# **Model-Based Optimization**

Principles and Trends

Robert Fourer
AMPL Optimization Inc.
4er@ampl.com

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# **Model-Based Optimization: Principles and Trends**

As optimization methods have been applied more broadly and effectively, a key factor in their success has been the adoption of a model-based approach. A researcher or analyst focuses on modeling the problem of interest, while the computation of a solution is left to general-purpose, off-the-shelf solvers; independent modeling languages and systems manage the difficulties of translating between the human modeler's ideas and the computer software's needs. This tutorial introduces model-based optimization with examples from the AMPL modeling language and various popular solvers; the presentation concludes by surveying current software, with special attention to the role of constraint programming.

# **Outline**

# Approaches to optimization

Model-based vs. Method-based

# Modeling languages for model-based optimization

- Motivation for modeling languages
- \* Algebraic modeling languages
- \* Executable vs. declarative languages
- Survey of modeling language software

# Solvers for model-based optimization

- Linear
- Nonlinear
- **❖** Global
- \* Constraint

# **Examples**

# Approaches to optimization

- Model-based vs. Method-based
  - \* Example: Balanced assignment

# Modeling languages for model-based optimization

- \* Executable vs. declarative languages
  - \* Example: gurobipy vs. AMPL
- Survey of modeling language software
  - \* Example: Balanced assignment in AMPL
  - \* Example: Nonlinear optimization in AMPL

# Solvers for model-based optimization

- Constraint
  - \* Example: Balanced assignment via CP in AMPL

# **Example:** Balanced Assignment

#### **Motivation**

meeting of employees from around the world

#### Given

- several employee categories (title, location, department, male/female)
- a specified number of project groups

### Assign

each employee to a project group

### So that

- the groups have about the same size
- \* the groups are as "diverse" as possible with respect to all categories

# **Method-Based** Approach

# Define an algorithm to build a balanced assignment

- Start with all groups empty
- Make a list of people (employees)
- For each person in the list:
  - \* Add to the group whose resulting "sameness" will be least

```
Initialize all groups G = { }
Repeat for each person p
   sMin = Infinity
   Repeat for each group G
      s = total "sameness" in <math>G \cup \{p\}
      if s < sMin then
         sMin = s
         GMin = G
   Assign person p to group GMin
```

# Method-Based Approach (cont'd)

# Define a computable concept of "sameness"

- Sameness of any two people:
  - \* Number of categories in which they are the same
- Sameness of a group:
  - \* Sum of the sameness of all pairs of people in the group

# Refine the algorithm to get better results

- \* Reorder the list of people
- Locally improve the initial "greedy" solution by swapping group members
- Seek further improvement through local search metaheuristics
  - \* What are the neighbors of an assignment?
  - \* How can two assignments combine to create a better one?

# **Model-Based** Approach

### Formulate a "minimal sameness" model

- Define decision variables for assignment of people to groups
  - \*  $x_{ij} = 1$  if person 1 assigned to group j
  - \*  $x_{ij} = 0$  otherwise
- Specify valid assignments through constraints on the variables
- Formulate sameness as an objective to be minimized
  - \* *Total sameness* = sum of the sameness of all groups

# Send to an off-the-shelf solver

- Choice of excellent linear-quadratic mixed-integer solvers
- Zero-one optimization is a special case

# **Model-Based Formulation**

### Given

```
P set of people
```

C set of categories of people

 $t_{ik}$  type of person *i* within category *k*, for all  $i \in P$ ,  $k \in C$ 

### and

*G* number of groups

 $g^{\min}$  lower limit on people in a group

 $g^{\text{max}}$  upper limit on people in a group

# Define

$$s_{i_1i_2} = |\{k \in C : t_{i_1k} = t_{i_2k}\}|, \text{ for all } i_1 \in P, i_2 \in P$$

$$sameness of persons i_1 \ and \ i_2$$

# **Model-Based Formulation** (cont'd)

### **Determine**

$$x_{ij} \in \{0,1\} = 1$$
 if person  $i$  is assigned to group  $j$   
= 0 otherwise, for all  $i \in P, j = 1,..., G$ 

### To minimize

$$\sum_{i_1 \in P} \sum_{i_2 \in P} s_{i_1 i_2} \sum_{j=1}^{G} x_{i_1 j} x_{i_2 j}$$
total sameness of all pairs of people in all groups

# Subject to

$$\sum_{j=1}^{G} x_{ij} = 1, \text{ for each } i \in P$$
each person must be assigned to one group

$$g^{\min} \leq \sum_{i \in P} x_{ij} \leq g^{\max}$$
, for each  $j = 1, ..., G$   
each group must be assigned an acceptable number of people

# **Model-Based Solution**

# Optimize with an off-the-shelf solver

### Choose among many alternatives

- Linearize and send to a mixed-integer linear solver
  - \* CPLEX, Gurobi, Xpress; CBC, MIPCL, SCIP
- Send quadratic formulation to a mixed-integer solver that automatically linearizes products involving binary variables
  - \* CPLEX, Gurobi, Xpress
- Send quadratic formulation to a nonlinear solver
  - **★** Mixed-integer nonlinear: Knitro, BARON
  - \* Continuous nonlinear (might come out integer): MINOS, Ipopt, ...

# Where Is the Work?

### Method-based

Programming an implementation of the method

### Model-based

Constructing a formulation of the model

# **Complications in Balanced Assignment**

# "Total Sameness" is problematical

- Hard for client to relate to goal of diversity
- Minimize "total variation" instead
  - \* Sum over all types: most minus least assigned to any group

# Client has special requirements

- ❖ No employee should be "isolated" within their group
  - **★** No group can have exactly one woman
  - \* Every person must have a group-mate from the same location and of equal or adjacent rank

# Room capacities are variable

- Different groups have different size limits
- **❖** *Minimize* "total deviation"
  - \* Sum over all types: greatest violation of target range for any group

# Method-Based (cont'd)

# Revise or replace the solution approach

- Total variation is less suitable to a greedy algorithm
- ❖ Total variation is harder to locally improve
- Client constraints are challenging to enforce

# Update or re-implement the method

Even small changes to the problem can necessitate major changes to the method and its implementation

# Model-Based (cont'd)

Replace the objective

Formulate additional constraints

Send back to the solver

# Model-Based (cont'd)

# To write new objective, add variables

 $y_{kl}^{\min}$  fewest people of category k, type l in any group,  $y_{kl}^{\max}$  most people of category k, type l in any group, for each  $k \in C$ ,  $l \in T_k = \bigcup_{i \in P} \{t_{ik}\}$ 

### Add defining constraints

$$y_{kl}^{\min} \le \sum_{i \in P: t_{ik} = l} x_{ij}$$
, for each  $j = 1, ..., G$ ;  $k \in C, l \in T_k$   
 $y_{kl}^{\max} \ge \sum_{i \in P: t_{ik} = l} x_{ij}$ , for each  $j = 1, ..., G$ ;  $k \in C, l \in T_k$ 

### Minimize total variation

$$\sum_{k \in C} \sum_{l \in T_k} (y_{kl}^{\max} - y_{kl}^{\min})$$

# Model-Based (cont'd)

To express client requirement for women in a group, let

$$Q = \{i \in P: t_{i,m/f} = \text{female}\}$$

### Add constraints

$$\sum_{i \in Q} x_{ij} = 0$$
 or  $\sum_{i \in Q} x_{ij} \ge 2$ , for each  $j = 1, \dots, G$ 

