Open Source Tools for Optimization in Python

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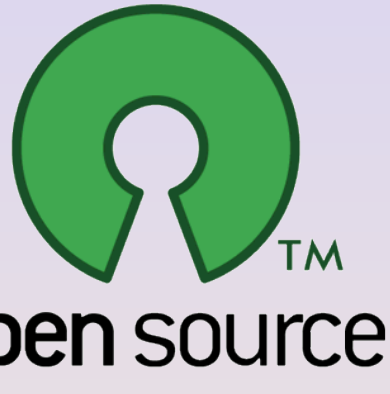

Sage Days Workshop
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Outline

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Caveats and Motivation

- Caveats
  - I have no idea about the background of the audience.
  - The talk may be either too basic or too advanced.
- Why am I here?
  - I'm not a Sage developer or user (yet!).
  - I'm hoping this will be a chance to get more involved in Sage development.
- Please ask lots of questions so as to guide me in what to dive into!

Mathematical Optimization

- Mathematical optimization provides a formal language for describing and analyzing optimization problems. Elements of the model:
  - Decision variables
  - Constraints
  - Objective Function
  - Parameters and Data
- The general form of a *mathematical optimization problem* is:

$$\text{min or max} \quad f(x) \tag{1}$$

$$\text{s.t.} \quad g_i(x) \left\{ \begin{array}{c} \leq \\ = \\ \geq \end{array} \right\} b_i \tag{2}$$

$$x \in X \tag{3}$$

where $X \subseteq \mathbb{R}^n$ might be a discrete set.

Types of Mathematical Optimization Problems

- The type of a mathematical optimization problem is determined primarily by
  - The form of the objective and the constraints.
  - The form of the set X.
- The most important factors in whether a mathematical optimization problem is "tractable" are the convexity of the objective function and the feasible region.
- Mathematical optimization problems are generally classified according to the following dichotomies.
  - Linear/nonlinear
  - Convex/nonconvex
  - Discrete/continuous
  - Stochastic/deterministic
- See the NEOS guide for a more detailed breakdown.

Quick Intro to Modeling and Analysis

Modeling and Analysis Process

- Develop a conceptual model of the system to be optimized.
- Formulate a corresponding mathematical optimization problem.
- Develop an "abstract" model using a modeling system.
- Populate the model with data to obtain an instance.
- "Solve" the resulting instance using appropriate software.
- Analyze the results.

These steps generally involve several different pieces of software working in concert.

- For optimization problems, the modeling is often done with an *algebraic modeling system*.
- Data can be obtained from a wide range of sources, including spreadsheets.
- Solution of the model is usually relegated to specialized software, depending on the type of model.

Example: Optimal Bond Portfolio

- A bond portfolio manager has $\$100K$ to allocate to two different bonds.

Bond	Yield	Maturity	Rating
A	4	3	A (2)
B	3	4	Aaa (1)

- The goal is to maximize total return subject to the following limits.
  - The average rating must be at most 1.5 (lower is better).
  - The average maturity must be at most 3.6 years.
- Any cash not invested will be kept in a non-interest bearing account and is assumed to have an implicit rating of 0 (no risk).

Bond Portfolio Model

- Let x_1 be the amount of Bond A to be purchased and x_2 the mount of Bond B to be purchased.
- Then the problem of determining the optimal portfolio can be formulated as follows.

Bond Portfolio Model

$$\begin{aligned}
\max \quad & 4x_1 + 3x_2 && (4)\\
\text{s.t.} \quad & x_1 + x_2 \leq 100 && (5)\\
& 2x_1 + x_2 \leq 150 && (6)\\
& 3x_1 + 4x_2 \leq 360 && (7)\\
& x_1, x_2 \geq 0 && (8)
\end{aligned}$$

Abstracting the Model

- The previous model is not very satisfactory from a practical perspective, since the basic parameters might change after the model is specified.
- An *abstract algebraic model* is a model that doesn't have values for the input data.
- Components of an abstract algebraic model are

Data

- Sets: Sets that index variables and constraints.
- Parameters: Specific values of numerical inputs.

Model

- Variables: Values in the model that need to be decided upon.
- Objective Function: A function of the variable values to be maximized or minimized.
- Constraints: Functions of the variable values that must lie within given bounds.

Abstract Bond Portfolio Model

- Let B be a set of bonds available for purchase and let F be a set of salient features of these bonds to be limited and/or optimized.
- Let x_b be the amount of bond b to be purchased.
- Let c_b be the value of the feature to be optimized for bond b and a_{fb} be the value of feature f for bond b.
- Finally, let L_f be the limit on the average value of feature f (assume are all are upper limits).

