Universitat d'Alacant
Universidad de Alicante

CAChemE

Introduction to Optimization Modeling in Python

PSE Summer School
Universitat Politècnica de Catalunya

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July 2019

Contents

- Install PYOMO and solvers
- Introduction to Python
- PYOMO Components
- Case Studies

https://github.com/CAChemE/

Install PYOMO and Solvers

PYOMO

- `conda install -c conda-forge pyomo`
- `conda install -c conda-forge pyomo.extras`

http://www.pyomo.org/installation/

SOLVERS

- glpk [LP, MILP] >> `conda install -c conda-forge glpk`

http://ftp.gnu.org/gnu/glpk/

- gurobi [LP, MILP] >> download and install. Free university license

http://www.gurobi.com/

- IPOPT [NLP] >> `conda install -c conda-forge ipopt`

https://www.coin-or.org/download/binary/

- SCIP [MINLP] >> download and add the solver installation to the path environment variable

http://scip.zib.de/#download

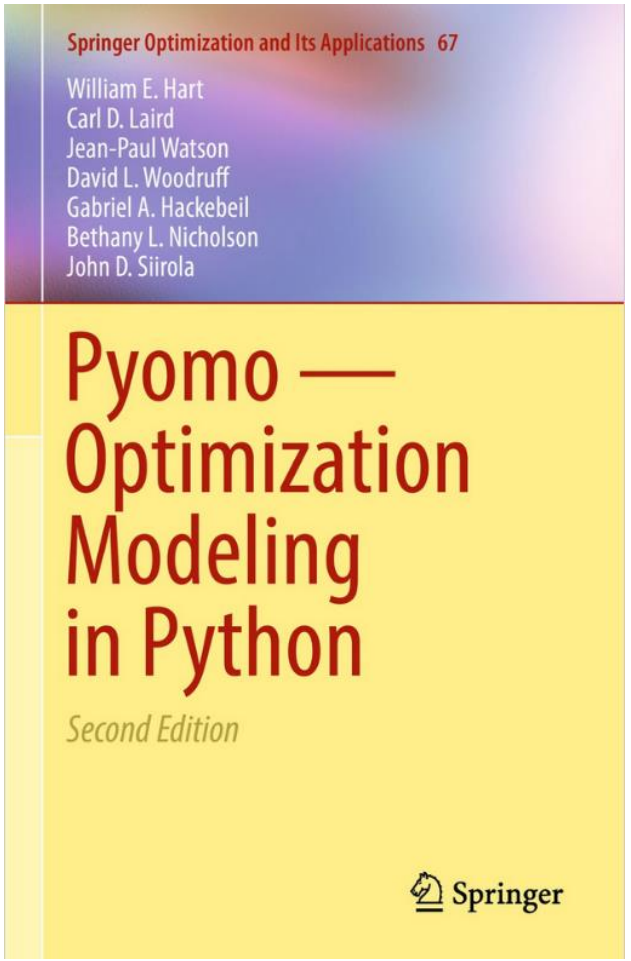
PYOMO Sources

Homepage:

http://www.pyomo.org/

https://software.sandia.gov/trac/pyomo

Book Reference



PYOMO Sources

GitHub

https://github.com/Pyomo

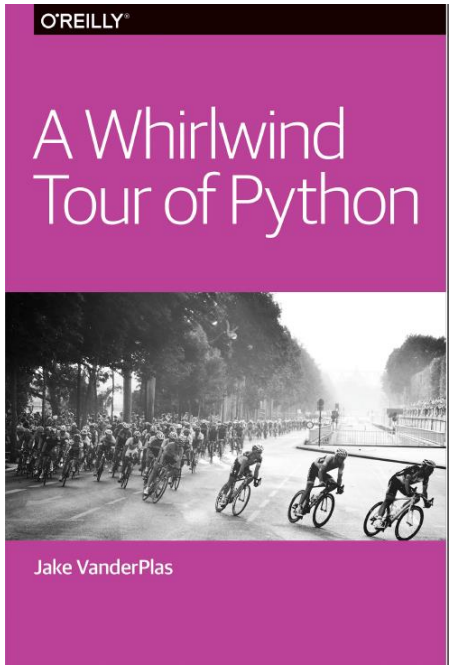
Help Forums

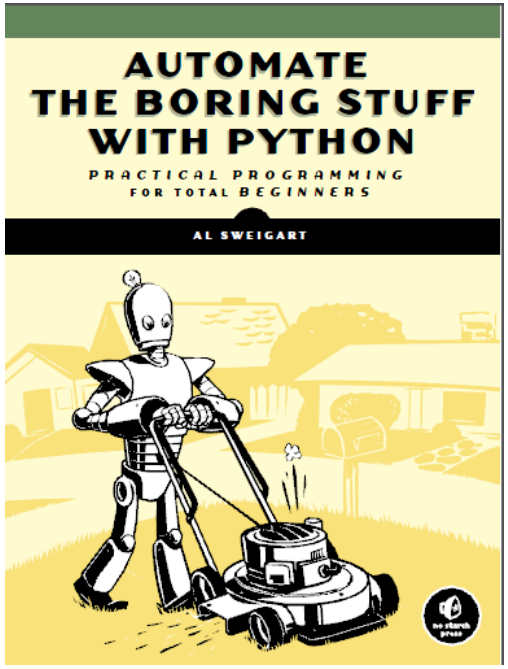
https://groups.google.com/forum/#!forum/pyomo-forum