# Model-Based (cont'd)

To express client requirement for women in a group, let

$$Q = \{i \in P: t_{i,m/f} = \text{female}\}$$

Define logic variables

$$z_j \in \{0,1\} = 1$$
 if any women assigned to group  $j$   
= 0 otherwise, for all  $j = 1, ..., G$ 

Add constraints relating logic variables to assignment variables

$$z_j = 0 \Rightarrow \sum_{i \in Q} x_{ij} = 0,$$
  
 $z_j = 1 \Rightarrow \sum_{i \in Q} x_{ij} \ge 2$ , for each  $j = 1, ..., G$ 

# Model-Based (cont'd)

To express client requirement for women in a group, let

$$Q = \{i \in P: t_{i,m/f} = \text{female}\}$$

Define logic variables

$$z_j \in \{0,1\} = 1$$
 if any women assigned to group  $j$   
= 0 otherwise, for all  $j = 1, ..., G$ 

Linearize constraints relating logic variables to assignment variables

$$2z_j \le \sum_{i \in Q} x_{ij} \le |Q| z_j$$
, for each  $j = 1, ..., G$ 

# Model-Based (cont'd)

# To express client requirements for group-mates, let

$$R_{l_1 l_2} = \{i \in P: t_{i,loc} = l_1, t_{i,rank} = l_2\}, \text{ for all } l_1 \in T_{loc}, l_2 \in T_{rank}$$

 $A_l \subseteq T_{\text{rank}}$ , set of ranks adjacent to rank l, for all  $l \in T_{\text{rank}}$ 

### Add constraints

$$\sum_{i \in R_{l_1 l_2}} x_{ij} = 0 \text{ or } \sum_{i \in R_{l_1 l_2}} x_{ij} + \sum_{l \in A_{l_2}} \sum_{i \in R_{l_1 l}} x_{ij} \ge 2,$$
for each  $l_1 \in T_{\text{loc}}, l_2 \in T_{\text{rank}}, j = 1, \dots, G$ 

# Model-Based (cont'd)

# To express client requirements for group-mates, let

$$R_{l_1 l_2} = \{i \in P: t_{i,loc} = l_1, t_{i,rank} = l_2\}, \text{ for all } l_1 \in T_{loc}, l_2 \in T_{rank}$$
  
 $A_l \subseteq T_{rank}, \text{ set of ranks adjacent to rank } l, \text{ for all } l \in T_{rank}$ 

# Define logic variables

$$w_{l_1 l_2 j} \in \{0,1\} = 1$$
 if group  $j$  has anyone from location  $l_1$  of rank  $l_2$   
= 0 otherwise, for all  $l_1 \in T_{loc}$ ,  $l_2 \in T_{rank}$ ,  $j = 1, ..., G$ 

# Add constraints relating logic variables to assignment variables

$$\begin{split} w_{l_1 l_2 j} &= 0 \ \Rightarrow \sum_{i \in R_{l_1 l_2}} x_{ij} = 0, \\ w_{l_1 l_2 j} &= 1 \ \Rightarrow \sum_{i \in R_{l_1 l_2}} x_{ij} + \sum_{l \in A_{l_2}} \sum_{i \in R_{l_1 l}} x_{ij} \geq 2, \\ & \text{for each } l_1 \in T_{\text{loc}}, \, l_2 \in T_{\text{rank}}, \, j = 1, \dots, G \end{split}$$

# Model-Based (cont'd)

# To express client requirements for group-mates, let

$$R_{l_1 l_2} = \{i \in P: t_{i,loc} = l_1, t_{i,rank} = l_2\}, \text{ for all } l_1 \in T_{loc}, l_2 \in T_{rank}$$
  
 $A_l \subseteq T_{rank}, \text{ set of ranks adjacent to rank } l, \text{ for all } l \in T_{rank}$ 

# Define logic variables

$$w_{l_1 l_2 j} \in \{0,1\} = 1$$
 if group  $j$  has anyone from location  $l_1$  of rank  $l_2$   
= 0 otherwise, for all  $l_1 \in T_{loc}$ ,  $l_2 \in T_{rank}$ ,  $j = 1, ..., G$ 

# Linearize constraints relating logic variables to assignment variables

$$\begin{split} w_{l_1 l_2 j} &\leq \sum_{i \in R_{l_1 l_2}} x_{ij} \leq \left| R_{l_1 l_2} \right| w_{l_1 l_2 j}, \\ \sum_{i \in R_{l_1 l_2}} x_{ij} + \sum_{l \in A_{l_2}} \sum_{i \in R_{l_1 l}} x_{ij} \geq 2 w_{l_1 l_2 j}, \\ & \text{for each } l_1 \in T_{\text{loc}}, \, l_2 \in T_{\text{rank}}, \, j = 1, \dots, G \end{split}$$

# Method-Based Remains Popular for . . .

# Heuristic approaches

- Simple heuristics
  - \* Greedy algorithms, local improvement methods
- Metaheuristics
  - \* Evolutionary methods, simulated annealing, tabu search, GRASP, . . .

# Situations hard to formulate mathematically

- Difficult combinatorial constraints
- Black-box objectives and constraints

# Large-scale, intensive applications

- Routing fleets of delivery trucks
- Finding shortest routes in mapping apps
- Deep learning for facial recognition

# Model-Based Has Become Common in . . .

### Diverse industries

- Manufacturing, distribution, supply-chain management
- ❖ Air and rail operations, trucking, delivery services
- Medicine, medical services
- \* Refining, electric power flow, gas pipelines, hydropower
- ❖ Finance, e-commerce, . . .

# Diverse fields

- Operations research & management science
- Business analytics
- Engineering & science
- ❖ Economics & finance

# Model-Based Has Become Standard for . . .

Diverse industries

Diverse fields

# Diverse kinds of users

- Anyone who took an "optimization" class
- Anyone else with a technical background
- Newcomers to optimization

### These have in common . . .

- ❖ Good algebraic formulations for off-the-shelf solvers
- Users focused on modeling

# **Trends Favor Model-Based Optimization**

# Model-based approaches have spread

- Model-based metaheuristics ("Matheuristics")
- ❖ Solvers for SAT, planning, *constraint programing*

# Off-the-shelf optimization solvers have kept improving

- Solve the same problems faster and faster
- Handle broader problem classes
- \* Recognize special cases automatically

# Optimization models have become easier to embed within broader methods

- ❖ Solver callbacks
- Model-based evolution of solver APIs
- ❖ APIs for optimization modeling systems