Abstract Bond Portfolio Model

$$\max \quad \sum_{b \in B} c_b x_b \tag{9}$$

$$\text{s.t.} \quad \sum_{f \in F} \sum_{b \in B} a_{fb} x_b \leq L_b \qquad \forall f \in F \tag{10}$$

$$x_b \geq 0 \qquad \forall b \in B \tag{11}$$

Outline

COIN-OR: Open Source Operations Research

The COIN-OR Foundation

- A non-profit foundation promoting the development and use of interoperable, open-source software for operations research.
- A consortium of researchers in both industry and academia dedicated to improving the state of computational research in OR.
- A venue for developing and maintaining standards.
- A forum for discussion and interaction between practitioners and researchers.

The COIN-OR Repository

- A collection of interoperable software tools for building optimization codes, as well as a few stand alone packages.
- A venue for peer review of OR software tools.
- A development platform for open source projects, including a wide range of project management tools.

What You Can Do With COIN-OR

- We currently have 50+ projects and more are being added all the time.
- COIN-OR has solvers for most common optimization problem classes.
  - Linear programming
  - Nonlinear programming
  - Mixed integer linear programming
  - Mixed integer nonlinear programming (convex and nonconvex)
  - Stochastic linear programming
  - Semidefinite programming
  - Graph problems
  - Combinatorial problems (VRP, TSP, SPP, etc.)
  - Graphics and visualization
- COIN-OR has various utilities for reading/building/manipulating/preprocessing optimization models and getting them into solvers.
- COIN-OR has overarching frameworks that support implementation of broad algorithm classes.
  - Parallel search
  - Branch and cut (and price)
  - Decomposition-based algorithms

The COIN-OR Optimization Suite

- COIN-OR distributes a free and open source suite of software that can handle all the classes of problems we'll discuss.
  - Clp (LP)
  - Cbc (MILP)
  - Ipopt (NLP)
  - SYMPHONY (MILP, BMILP)
  - DIP (MILP)
  - Bonmin (Convex MINLP)
  - Couenne (Non-convex MINLP)
  - Optimization Services (Interface)
- COIN also develops standards and interfaces that allow software components to interoperate.
- Check out the Web site for the project at `http://www.coin-or.org`

Modular Structure of the Suite

- One of the hallmarks of good open source tools is *modularity*.
- The suite is made up of building blocks with well-defined interfaces that allow construction of higher level tools.
- There have been 75 authors over time and most have never coordinated directly with each other!
- This is the open source model of development.

Basic Building Blocks: CoinUtils

The CoinUtils project contains a wide range of low-level utilities used in almost every project in suite.

- Factorization
- File parsing
- Sparse matrix and array storage
- Presolve
- Memory management
- Model building
- Parameter parsing
- Timing
- Basic data structures

Basic Building Blocks: Open Solver Interface

Uniform API for a variety of solvers:

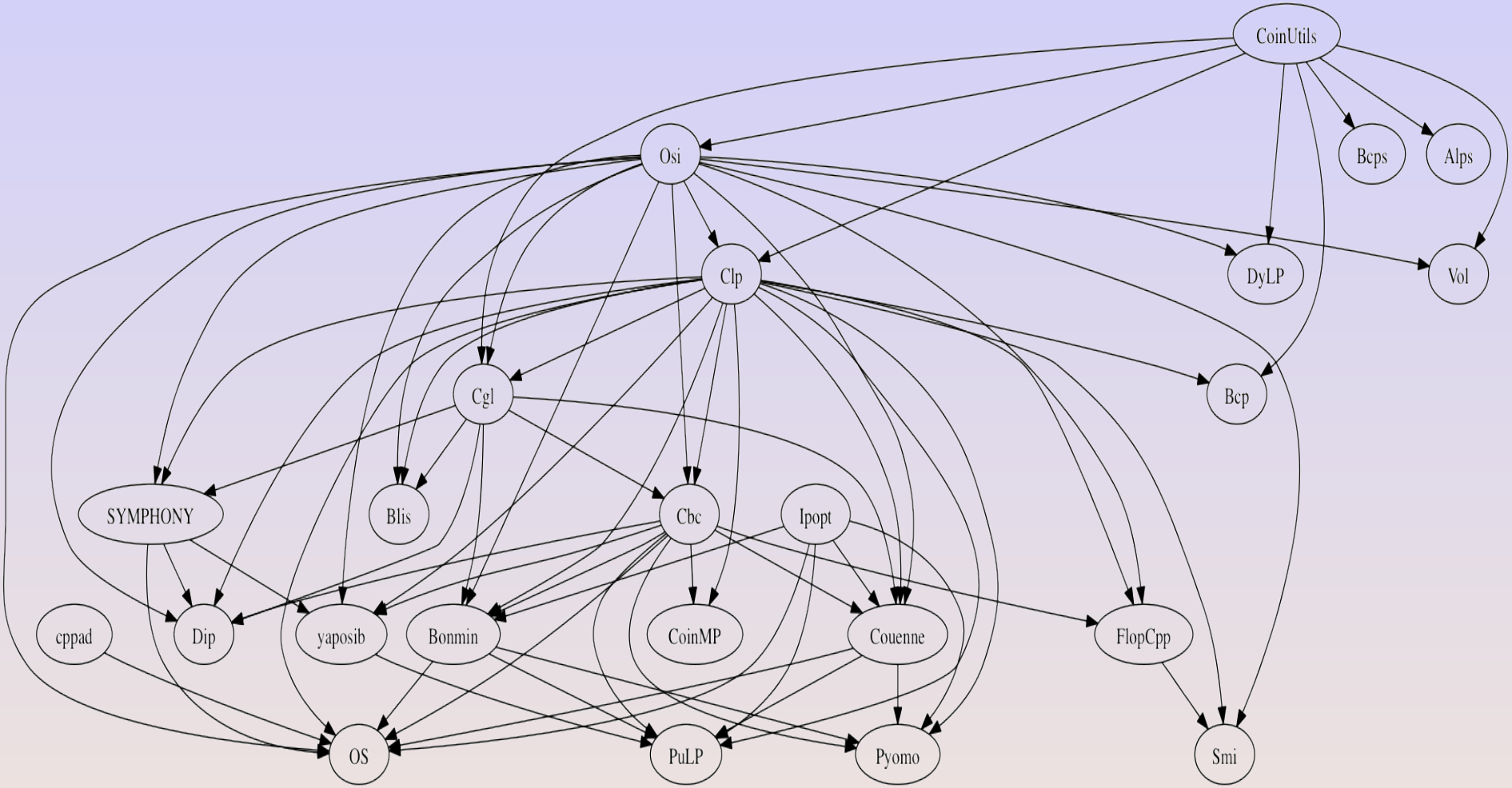
- CBC
- CLP
- CPLEX
- DyLP
- FortMP
- XPRESS-MP
- GLPK
- Mosek
- OSL
- Soplex
- SYMPHONY
- Volume Algorithm

- Read input from MPS or CPLEX LP files or construct instances using COIN-OR data structures.
- Manipulate instances and output to MPS or LP file.
- Set solver parameters.
- Calls LP solver for LP or MIP LP relaxation.
- Manages interaction with dynamic cut and column generators.
- Calls MIP solver.
- Returns solution and status information.

Building Blocks: Cut Generator Library

- A collection of cutting-plane generators and management utilities.
- Interacts with OSI to inspect problem instance and solution information and get violated cuts.
- Cuts include:
  - Combinatorial cuts: AllDifferent, Clique, KnapsackCover, OddHole
  - Flow cover cuts
  - Lift-and-project cuts
  - Mixed integer rounding cuts
  - General strengthening: DuplicateRows, Preprocessing, Probing, SimpleRounding

Optimization Suite Dependency Graph



Getting the COIN-OR Optimization Suite

- Source builds out of the box on Windows, Linux, OSX using the Gnu autotools (or with Visual Studio project files on Windows).
- Source is available from

```
https://www.coin-or.org
https://github.com/coin-or
```

- Packages are available to install on many Linux distros.
- Homebrew recipes are available for many projects on OSX (we are working on this).
- Binaries are automatically built and deployed here:

```
https://bintray.com/coin-or/download
```

- For many more details, see Lecture 1 of this tutorial (slightly out of date now):

```
http://coral.ie.lehigh.edu/ ted/teaching/coin-or
```

Outline

Modeling Software

Most existing modeling software can be used with COIN solvers.