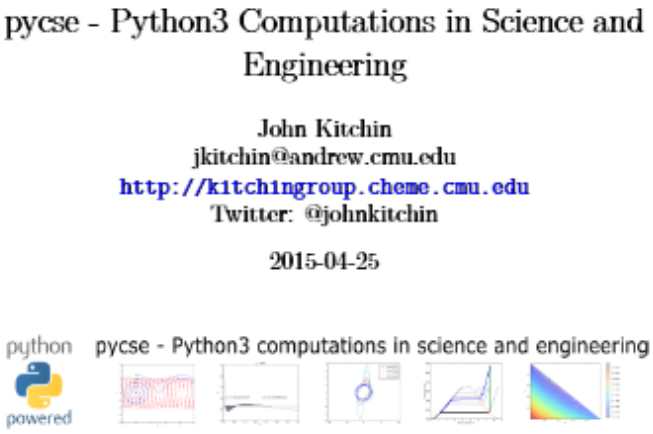
Stack Overflow

https://stackoverflow.com/questions/tagged/pyomo

PYTHON Sources



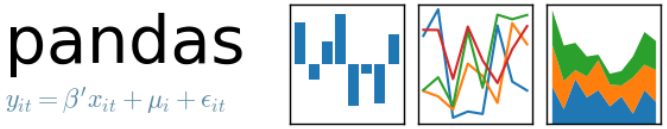



pycse - Python3 Computations in Science and Engineering

John Kitchin
jkitchin@andrew.cmu.edu
http://kitchingroup.cheme.cmu.edu
Twitter: @johnkitchin

2015-04-25

PYTHON Sources



PYOMO Components

PYOMO Components

Example: Machinery Problem

A company manufacture four types of machinery. The factory is divided in three sections. The first section has available 960 h/week, the second 1110 h/week and the third 400 h/week. Each machinery unit requires the following time at each section

Plants	hours per machinery			Profit [units/machinery]
	Machining	Painting	Assembly	
Machinery 1	6	3	2	12
Machinery 2	4	3	1	8
Machinery 3	4	6	2	12
Machinery 4	8	9	1	17

Determine the number of units of machinery for each type that should be manufacture per week to maximize the profit.

PYOMO Components

Example: Machinery Problem

Nomenclature

- m ➔ machinery type (set)
- s ➔ factory section (set)
- $profit_m$ ➔ profit per machinery type (parameter)
- b_s ➔ time availability in each section per week (parameter)
- $T_{m,s}$ ➔ time required for each machinery type in each section (parameter)
- x_m ➔ number of units of machinery for each type (variable)