# Modeling Languages for Model-Based Optimization

### Background

- The modeling lifecycle
- Matrix generators
- Modeling languages

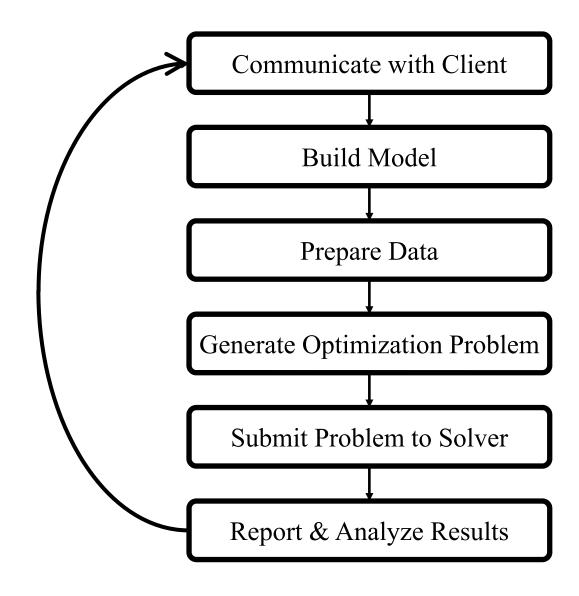
# Algebraic modeling languages

- Design approaches: declarative, executable
- \* Example: AMPL vs. gurobipy
- Survey of available software

# Balanced assignment model in AMPL

- \* Formulation
- Solution

# The Optimization Modeling Lifecycle



# Managing the Modeling Lifecycle

# Goals for optimization software

- \* Repeat the cycle quickly and reliably
- \* Get results before client loses interest
- Deploy for application

# Complication: two forms of an optimization problem

- ❖ Modeler's form
  - \* Mathematical description, easy for people to work with
- Solver's form
  - \* Explicit data structure, easy for solvers to compute with

# Challenge: translate between these two forms

### **Matrix Generators**

# Write a program to generate the solver's form

- \* Read data and compute objective & constraint coefficients
- \* Communicate with the solver via its API
- Convert the solver's solution for viewing or processing

#### Some attractions

- Ease of embedding into larger systems
- \* Access to advanced solver features

# Serious disadvantages

- Difficult environment for modeling
  - \* program does not resemble the modeler's form
  - \* model is not separate from data
- Very slow modeling cycle
  - \* hard to check the program for correctness
  - \* hard to distinguish modeling from programming errors

[1980] Over the past seven years we have perceived that the size distribution of general structure LP problems being run on commercial LP codes has remained about stable. . . . A 3000 constraint LP model is still considered large and very few LP problems larger than 6000 rows are being solved on a production basis. . . . That this distribution has not noticeably changed despite a massive change in solution economics is unexpected.

We do not feel that the linear programming user's most pressing need over the next few years is for a new optimizer that runs twice as fast on a machine that costs half as much (although this will probably happen). Cost of optimization is just not the dominant barrier to LP model implementation. The process required to manage the data, formulate and build the model, report on and analyze the results costs far more, and is much more of a barrier to effective use of LP, than the cost/performance of the optimizer.

Why aren't more larger models being run? It is not because they could not be useful; it is because we are not successful in using them. . . . They become unmanageable. LP technology has reached the point where anything that can be formulated and understood can be optimized at a relatively modest cost.

C.B. Krabek, R.J. Sjoquist and D.C. Sommer, The APEX Systems: Past and Future. *SIGMAP Bulletin* **29** (April *1980*) 3–23.

# **Modeling Languages**

### Describe your model

- Write your symbolic model in a computer-readable modeler's form
- Prepare data for the model
- Let computer translate to & from the solver's form

### Limited drawbacks

- Need to learn a new language
- ❖ Incur overhead in translation
- \* Make formulations clearer and hence easier to steal?

### Great advantages

- Faster modeling cycles
- More reliable modeling
- More maintainable applications

[1982] The aim of this system is to provide one representation of a model which is easily understood by both humans and machines. . . . With such a notation, the information content of the model representation is such that a machine can not only check for algebraic correctness and completeness, but also interface automatically with solution algorithms and report writers.

... a significant portion of total resources in a modeling exercise ... is spent on the generation, manipulation and reporting of models. It is evident that this must be reduced greatly if models are to become effective tools in planning and decision making.

The heart of it all is the fact that solution algorithms need a data structure which, for all practical purposes, is impossible to comprehend by humans, while, at the same time, meaningful problem representations for humans are not acceptable to machines. We feel that the two translation processes required (to and from the machine) can be identified as the main source of difficulties and errors. GAMS is a system that is designed to eliminate these two translation processes, thereby lifting a technical barrier to effective modeling . . .

J. Bisschop and A. Meeraus, On the Development of a General Algebraic Modeling System in a Strategic Planning Environment. *Mathematical Programming Study* **20** (*1982*) 1–29.

[1983] These two forms of a linear program — the modeler's form and the algorithm's form — are not much alike, and yet neither can be done without. Thus any application of linear optimization involves translating the one form to the other. This process of translation has long been recognized as a difficult and expensive task of practical linear programming.

In the traditional approach to translation, the work is divided between modeler and machine. . . .

There is also a quite different approach to translation, in which as much work as possible is left to the machine. The central feature of this alternative approach is a *modeling language* that is written by the modeler and translated by the computer. A modeling language is not a programming language; rather, it is a declarative language that expresses the modeler's form of a linear program in a notation that a computer system can interpret.

R. Fourer, Modeling Languages Versus Matrix Generators for Linear Programming. *ACM Transactions on Mathematical Software* **9** (1983) 143–183.

# Algebraic Modeling Languages

# Designed for a model-based approach

- Define data in terms of sets & parameters
  - \* Analogous to database keys & records
- Define decision variables
- Minimize or maximize an algebraic function of decision variables
- Subject to algebraic equations or inequalities that constrain the values of the variables

# Advantages

- \* Familiar
- \* Powerful
- Proven

#### Algebraic Modeling Languages

# **Overview**

# Design alternatives

- \* Executable: object libraries for programming languages
- \* Declarative: specialized optimization languages

# Design comparison

❖ Executable versus declarative using one simple example

### Survey

- Solver-independent vs. solver-specific
- Proprietary vs. free
- Notable specific features

## **Executable**

### Concept

- Create an algebraic modeling language inside a general-purpose programming language
- ❖ Redefine operators like + and <= to return constraint objects rather than simple values

### Advantages

- Ready integration with applications
- Good access to advanced solver features

## Disadvantages

- Programming issues complicate description of the model
- Modeling and programming bugs are hard to separate
- Efficiency issues are more of a concern

## **Declarative**

### Concept

- Design a language specifically for optimization modeling
  - \* Resembles mathematical notation as much as possible
- Extend to command scripts and database links
- Connect to external applications via APIs

### Disadvantages

- ❖ Adds a system between application and solver
- ❖ Does not have a full object-oriented programming framework

### Advantages

- Streamlines model development
- ❖ Promotes validation and maintenance of models
- Can provide APIs for many popular programming languages

# Comparison: Executable vs. Declarative

### Two representative widely used systems

- **❖** Executable: *gurobipy* 
  - \* Python modeling interface for Gurobi solver
  - \* http://gurobi.com
- ❖ Declarative: *AMPL* 
  - \* Specialized modeling language with multi-solver support
  - \* http://ampl.com

### Data

## gurobipy

Assign values to Python lists and dictionaries

```
commodities = ['Pencils', 'Pens']

nodes = ['Detroit', 'Denver',
  'Boston', 'New York', 'Seattle']

arcs, capacity = multidict({
    ('Detroit', 'Boston'): 100,
    ('Detroit', 'New York'): 80,
    ('Detroit', 'Seattle'): 120,
    ('Denver', 'Boston'): 120,
    ('Denver', 'New York'): 120,
    ('Denver', 'New York'): 120,
    ('Denver', 'Seattle'): 120 })
```

