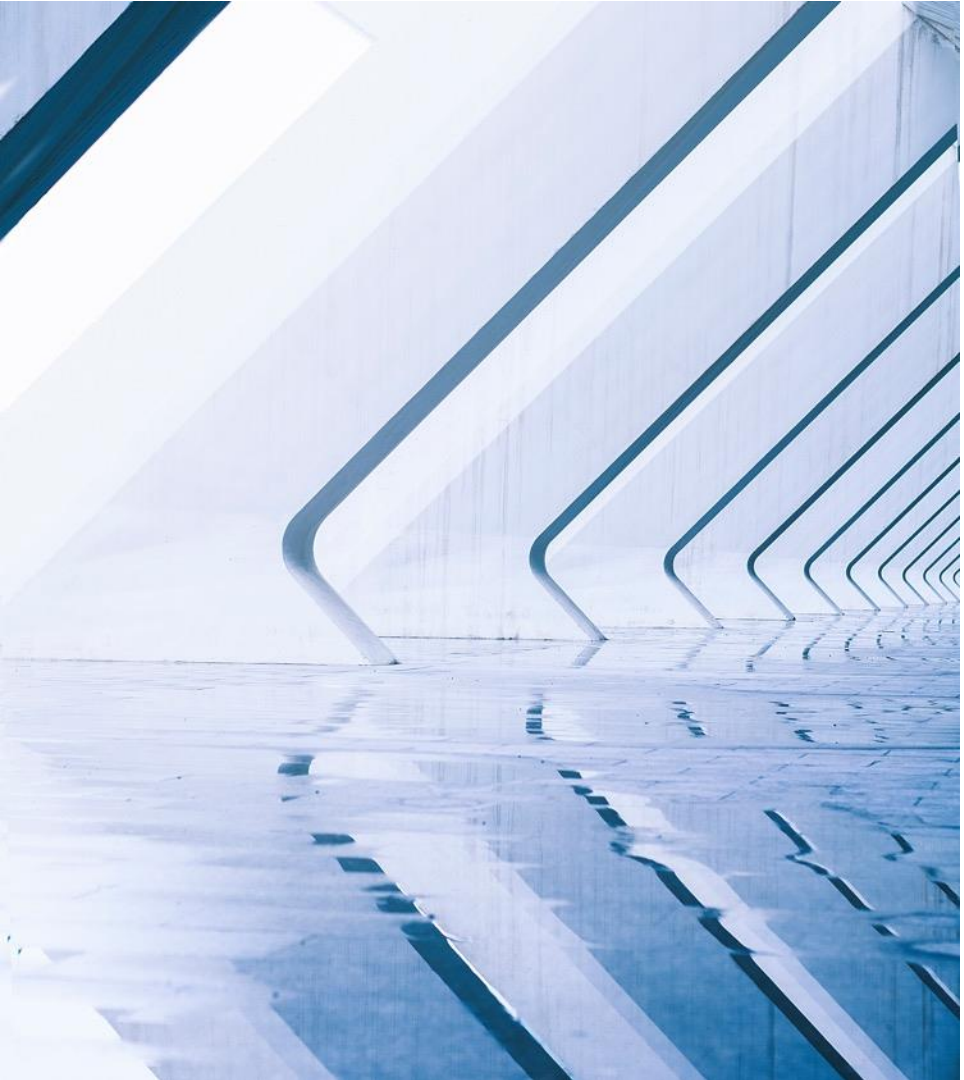
- Try to stress-test your model
  - Do the solutions for corner cases make sense?
  - Always ensure your solutions are at least two-opt.
- A solution is only always optimal (or [in]feasible) w.r.t. your model
  - ...and the data that was fed into your model
  - Slight violations might still be tolerable in practice
  - Often enough solving to exact optimality is not required (e.g., due to inaccurate data)
- Be prepared for a pushback

Quiz time

- A product of binary variables
  a) Is a nonlinear structure and requires an MINLP solver
  b) Needs to be linearly approximated by the modeller
  c) Is a structure that many MIP solvers support
- Indicator constraints model…
  a) If-then relations
  b) If-then-else relations
  c) If-and-only-if relations
- What is a good rule of thumb to keep numerics under control?
  a) Don‘t mix continuous and integer variables in one constraint
  b) Don‘t mix inequalities and equations in one model
  c) Don‘t use coefficients that span more than six orders of magnitude

Quiz time

- A product of binary variables
  a) Is a nonlinear structure and requires an MINLP solver
  b) Needs to be linearly approximated by the modeller
  c) Is a structure that many MIP solvers support
- Indicator constraints model...
  a) If-then relations
  b) If-then-else relations
  c) If-and-only-if relations
- What is a good rule of thumb to keep numerics under control?
  a) Don‘t mix continuous and integer variables in one constraint
  b) Don‘t mix inequalities and equations in one model
  c) Don‘t use coefficients that span more than six orders of magnitude



FICO

Thank You!

Timo Berthold