- Commercial Systems
  - GAMS
  - MPL
  - AMPL
  - AIMMS
- Python-based Open Source Modeling Languages and Interfaces
  - Pyomo
  - PuLP/Dippy
  - CyLP (provides API-level interface)
  - yaposib

Modeling Software (cont'd)

- Other Front Ends (mostly open source)
  - FLOPC++ (algebraic modeling in C++)
  - CMPL
  - MathProg.jl (modeling language built in Julia)
  - GMPL (open-source AMPL clone)
  - ZMPL (stand-alone parser)
  - SolverStudio (spreadsheet plug-in: www.OpenSolver.org)
  - Open Office spreadsheet
  - R (RSymphony Plug-in)
  - Matlab (OPTI)
  - Mathematica
  - *Sage*!

How They Interface

- Although not required, it's useful to know something about how modeling languages interface with solvers.
- In many cases, modeling languages interface with solvers by writing out an intermediate file that the solver then reads in.
- It is also possible to generate these intermediate files directly from a custom-developed code.
- Common file formats
  - MPS format: The original standard developed by IBM in the days of Fortran, not easily human-readable and only supports (integer) linear modeling.
  - LP format: Developed by CPLEX as a human-readable alternative to MPS.
  - .nl format: AMPL's intermediate format that also supports non-linear modeling.
  - OSIL: an open, XML-based format used by the Optimization Services framework of COIN-OR.
- Several projects use Python C Extensions to get the data into the solver through memory.

Outline

Where to Get the Examples

- The remainder of the talk will review a wide range of examples.
- These and many other examples of modeling with Python-based modeling languages can be found at the below URLs.

`https://github.com/tkralphs/FinancialModels`

`http://projects.coin-or.org/browser/Dip/trunk/Dip/src/dippy/examples`

`https://github.com/Pyomo/PyomoGallery/wiki`

`https://github.com/coin-or/pulp/tree/master/examples`
`https://pythonhosted.org/PuLP/CaseStudies`

PuLP: Algebraic Modeling in Python

- PuLP is a modeling language in COIN-OR that provides data types for Python that support algebraic modeling.
- PuLP only supports development of linear models.
- Main classes
  - `LpProblem`
  - `LpVariable`
- Variables can be declared individually or as "dictionaries" (indexed sets).
- We do not need an explicit notion of a parameter or set here because Python provides data structures we can use.
- In PuLP, models are technically "concrete," since the model is always created with knowledge of the data.
- However, it is still possible to maintain a separation between model and data.
- Developer: Stuart Mitchell

```
pip install pulp
```

Simple PuLP Model (bonds_simple-PuLP.py)

```
from pulp import LpProblem, LpVariable, lpSum, LpMaximize, value

prob = LpProblem("Dedication Model", LpMaximize)

X1 = LpVariable("X1", 0, None)
X2 = LpVariable("X2", 0, None)

prob += 4*X1 + 3*X2
prob += X1 + X2 <= 100
prob += 2*X1 + X2 <= 150
prob += 3*X1 + 4*X2 <= 360

prob.solve()

print 'Optimal total cost is: ', value(prob.objective)

print "X1 :", X1.varValue
print "X2 :", X2.varValue
```

PuLP Model: Bond Portfolio Example (bonds-PuLP.py)

```
from pulp import LpProblem, LpVariable, lpSum, LpMaximize, value

from bonds import bonds, max_rating, max_maturity, max_cash

prob = LpProblem("Bond Selection Model", LpMaximize)

buy = LpVariable.dicts('bonds', bonds.keys(), 0, None)

prob += lpSum(bonds[b]['yield'] * buy[b] for b in bonds)

prob += lpSum(buy[b] for b in bonds) <= max_cash, "cash"

prob += (lpSum(bonds[b]['rating'] * buy[b] for b in bonds)
         <= max_cash*max_rating, "ratings")

prob += (lpSum(bonds[b]['maturity'] * buy[b] for b in bonds)
         <= max_cash*max_maturity, "maturities")
```

PuLP Data: Bond Portfolio Example (bonds_data.py)

```
bonds = {'A' : {'yield'    : 4,
                'rating'   : 2,
                'maturity' : 3,},

         'B' : {'yield'    : 3,
                'rating'   : 1,
                'maturity' : 4,},
        }

max_cash = 100
max_rating = 1.5
max_maturity = 3.6
```

Notes About the Model

- We can use Python's native `import` mechanism to get the data.
- Note, however, that the data is read and stored *before* the model.
- This means that we don't need to declare sets and parameters.
- Constraints
  - Naming of constraints is optional and only necessary for certain kinds of post-solution analysis.
  - Constraints are added to the model using an intuitive syntax.
  - Objectives are nothing more than expressions without a right hand side.
- Indexing
  - Indexing in Python is done using the native dictionary data structure.
  - Note the extensive use of comprehensions, which have a syntax very similar to quantifiers in a mathematical model.