Provide data later in a separate file

#### AMPL

Define symbolic model sets and parameters

```
set COMMODITIES;
set NODES;
set ARCS within {NODES, NODES};
param capacity {ARCS} >= 0;
```

```
set COMMODITIES := Pencils Pens ;
set NODES := Detroit Denver
Boston 'New York' Seattle ;
param: ARCS: capacity:
    Boston 'New York' Seattle :=
Detroit 100 80 120
Denver 120 120 120 ;
```

## Data (cont'd)

## gurobipy

```
inflow = {
    ('Pencils', 'Detroit'): 50,
    ('Pencils', 'Denver'): 60,
    ('Pencils', 'Boston'): -50,
    ('Pencils', 'New York'): -50,
    ('Pencils', 'Seattle'): -10,
    ('Pens', 'Detroit'): 60,
    ('Pens', 'Denver'): 40,
    ('Pens', 'Boston'): -40,
    ('Pens', 'New York'): -30,
    ('Pens', 'Seattle'): -30 }
```

```
param inflow {COMMODITIES,NODES};
```

## Data (cont'd)

### gurobipy

```
cost = {
    ('Pencils', 'Detroit', 'Boston'): 10,
    ('Pencils', 'Detroit', 'New York'): 20,
    ('Pencils', 'Detroit', 'Seattle'): 60,
    ('Pencils', 'Denver', 'Boston'): 40,
    ('Pencils', 'Denver', 'New York'): 40,
    ('Pencils', 'Denver', 'Seattle'): 30,
    ('Pens', 'Detroit', 'Boston'): 20,
    ('Pens', 'Detroit', 'New York'): 20,
    ('Pens', 'Detroit', 'Seattle'): 80,
    ('Pens', 'Denver', 'Boston'): 60,
    ('Pens', 'Denver', 'Boston'): 70,
    ('Pens', 'Denver', 'New York'): 70,
    ('Pens', 'Denver', 'Seattle'): 30 }
```

# Data (cont'd)

```
param cost {COMMODITIES,ARCS} >= 0;
```

```
param cost
 [Pencils,*,*] (tr) Detroit Denver :=
    Boston
                           40
                    10
    'New York'
                    20
                           40
                    60
    Seattle
                           30
 [Pens,*,*] (tr) Detroit Denver :=
    Boston
                    20
                           60
    'New York'
                    20
                           70
    Seattle
                    80
                           30
```

### Model

## gurobipy

## (Note on Summations)

### gurobipy quicksum

```
m.addConstrs(
  (quicksum(flow[h,i,j] for i,j in arcs.select('*',j)) + inflow[h,j] ==
   quicksum(flow[h,j,k] for j,k in arcs.select(j,'*'))
   for h in commodities for j in nodes), "node")
```

#### quicksum (data)

A version of the Python sum function that is much more efficient for building large Gurobi expressions (LinExpr or QuadExpr objects). The function takes a list of terms as its argument.

Note that while quicksum is much faster than sum, it isn't the fastest approach for building a large expression. Use addTerms or the LinExpr() constructor if you want the quickest possible expression construction.

## Model (cont'd)

```
var Flow {COMMODITIES,ARCS} >= 0;
minimize TotalCost:
    sum {h in COMMODITIES, (i,j) in ARCS} cost[h,i,j] * Flow[h,i,j];
subject to Capacity {(i,j) in ARCS}:
    sum {h in COMMODITIES} Flow[h,i,j] <= capacity[i,j];
subject to Conservation {h in COMMODITIES, j in NODES}:
    sum {(i,j) in ARCS} Flow[h,i,j] + inflow[h,j] =
    sum {(j,i) in ARCS} Flow[h,j,i];</pre>
```

## **Solution**

## gurobipy

# Solution (cont'd)

```
ampl: solve;
Gurobi 8.0.0: optimal solution; objective 5500
2 simplex iterations
ampl: display Flow;
Flow [Pencils,*,*]
       Boston 'New York' Seattle :=
                  50
                          10
Denver
Detroit 50
                           0
 [Pens,*,*]
       Boston 'New York' Seattle
                                  :=
Denver
          10
                          30
Detroit 30
                  30
```

## **Integration with Solvers**

## gurobipy

- Works closely with the Gurobi solver:
   callbacks during optimization, fast re-solves after problem changes
- Offers convenient extended expressions: min/max, and/or, if-then-else

- Supports all popular solvers
- Extends to general nonlinear and logic expressions
   Connects to nonlinear function libraries and user-defined functions
- Automatically computes nonlinear function derivatives

## **Integration with Applications**

## gurobipy

- Everything can be developed in Python
  - \* Extensive data, visualization, deployment tools available
- ❖ Limited modeling features also in C++, C#, Java

- Modeling language extended with loops, tests, assignments
- ❖ Application programming interfaces (APIs) for calling AMPL from C++, C#, Java, MATLAB, Python, R
  - \* Efficient methods for data interchange
- ❖ Add-ons for streamlined deployment
  - \* QuanDec by Cassotis
  - \* Opalytics Cloud Platform

# **Software Survey**

## Solver-specific

- Associated with popular commercial solvers
- \* Executable and declarative alternatives

## Solver-independent

- Support multiple solvers and solver types
- ❖ Mostly commercial/declarative and free/executable

#### Survey

# **Solver-Specific**

#### Declarative, commercial

- ❖ OPL for CPLEX (IBM)
- ❖ MOSEL\* for Xpress (FICO)
- ❖ OPTMODEL for SAS/OR (SAS)

### Executable, commercial

- ❖ Concert Technology C++ for CPLEX
- gurobipy for Gurobi
- sasoptpy for SAS Optimization

#### Survey

# Solver-Independent

### Declarative, commercial

- \* AIMMS
- \* AMPL
- \* GAMS
- \* MPL

### Declarative, free

- \* CMPL
- ❖ GMPL / MathProg

### Executable, free

- PuLP; Pyomo / Python
- ❖ YALMIP; CVX / MATLAB
- JuMP / Julia
- **❖** FLOPC++ / C++

## **Trends**

### Commercial, declarative modeling systems

- ❖ Established lineup of solver-independent modeling systems that represent decades of development and support
- Extended with scripting, APIs, data tools to promote integration with broader applications

### Commercial, executable modeling systems

- Increasingly essential to commercial solver offerings
- ❖ Becoming the recommended APIs for solvers

### Free, executable modeling systems

- ❖ A major current focus of free optimization software development
- Interesting new executable modeling languages
   have become easier to develop than interesting new solvers

# **Special Notes**

#### Notable cases not detailed earlier . . .

- \* AIMMS (solver-independent, commercial, declarative) has extensive application development tools built in
- \* CMPL (solver-independent, free, declarative) has an IDE, Python and Java APIs, and remote server support
- ❖ GMPL/MathProg (solver-independent, free, declarative) is a free implementation of mainly a subset of AMPL
- ❖ JuMP (solver-independent, free, executable) claims greater efficiency through use of a new programming language, Julia
- MOSEL for Xpress (solver-specific, commercial)

   a hybrid of declarative and executable,
   has recently been made free and may accept other solvers