$$\max_x : \sum_m profit_m \, x_m$$

Objective function

$$s.t. \quad \sum_m T_{m,s} \, x_m \leq b_i \qquad \forall s$$

Factory section time limit

$$x_m \in \mathbb{Z}$$

Model Structure

```
from pyomo.environ import *

m = ConcreteModel()

M = m.M = Set(initialize =  ['m1', 'm2', 'm3', 'm4'])
S = m.S = Set(initialize =  ['s1', 's2', 's3'])

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time_x_section = {
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x = m.x = Var( M, within = PositiveIntegers)

m.value = Objective(
expr = sum( profit[i] * m.x[i] for i in M),
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def constraint_rule(m, j):
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Constraint functions declaration

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```

Solver call

Case Studies

Assignment Problem

In this problem, we have a number of people “p” and a number of tasks “t”. Each person has a suitability coefficient “SC”, which represents how effectively can a person “p” perform a task “t”. The objective is to maximize the total suitability of the system. For this example, the following data is presented:

PEOPLE: Pedro, Marta, Laura
TASKS: Accountant, Sell Manager, Human Resources
SUITABILITY COEFFICIENTS:

Person	SC Accountant	SC Sell Manager	SC Human Resources
Pedro	11	5	2
Marta	15	12	8
Laura	3	1	10

Assignment Problem

Mathematical Model

$$\max\left(\sum_{p,t} C_{p,t} y_{p,t}\right)$$

Maximize the suitability of the assignment

$$s.t.$$

$$\sum_{t} y_{p,t} = 1 \qquad \forall p$$

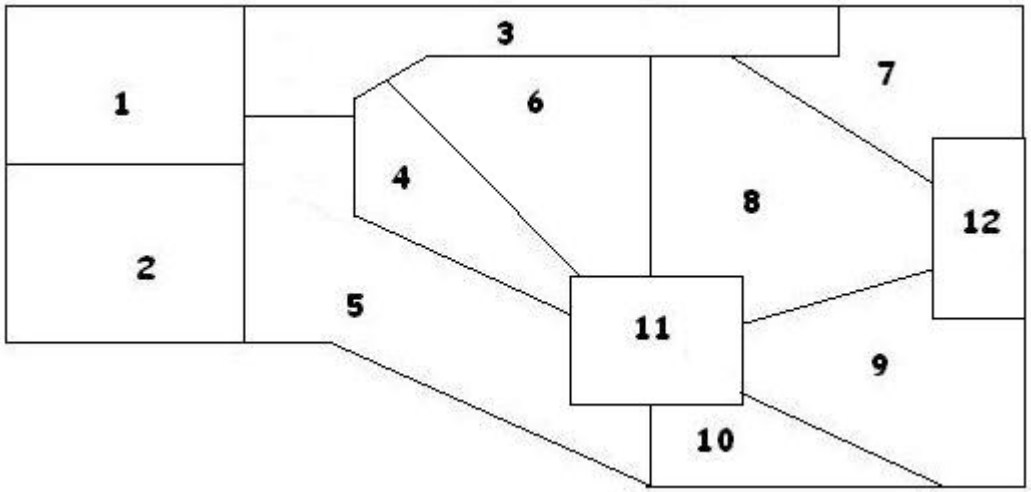
Each person can only perform one job

$$\sum_{p} y_{p,t} = 1 \qquad \forall t$$

Each job must be performed by one and only one person

Set Covering Problem

In this problem, we have a number of zones in which we may or may not install awesome new firefighter stations. However, the mayor of the city is a bit stingy, and wants us to install the absolute minimum number of stations possible. Having the following map of the zone:



And considering that a single station can only provide service to the zones in its immediate neighborhood, what stations should be built?

Set Covering Problem

Mathematical Model

$$\min(\sum_i y_i)$$

Minimize the number of stations

$$s.t.$$

$$\sum_i C_{i',i} y_i \geq 1 \qquad \forall i'$$

Service constraint

Knap-Sack Problem

In this problem, we are adventurous thieves. We want to loot all of the treasures that we can before the guards arrive. Since it will not be possible to come back to loot whatever we leave behind, we must ensure that we maximize the benefit of what we steal. Our horse can handle up until 2500 g of weight (It's a tiny pony) and a volume of 2000 cm3. Considering the loot table, what should we carry out there to sell?

Item	Market Price	Volume (cm3)	Unit Weight (g)	Units available
Chest	50	1000	2000	1
Ring	5	2	20	10