Notes About the Data Import

- We are storing the data about the bonds in a "dictionary of dictionaries."
- With this data structure, we don't need to separately construct the list of bonds.
- We can access the list of bonds as `bonds.keys()`.
- Note, however, that we still end up hard-coding the list of features and we must repeat this list of features for every bond.
- We can avoid this using some advanced Python programming techniques, but how to do this with SolverStudio later.

Bond Portfolio Example: Solution in PuLP

```
prob.solve()

epsilon = .001

print 'Optimal purchases:'
for i in bonds:
    if buy[i].varValue > epsilon:
        print 'Bond', i, ":", buy[i].varValue
```

More Complexity: Facility Location Problem

- We have n locations and m customers to be served from those locations.
- There is a fixed cost c_j and a capacity W_j associated with facility j.
- There is a cost d_{ij} and demand w_{ij} for serving customer i from facility j.
- We have two sets of binary variables.
  - y_j is 1 if facility j is opened, 0 otherwise.
  - x_{ij} is 1 if customer i is served by facility j, 0 otherwise.

Capacitated Facility Location Problem

$$
\begin{aligned}
\min \quad & \sum_{j=1}^{n} c_j y_j + \sum_{i=1}^{m} \sum_{j=1}^{n} d_{ij} x_{ij} & \\
\text{s.t.} \quad & \sum_{j=1}^{n} x_{ij} = 1 & \forall i \\
& \sum_{i=1}^{m} w_{ij} x_{ij} \leq W_j & \forall j \\
& x_{ij} \leq y_j & \forall i, j \\
& x_{ij}, y_j \in \{0, 1\} & \forall i, j
\end{aligned}
$$

PuLP Model: Facility Location Example

```
from products   import REQUIREMENT, PRODUCTS
from facilities import FIXED_CHARGE, LOCATIONS, CAPACITY

prob = LpProblem("Facility_Location")

ASSIGNMENTS = [(i, j) for i in LOCATIONS for j in PRODUCTS]
assign_vars = LpVariable.dicts("x", ASSIGNMENTS, 0, 1, LpBinary)
use_vars    = LpVariable.dicts("y", LOCATIONS, 0, 1, LpBinary)

prob += lpSum(use_vars[i] * FIXED_COST[i] for i in LOCATIONS)

for j in PRODUCTS:
    prob += lpSum(assign_vars[(i, j)] for i in LOCATIONS) == 1

for i in LOCATIONS:
    prob += lpSum(assign_vars[(i, j)] * REQUIREMENT[j]
                  for j in PRODUCTS) <= CAPACITY * use_vars[i]

prob.solve()

for i in LOCATIONS:
    if use_vars[i].varValue > 0:
        print "Location ", i, " is assigned: ",
        print [j for j in PRODUCTS if assign_vars[(i, j)].varValue > 0]
```

PuLP Data: Facility Location Example

```
# The requirements for the products
REQUIREMENT = {
    1 : 7,
    2 : 5,
    3 : 3,
    4 : 2,
    5 : 2,
}
# Set of all products
PRODUCTS = REQUIREMENT.keys()
PRODUCTS.sort()
# Costs of the facilities
FIXED_COST = {
    1 : 10,
    2 : 20,
    3 : 16,
    4 : 1,
    5 : 2,
}
# Set of facilities
LOCATIONS = FIXED_COST.keys()
LOCATIONS.sort()
# The capacity of the facilities
CAPACITY = 8
```

DIP/DipPy: Decomposition-based Modeling and Solution

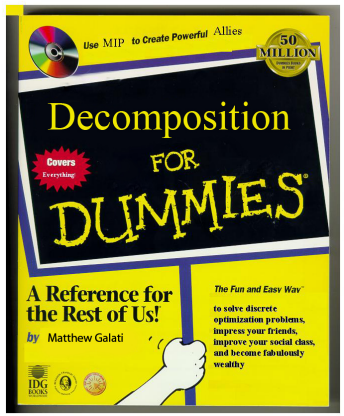
DIP (w/ M. Galati and J. Wang)

A software framework and stand-alone solver for implementation and use of a variety of decomposition-based algorithms.

- Decomposition-based algorithms have traditionally been difficult to implement and compare.
- Abstracts the common, generic elements of these methods.
  - Key: API is in terms of the compact formulation.
  - The framework takes care of reformulation and implementation.
  - DIP is now a *fully generic* decomposition-based parallel MILP solver.