# **Balanced Assignment Revisited**

#### Given

```
P set of people
```

C set of categories of people

 $t_{ik}$  type of person *i* within category *k*, for all  $i \in P$ ,  $k \in C$ 

#### and

```
G number of groups
```

 $g^{\min}$  lower limit on people in a group

 $g^{\text{max}}$  upper limit on people in a group

### Define

$$T_k = \bigcup_{i \in P} \{t_{ik}\}, \text{ for all } k \in C$$
  
set of all types of people in category  $k$ 

# Balanced Assignment Revisited in AMPL

#### Sets, parameters

# **Balanced Assignment**

#### **Determine**

```
x_{ij} \in \{0,1\} = 1 if person i is assigned to group j = 0 otherwise, for all i \in P, j = 1, ..., G y_{kl}^{\min} fewest people of category k, type l in any group, y_{kl}^{\max} most people of category k, type l in any group, for each k \in C, l \in T_k
```

#### Where

$$y_{kl}^{\min} \le \sum_{i \in P: t_{ik} = l} x_{ij}$$
, for each  $j = 1, ..., G$ ;  $k \in C, l \in T_k$   
 $y_{kl}^{\max} \ge \sum_{i \in P: t_{ik} = l} x_{ij}$ , for each  $j = 1, ..., G$ ;  $k \in C, l \in T_k$ 

# Balanced Assignment in AMPL

### Variables, defining constraints

```
var Assign {i in PEOPLE, j in 1..numberGrps} binary;
              # Assign[i,j] is 1 if and only if
              # person i is assigned to group j
var MinType {k in CATEG, TYPES[k]};
var MaxType {k in CATEG, TYPES[k]};
              # fewest and most people of each type, over all groups
subj to MinTypeDefn {j in 1..numberGrps, k in CATEG, l in TYPES[k]}:
  MinType[k,1] <= sum {i in PEOPLE: type[i,k] = 1} Assign[i,j];</pre>
subj to MaxTypeDefn {j in 1..numberGrps, k in CATEG, l in TYPES[k]}:
   MaxType[k,1] >= sum {i in PEOPLE: type[i,k] = 1} Assign[i,j];
              # values of MinTypeDefn and MaxTypeDefn variables
              # must be consistent with values of Assign variables
```

$$y_{kl}^{\max} \ge \sum_{i \in P: t_{ik} = l} x_{ij}$$
, for each  $j = 1, \dots, G$ ;  $k \in C$ ,  $l \in T_k$ 

# **Balanced Assignment**

#### *Minimize*

$$\sum_{k \in C} \sum_{l \in T_k} (y_{kl}^{\max} - y_{kl}^{\min})$$

sum of inter-group variation over all types in all categories

### Subject to

$$\sum_{j=1}^{G} x_{ij} = 1, \text{ for each } i \in P$$

each person must be assigned to one group

$$g^{\min} \le \sum_{i \in P} x_{ij} \le g^{\max}$$
, for each  $j = 1, ..., G$ 

each group must be assigned an acceptable number of people

# Balanced Assignment in AMPL

### Objective, assignment constraints

```
minimize TotalVariation:
    sum {k in CATEG, l in TYPES[k]} (MaxType[k,1] - MinType[k,1]);
          # Total variation over all types

subj to AssignAll {i in PEOPLE}:
    sum {j in 1..numberGrps} Assign[i,j] = 1;
          # Each person must be assigned to one group

subj to GroupSize {j in 1..numberGrps}:
    minInGrp <= sum {i in PEOPLE} Assign[i,j] <= maxInGrp;
          # Each group must have an acceptable size</pre>
```

$$g^{\min} \le \sum_{i \in P} x_{ij} \le g^{\max}$$
, for each  $j = 1, \dots, G$ 

# **Balanced Assignment**

## Define also

$$Q = \{i \in P: t_{i,m/f} = \text{female}\}$$

#### **Determine**

$$z_j \in \{0,1\} = 1$$
 if any women assigned to group  $j$   
= 0 otherwise, for all  $j = 1, ..., G$ 

### Subject to

$$2z_j \le \sum_{i \in Q} x_{ij} \le |Q| z_j$$
, for each  $j = 1, ..., G$   
each group must have either  
no women  $(z_j = 0)$  or  $\ge 2$  women  $(z_j = 1)$ 

# Balanced Assignment in AMPL

### Supplemental constraints

```
set WOMEN = {i in PEOPLE: type[i,'m/f'] = 'F'};
var WomenInGroup {j in 1..numberGrps} binary;
subj to Min2WomenInGroupLO {j in 1..numberGrps}:
    2 * WomenInGroup[j] <= sum {i in WOMEN} Assign[i,j];
subj to Min2WomenInGroupUP {j in 1..numberGrps}:
    sum {i in WOMEN} Assign[i,j] <= card(WOMEN) * WomenInGroup[j];</pre>
```

$$2z_j \le \sum_{i \in Q} x_{ij} \le |Q| z_j$$
, for each  $j = 1, \dots, G$ 

#### Balanced Assignment

# **Modeling Language Data**

### 210 people

```
set PEOPLE :=
   BIW
          AJH
                  FWI
                         IGN
                                KWR
                                       KKI
                                               HMN
                                                      SML
                                                             RSR
                                                                    TBR
   KRS
          CAE
                         CAR
                                PSL
                                       BCG
                                              DJA
                                                      AJT
                                                             JPY
                                                                    HWG
                  MPO
   TLR
          MRL
                  JDS
                         JAE
                                TEN
                                       MKA
                                               NMA
                                                      PAS
                                                             DLD
                                                                    SCG
          FTR
                  GCY
                         OGZ
                                SME
                                       KKA
                                               MMY
                                                             ASA
                                                                    JLN
   VAA
                                                      API
                                                                    JSG
   JRT
          SJO
                  WMS
                         RLN
                                WLB
                                       SGA
                                               MRE
                                                      SDN
                                                             HAN
   AMR
          DHY
                  JMS
                         AGI
                                RHE
                                       BLE
                                               SMA
                                                      BAN
                                                             JAP
                                                                    HER
   MES
          DHE
                  SWS
                         ACI
                                       TWD
                                               MMA
                                                                    LHS
                                RJY
                                                      JJR
                                                             MFR
   JAD
          CWU
                  PMY
                         CAH
                                SJH
                                       EGR
                                               JMQ
                                                      GGH
                                                                    JWR
                                                             MMH
   MJR
          EAZ
                  WAD
                         LVN
                                DHR
                                       ABE
                                               LSR
                                                      MBT
                                                             AJU
                                                                    SAS
          RFS
                                                                    CGS
   JRS
                  TAR
                         DLT
                                HJO
                                       SCR
                                               CMY
                                                      GDE
                                                             MSL
   HCN
          JWS
                  RPR
                         RCR
                                RLS
                                       DSF
                                               MNA
                                                             PSY
                                                                    MET
                                                      MSR
          RVY
                  PWS
                         CTS
                                KLN
                                       RDN
                                               ANV
                                                             FSM
                                                                    KWN
   DAN
                                                      LMN
   CWT
          PMO
                  EJD
                         AJS
                                SBK
                                       JWB
                                               SNN
                                                      PST
                                                             PSZ
                                                                    AWN
          RGR
   DCN
                  CPR
                         NHI
                                HKA
                                       VMA
                                               DMN
                                                      KRA
                                                             CSN
                                                                    HRR
   SWR
          LLR
                  AVI
                         RHA
                                KWY
                                       MLE
                                               FJL
                                                      ES<sub>0</sub>
                                                             TJY
                                                                    WHF
   TBG
          FEE
                  MTH
                                WFS
                                               SOL
                                                      ASO
                                                                    RGE
                         RMN
                                       CEH
                                                             MDI
                                                                    HMG
   LVO
          ADS
                  CGH
                         RHD
                                MBM
                                       MRH
                                               RGF
                                                      PSA
                                                             TTI
          CFS
   ECA
                  MKN
                         SBM
                                RCG
                                       JMA
                                               EGL
                                                      UJT
                                                             ETN
                                                                    GWZ
   MAI
          DBN
                  HFE
                         PS<sub>0</sub>
                                APT
                                       JMT
                                               RJE
                                                      MRZ
                                                                    XYF
                                                             MRK
   JCO
          PSN
                  SCS
                         RDL
                                TMN
                                       CGY
                                               GMR
                                                      SER
                                                             RMS
                                                                    JEN
                  DGR
   DWO
          REN
                         DET
                                FJT
                                       RJZ
                                               MBY
                                                      RSN
                                                             REZ
                                                                    BLW ;
```