Necklace	3	10	300	1
Mirror	20	500	1000	1
Bracelet	16	15	300	15
Ruby	5	3	75	1
Parfum	1	100	100	1
Diamond	30	5	50	1
Gold goblet	12	250	500	1
Spice	40	100	100	1

Knap-Sack Problem

Mathematical Model

$$\max(\sum_i MP_i n_i)$$ Maximize Profit

$$s.t.$$

$$\sum_i V_i n_i \leq 2000$$ Volume constraint

$$\sum_i W_i n_i \leq 2500$$ Weight constraint

$$n_i \leq N_i \qquad \forall i$$ Amount constraint

Sudoku problem

Nomenclature

r ➔ rows | **c** ➔ columns | **k** ➔ value

$y_{r,c,k}$ ➔ binary variable. $y_{r,c,k} = 1$ means cell [r. c] is assigned number k

	c1	c2	c3	c4	c5	c6	c7	c8	c9
r1	5	3			7				
r2	6			1	9	5			
r3		9	8					6	
r4	8				6				3
r5	4			8					1
r6	7				2				6
r7		6					2	8	
r8				4	1				5
r9					8			7	9

Every position in the Sudoku is filled

$$\sum_k y_{r,c,k} = 1 \quad \forall r, c$$

Cells in the same column must be assigned distinct numbers

$$\sum_r y_{r,c,k} = 1 \quad \forall c, k$$

Cells in the same row must be assigned distinct numbers

$$\sum_c y_{r,c,k} = 1 \quad \forall r, k$$

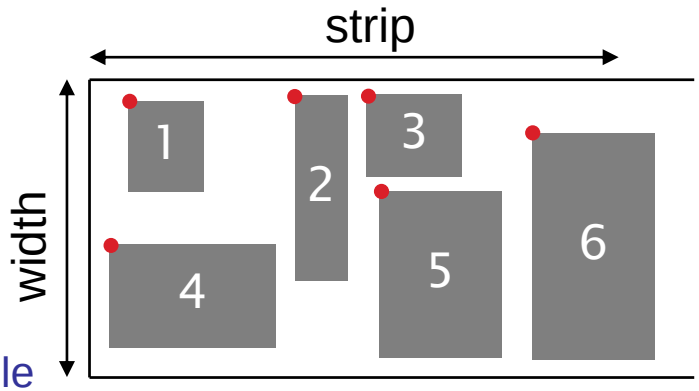
Cells in the same 3x3 grid must be assigned distinct numbers

$$\sum_{r=3p-2}^{3p} \sum_{c=3q-2}^{3q} y_{r,c,k} = 1 \quad \forall k,\ p, q = 1, 2, 3$$

Strip packing 2D problem

Nomenclature

- **i** ➔ rectangles, i = {1,2,…,n}
- **lt** ➔ length of the strip
- **(x_i,y_i)** ➔ rectangle coordinates
- L_i, H_i ➔ Length and height of rectangle i
- W ➔ Width of the strip
- UB_i ➔ Upper bound for the x-coordinate of every rectangle



GDP Formulation

Source: Sawaya & Grossmann (2005), https://doi.org/10.1016/j.compchemeng.2005.04.004

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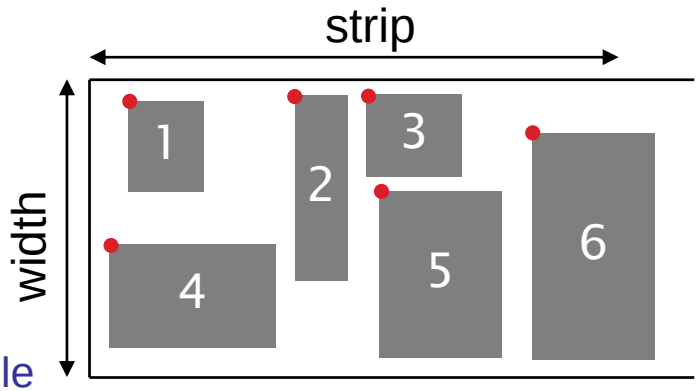

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GDP Formulation

$$\min \; lt$$

$$s.t \quad lt \geq x_i + L_i \qquad \forall i \in N$$

[redacted]

$$Y^1_{i,j} \vee Y^2_{i,j} \vee Y^3_{i,j} \vee Y^4_{i,j} \qquad \forall i,j \in N, i < j$$

$$x_i \leq UB - L_i \qquad \forall i \in N$$

$$H_i \leq y_i \leq W \qquad \forall i \in N$$

$$lt, x_i, y_i \in \mathbb{R}$$

$$Y_{i,j} \in \{Ture, False\}$$

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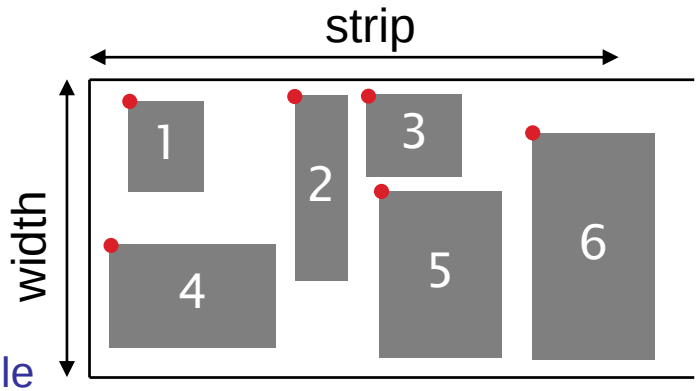

MILP Formulation [Big-M]

$$\min\ lt$$

$$s.t\quad lt \geq x_i + L_i \qquad \forall i \in N$$

$$y_j - H_j \geq y_i - M_{ij}^1\ 1 - w_{ij}^1 \qquad \forall i,j \in N, i < j$$

$$x_i + L_i \leq x_j + M_{ij}^2\ 1 - w_{ij}^2 \qquad \forall i,j \in N, i < j$$

$$y_i - H_i \geq y_j - M_{ij}^3\ 1 - w_{ij}^3 \qquad \forall i,j \in N, i < j$$

$$x_j + L_j \leq x_i + M_{ij}^4\ 1 - w_{ij}^4 \qquad \forall i,j \in N, i < j$$

$$\sum_{d \in D} w_{ij}^d = 1 \qquad \forall i,j \in N, i < j$$

$$x_i \leq UB - L_i \qquad \forall i \in N$$

$$H_i \leq y_i \leq W \qquad \forall i \in N$$

$$lt, x_i, y_i \in \mathbb{R}, \qquad w_{i,j} \in \{0,1\}$$

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