DipPy (w/ M. O'Sullivan)

- PuLP plus a Python C extension.
- User can express decompositions in a "natural" way.
- Allows access to multiple decomposition methods and callbacks.



⇐ *Joke* !

DipPy Basics: Facility Location Example

```
from products   import REQUIREMENT, PRODUCTS
from facilities import FIXED_CHARGE, LOCATIONS, CAPACITY

prob = dippy.DipProblem("Facility_Location")

ASSIGNMENTS = [(i, j) for i in LOCATIONS for j in PRODUCTS]
assign_vars = LpVariable.dicts("x", ASSIGNMENTS, 0, 1, LpBinary)
use_vars    = LpVariable.dicts("y", LOCATIONS, 0, 1, LpBinary)

prob += lpSum(use_vars[i] * FIXED_COST[i] for i in LOCATIONS)

for j in PRODUCTS:
    prob += lpSum(assign_vars[(i, j)] for i in LOCATIONS) == 1

for i in LOCATIONS:
    prob.relaxation[i] += lpSum(assign_vars[(i, j)] * REQUIREMENT[j]
                          for j in PRODUCTS) <= CAPACITY * use_vars[i]

dippy.Solve(prob, doPriceCut:1)

for i in LOCATIONS:
    if use_vars[i].varValue > 0:
        print "Location ", i, " is assigned: ",
        print [j for j in PRODUCTS if assign_vars[(i, j)].varValue > 0]
```

DipPy Callbacks

```
def solve_subproblem(prob, index, redCosts, convexDual):
    ...
    return knapsack01(obj, weights, CAPACITY)
def knapsack01(obj, weights, capacity):
    ...
    return solution
def first_fit(prob):
    ...
    return bvs
prob.init_vars = first_fit
def choose_branch(prob, sol):
    ...
    return ([], down_branch_ub, up_branch_lb, [])
def generate_cuts(prob, sol):
    ...
    return new_cuts
def heuristics(prob, xhat, cost):
    ...
    return sols
dippy.Solve(prob, {'doPriceCut': '1'})
```

CyLP: Low-level Modeling and API for Cbc/Clp/Cgl

- CyLP provides a low-level modeling language for accessing details of the algorithms and low-level parts of the API.
- The included modeling language is “close to the metal”, works directly with numerical data with access to low-level data structures.
- Clp
  - Pivot-level control of algorithm in Clp.
  - Access to fine-grained results of solve.
- Cbc
  - Python classes for customization
- Cgl
  - Python class for building cut generators wrapped around Cgl.
- Developers: Mehdi Towhidi and Dominique Orban

CyLP: Accessing the Tableaux

```
lp = CyClpSimplex()
x = lp.addVariable('x', numVars)
lp += x_u >= x >= 0

lp += A * x <= b if cons_sense == '<=' else A * x >= b

lp.objective = -c * x if obj_sense == 'Max' else c * x
lp.primal(startFinishOptions = 1)
numCons = len(b)
print 'Current solution is', lp.primalVariableSolution['x']
print 'Current tableaux is', lp.tableaux
for row in range(lp.nConstraints):
    print 'Variables basic in row', row, 'is', lp.basicVariables[r
    print 'and has value' lp.rhs[row]
```

yaposib: Python Bindings for OSI (C.-M. Duquesne)

Provides Python bindings to any solver with an OSI interface

```
solver = yaposib.available_solvers()[0]

for filename in sys.argv[1:]:

    problem = yaposib.Problem(solver)

    print("Will now solve %s" % filename)
    err = problem.readMps(filename)
    if not err:
        problem.solve()
        if problem.status == 'optimal':
            print("Optimal value: %f" % problem.obj.value)
            for var in problem.cols:
                print("\t%s = %f" % (var.name, var.solution))
        else:
            print("No optimal solution could be found.")
```

Pyomo

- An algebraic modeling language in Python similar to PuLP.
- Can import data from many sources, including AMPL-style data files.
- More powerful, includes support for nonlinear modeling.
- Allows development of both concrete models (like PuLP) and abstract models (like other AMLs).
- Also include PySP for stochastic Programming.
- Primary classes
  - `ConcreteModel`, `AbstractModel`
  - `Set`, `Parameter`
  - `Var`, `Constraint`
- Developers: Bill Hart, John Siirola, Jean-Paul Watson, David Woodruff, and others...
- More on Wednesday 9:00 AM!

Thank You!

- There seems to be great potential in incorporating more of what COIN-OR offffers into Sage.
- I'd be happy to hear from anyone who agrees about potential future projects.

Questions?