# **Modeling Language Data**

4 categories, 18 types, 12 groups, 16-19 people/group

```
set CATEG := dept loc 'm/f' title ;
param type:
                loc
                    'm/f' title
     dept
BIW
      NNE
            Peoria
                              Assistant
      WSW
KRS
            Springfield
                              Assistant
TLR
      NNW
            Peoria
                              Adjunct
      NNW
VAA
            Peoria
                              Deputy
JRT
      NNE
            Springfield
                              Deputy
      SSE
AMR
            Peoria
                              Deputy
MES
      NNE
            Peoria
                              Consultant
JAD
      NNE
           Peoria
                              Adjunct
MJR
      NNE
            Springfield
                              Assistant
JRS
      NNE
            Springfield
                              Assistant
HCN
      SSE
            Peoria
                              Deputy
DAN
      NNE
            Springfield
                              Adjunct
param numberGrps := 12 ;
param minInGrp := 16 ;
param maxInGrp := 19 ;
```

## **Modeling Language Solution**

Model + data = problem instance to be solved (CPLEX)

```
ampl: model BalAssign.mod;
ampl: data BalAssign.dat;
ampl: option solver cplex;
ampl: option show_stats 1;
ampl: solve;
2568 variables:
        2532 binary variables
        36 linear variables
678 constraints, all linear; 26328 nonzeros
        210 equality constraints
        456 inequality constraints
        12 range constraints
1 linear objective; 36 nonzeros.
CPLEX 12.8.0.0: optimal integer solution; objective 16
115096 MIP simplex iterations
1305 branch-and-bound nodes
                                                              10.5 sec
```

## **Modeling Language Solution**

Model + data = problem instance to be solved (Gurobi)

```
ampl: model BalAssign.mod;
ampl: data BalAssign.dat;
ampl: option solver gurobi;
ampl: option show_stats 1;
ampl: solve;
2568 variables:
        2532 binary variables
        36 linear variables
678 constraints, all linear; 26328 nonzeros
        210 equality constraints
        456 inequality constraints
        12 range constraints
1 linear objective; 36 nonzeros.
Gurobi 8.0.0: optimal solution; objective 16
483547 simplex iterations
808 branch-and-cut nodes
                                                             108.8 sec
```

# Balanced Assignment (logical)

## Define also

$$Q = \{i \in P: t_{i,m/f} = \text{female}\}$$

#### **Determine**

$$z_j \in \{0,1\} = 1$$
 if any women assigned to group  $j$   
= 0 otherwise, for all  $j = 1, ..., G$ 

#### Where

$$z_j = 0 \Rightarrow \sum_{i \in Q} x_{ij} = 0,$$
  
 $z_j = 1 \Rightarrow \sum_{i \in Q} x_{ij} \ge 2$ , for each  $j = 1, ..., G$ 

# Balanced Assignment in AMPL

### Supplemental logical constraints

$$z_j = 0 \Rightarrow \sum_{i \in Q} x_{ij} = 0,$$
  
 $z_j = 1 \Rightarrow \sum_{i \in Q} x_{ij} \ge 2$ , for each  $j = 1, ..., G$ 

#### Balanced Assignment

# Balanced Assignment in AMPL

#### Send to "linear" solver

```
ampl: model BalAssignWomen.mod
ampl: data BalAssign.dat
ampl: option solver gurobi;
ampl: solve
2568 variables:
         2184 binary variables
         348 nonlinear variables
         36 linear variables
654 algebraic constraints, all linear; 25632 nonzeros
         210 equality constraints
         432 inequality constraints
         12 range constraints
12 logical constraints
1 linear objective; 29 nonzeros.
Gurobi 8.0.0: optimal solution; objective 16
265230 simplex iterations
756 branch-and-cut nodes
                                                              42.8 sec
```

#### Balanced Assignment

# Balanced Assignment in AMPL (refined)

#### Add bounds on variables

```
var MinType {k in CATEG, t in TYPES[k]}
  <= floor (card {i in PEOPLE: type[i,k] = t} / numberGrps);
var MaxType {k in CATEG, t in TYPES[k]
  >= ceil (card {i in PEOPLE: type[i,k] = t} / numberGrps);
```

```
ampl: solve

Presolve eliminates 72 constraints.
...

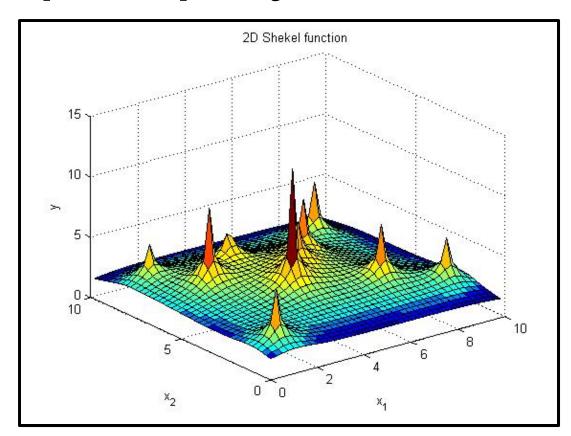
Gurobi 8.0.0: optimal solution; objective 16
1617 simplex iterations
1 branch-and-cut nodes

0.16 sec
```

# Nonlinear Optimization in AMPL

## Example: Shekel function

https://en.wikipedia.org/wiki/Shekel\_function



## **Mathematical Formulation**

### Given

*m* number of locally optimal points

*n* number of variables

### and

 $a_{ij}$  for each i = 1,...,m and j = 1,...,n $c_i$  for each i = 1,...,m

### **Determine**

 $x_i$  for each j = 1, ..., n

### to maximize

$$\sum_{i=1}^{m} 1/(c_i + \sum_{j=1}^{n} (x_j - a_{ij})^2)$$

# **Modeling Language Formulation**

Symbolic model (AMPL)

```
param m integer > 0;
param n integer > 0;
param a {1..m, 1..n};
param c {1..m};

var x {1..n};

maximize objective:
    sum {i in 1..m} 1 / (c[i] + sum {j in 1..n} (x[j] - a[i,j])^2);
```

$$\sum_{i=1}^{m} 1/(c_i + \sum_{j=1}^{n} (x_j - a_{ij})^2)$$

# **Modeling Language Data**

Explicit data (independent of model)

# **Modeling Language Solution**

Model + data = problem instance to be solved

```
ampl: model shekelEX.mod;
ampl: data shekelEX.dat;
ampl: option solver knitro;
ampl: solve;
Knitro 10.3.0: Locally optimal solution.
objective 5.055197729; feasibility error 0
6 iterations; 9 function evaluations
ampl: display x;
x [*] :=
1 1.00013
 1.00016
3 1.00013
4 1.00016
```

# **Modeling Language Solution**

... again with multistart option

```
ampl: model shekelEX.mod;
ampl: data shekelEX.dat;
ampl: option solver knitro;
ampl: option knitro_options 'ms_enable=1 ms_maxsolves=100';
ampl: solve;
Knitro 10.3.0: Locally optimal solution.
objective 10.15319968; feasibility error 0
43 iterations; 268 function evaluations
ampl: display x;
x [*] :=
1 4.00004
2 4.00013
3 4.00004
4 4.00013
```

# Solution (cont'd)

... again with a "global" solver

```
ampl: model shekelEX.mod;
ampl: data shekelEX.dat;
ampl: option solver baron;
ampl: solve;
BARON 17.10.13 (2017.10.13):
43 iterations, optimal within tolerances.
Objective 10.15319968
ampl: display x;
x [*] :=
1 4.00004
2 4.00013
3 4.00004
4 4.00013
```

# **Solvers for Model-Based Optimization**

Off-the-shelf solvers for broad problem classes

Three widely used types

- "Linear"
- \* "Nonlinear"
- "Global"

## "Linear" Solvers

## Require objective and constraint coefficients

## Linear objective and constraints

- Continuous variables
  - \* Primal simplex, dual simplex, interior-point
- Integer (including zero-one) variables
  - **★** Branch-and-bound + feasibility heuristics + cut generation
  - \* Automatic transformations to integer: piecewise-linear, discrete variable domains, indicator constraints
  - \* "Callbacks" to permit problem-specific algorithmic extensions

## Quadratic extensions

- Convex elliptic objectives and constraints
- Convex conic constraints
- ❖ Variable × binary in objective
  - \* Transformed to linear (or to convex if binary × binary)

# "Linear" Solvers (cont'd)

## CPLEX, Gurobi, Xpress

- Dominant commercial solvers
- Similar features
- Supported by many modeling systems

## SAS Optimization, MATLAB intlinprog

- Components of widely used commercial analytics packages
- ❖ SAS performance within 2x of the "big three"

### **MOSEK**

Commercial solver strongest for conic problems

### CBC, MIPCL, SCIP

- Fastest noncommercial solvers
- ❖ Effective alternatives for easy to moderately difficult problems
- ❖ MIPCL within 7x on some benchmarks

## "Nonlinear" Solvers

## Require function and derivative evaluations

### Continuous variables

- Smooth objective and constraint functions
- Locally optimal solutions
- Variety of methods
  - \* Interior-point, sequential quadratic, reduced gradient

## Extension to integer variables

## "Nonlinear" Solvers

### **Knitro**

- Most extensive commercial nonlinear solver
- Choice of methods; automatic choice of multiple starting points
- Parallel runs and parallel computations within methods
- Continuous and integer variables

## CONOPT, LOQO, MINOS, SNOPT

- Highly regarded commercial solvers for continuous variables
- Implement a variety of methods

## Bonmin, Ipopt

- Highly regarded free solvers
  - \* Ipopt for continuous problems via interior-point methods
  - **★** Bonmin extends to integer variables

## "Global" Solvers

## Require expression graphs (or equivalent)

## Nonlinear + global optimality

- Substantially harder than local optimality
- Smooth nonlinear objective and constraint functions
- Continuous and integer variables

### **BARON**

Dominant commercial global solver

### Couenne

Highly regarded noncommercial global solver

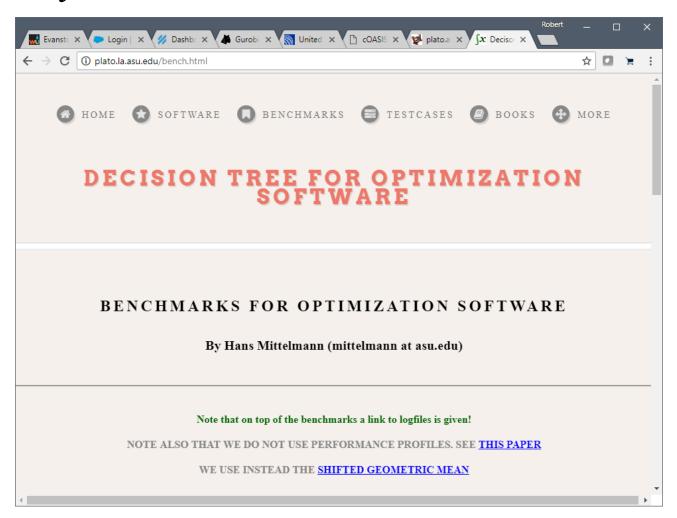
### LGO

- High-quality solutions, may be global
- Objective and constraint functions may be nonsmooth

Off-the-Shelf Solvers

## **Benchmarks**

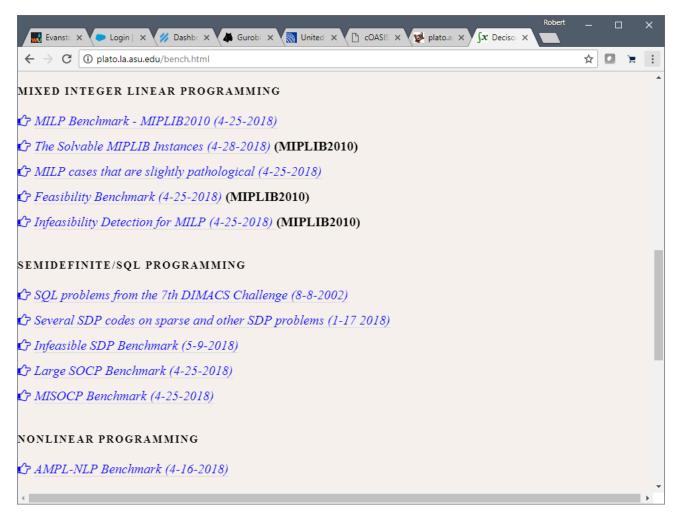
## Prof. Hans Mittelmann's benchmark website



### Off-the-Shelf Solvers

## **Benchmarks**

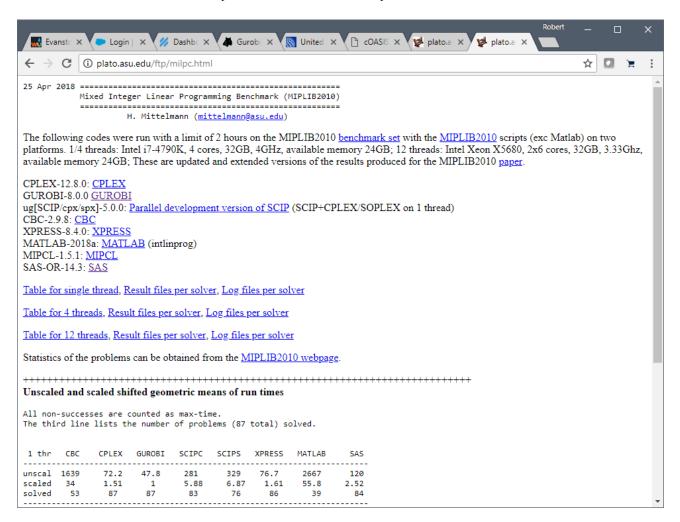
## By problem type and test set



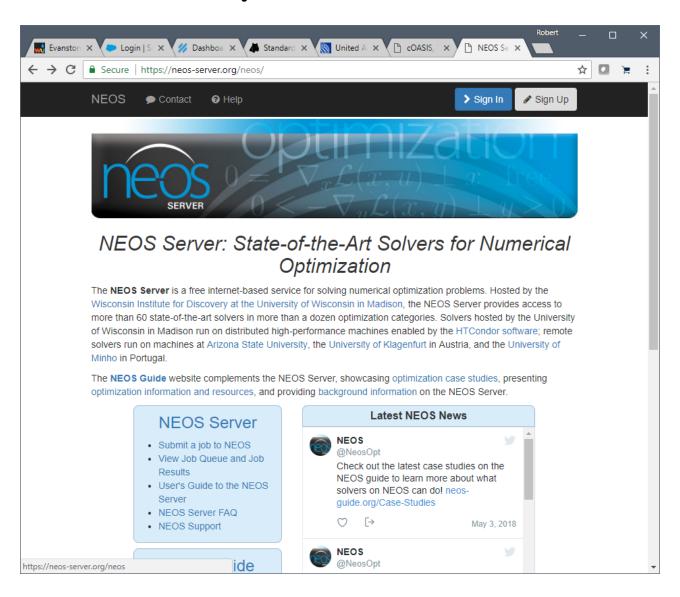
### Off-the-Shelf Solvers

## **Benchmarks**

### Documentation, summaries, links to detailed results

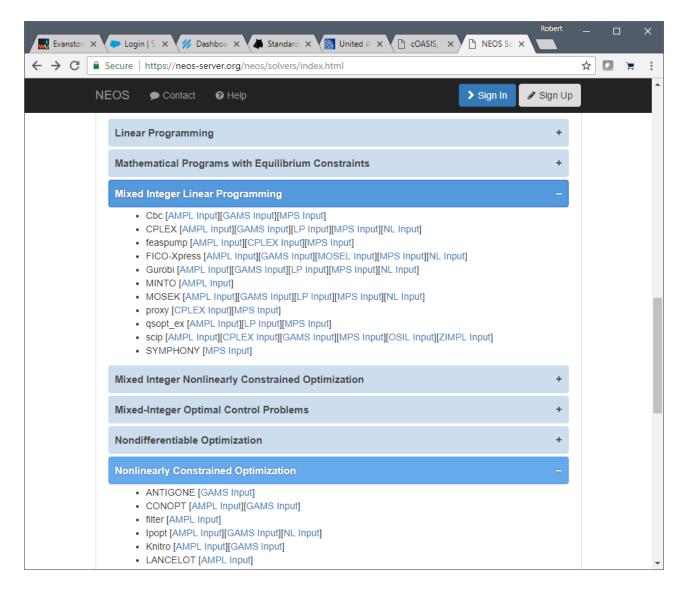


# **Curious? Try Them Out on NEOS!**



#### NEOS Server

# Solver & Language Listing



## **About the NEOS Server**

### Solvers

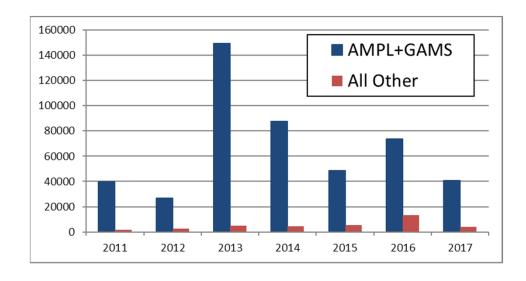
- ❖ 18 categories, 60+ solvers
- Commercial and noncommercial choices
- ❖ Almost all of the most popular ones

## *Inputs*

- Modeling languages: AMPL, GAMS, . . .
- ❖ Lower-level formats: MPS, LP, . . .

## *Interfaces*

- Web browser
- Special solver ("Kestrel") for AMPL and GAMS
- Python API



# **About the NEOS Server** (cont'd)

### Limits

- \* 8 hours
- **❖** 3 GBytes

## **Operation**

- Requests queued centrally, distributed to various servers for solving
- ❖ 650,000+ requests served in the past year, about 1800 per day or 75 per hour
- ❖ 17,296 requests on peak day (15 March 2018)

### Between method-based and model-based

- \* Relies on solvers
- ❖ Focus of the work may be on methods or may be on modeling

### Method-based view

❖ CP solver as a framework for implementation

### Model-based view

CP solver as an alternative type

## Method-Based vs. Model-Based

### Method-based view

- Define global constraints to express the problem
- ❖ Implement methods required to use the constraints in the solver
  - \* *Filtering*, checking, explanation, counting, reification, . . .
- Program the search procedure for the solver
  - \* Possibly add constraints via restrictions to the search

### Model-based view

- Write a model naturally without linearizing
  - \* Not-linear operators: min, max, abs
  - \* Logic operators: and, or, not, if-then
  - \* Global constraints: alldiff, atleast, atmost
  - \* Variables as indices
- Send to an off-the-shelf CP solver

# **CP Approach** to Balanced Assignment

## Fewer variables with larger domains

### Balanced Assignment

# **CP** Approach

## Global constraint for assignment to groups

### Balanced Assignment

# **CP** Approach

## Disjunctive constraint for women in a group

### Balanced Assignment

# **CP** Approach

### Solve with IBM ILOG CP

```
ampl: model BalAssign+CP.mod
ampl: data BalAssign.dat
ampl: option solver ilogcp;
ampl: solve;
246 variables:
        36 integer variables
        210 nonlinear variables
444 algebraic constraints, all nonlinear; 23112 nonzeros
        432 inequality constraints
        12 range constraints
12 logical constraints
1 linear objective; 28 nonzeros.
ilogcp 12.7.0: optimal solution
512386 choice points, 232919 fails, objective 16
                                                               5.3 sec
```

# Algebraic Modeling Languages for CP

### $IBM \ CPLEX \ C++API$

Executable, solver-specific

### IBM CPLEX OPL

Declarative, solver-specific

### **MiniZinc**

Declarative, solver-independent

# **Summary: Model-Based Optimization**

## Division of labor

- Analysts who build symbolic optimization models
- Developers who create general-purpose solvers

A successful approach across very diverse application areas

# Modeling languages (like AMPL) bridge the gap between models and solvers

- Translate between modeler's form and algorithm's form
- Maintain independence of model and data
- Offer independence of model and data from solver