### **Modeling, not Programming** Model-Based Optimization in AMPL

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### **Optimization in Analytics**

Goals

Features

**Applications** 

Steps

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### **Optimization** Goals

#### Given a recurring need to make many interrelated decisions

Purchases, production and shipment amounts, assignments, . . .

#### Consistently make highly desirable choices

By applying concepts of mathematical optimization

- Ways of describing problems (formulations)
- Ways of solving problems (algorithms)

### **Optimization** *Features*

Large numbers of decision variables

\* Thousands to millions

An objective function

✤ Minimize or maximize

#### Various constraint types

- ✤ 10-20 distinct types, though large numbers of each type
- \* Few variables involved in each constraint

#### Numerous scenarios with different data

\* Can't characterize all possible solutions in advance

## **Optimization** Applications



#### Energy and Utilities

✤ power networks, gas pipelines, hydroelectric power, water distribution

#### Production

- mining, steel, chemicals, oil refining, forestry and paper
- cars & trucks, paper products, processed foods

#### Transportation

✤ airlines, trucking, package delivery

#### Services

supply chain, hospitals & medicine, construction management

#### *Communications*

telecommunications, professional networking, file hosting

#### Finance

✤ software tools, investment management, commodity management

#### Advanced Technologies

✤ artificial intelligence, distributed computing, biotechnology

### **Optimization** *Development* Steps



### **Optimization** *Development Cycle*



### **Optimization** *Development Cycle*

#### Goals for optimization practitioners

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

#### Goals for optimization software

- Promote fast prototyping
- ✤ Facilitate integration with application systems
- Encourage long-term maintenance



### **Overview**

#### Modeling, not programming

#### Comparison of approaches

- Optimization: Model-based or method-based?
- Model-based optimization: Modeling language or programming language?
- Modeling languages: Declarative or executable?

#### Case studies

- Packing shipments
- ✤ Designing aircraft
- Managing power grids
- Assigning students to classes

## **Approaches to Optimization**

#### Method-based approach

\* *Program* a method (algorithm) for computing solutions

#### Model-based approach

\* *Formulate* a description (model) of the desired solutions

#### Which should you prefer?

- ✤ For simple problems, any approach can work
- ✤ But the application development cycle introduces *complications*...



## **Example:** Supply Chain Optimization

#### Motivation

Ship products efficiently to meet demands

#### Context

- a transportation network\* locations O
  - \* links  $\longrightarrow$
- ✤ supplies ---> at locations
- ♦ demands ---> at locations
- ✤ capacities on links
- ✤ shipping costs on links



## **Supply Chain Optimization**

#### Decide

✤ how much of each product to ship on each link

#### So that

- ✤ shipping costs are kept low
- shipments on each link respect capacity of the link
- supplies, demands, and shipments are in balance at each location

Two approaches . . .



## Supply-Chain Optimization Method-Based Approach

#### Program a method to build a shipping plan

\* *method:* says how to compute a solution

#### Order-driven

- Develop rules for how each order should be met
  - \* Given some demand and given available capacity, determine where to ship it from and which route to use
- Fill orders one by one, according to the rules
  \* Decrement capacity as each one is filled

#### Route-driven

- ✤ Repeat until all demands are met
  - \* Choose a shipping route and a product
  - \* Add as much flow as possible of that product along that route without exceeding supply, demand, or capacity

## Supply-Chain Optimization Method-Based Approach

#### Program refinements to the method to get better results . . .

#### Enhance the method

- ✤ Fill large order first, or
- Consider the least expensive routes first

#### Improve the initial solution

Look for simple exchanges that reduce cost

#### Apply metaheuristic concepts

- Systematically search for local improvements
  \* simulated annealing, tabu search, GRASP
- Combine solutions to evolve better ones
  - **\*** evolutionary methods, particle swarm optimization

... usually no optimal method is available

## Supply-Chain Optimization Model-Based Approach

#### Formulate a minimum shipping cost model

- \* *model:* says what a solution should satisfy
- Identify amounts shipped as the decisions of the model (variables)
- Specify feasible shipment amounts by writing equations that the variables must satisfy (*constraints*)
- Write total shipping cost as a summation over the variables (*objective*)
- Collect costs, capacities, supplies, demands (data)

#### Send to a solver that computes solutions

- ✤ Available ready to run, without programming
- Handles very broad problem classes efficiently
  - \* Ex: Linear constraints and objective, continuous or integer variables
- Exploits provably optimal algorithms

## Supply-Chain Optimization Model-Based Formulation

#### Given

- *P* set of products
- *N* set of network locations
- $A \subseteq N \times N$  set of links connecting locations

#### and

- $u_{ij}$  capacity of link from *i* to *j*, for each  $(i, j) \in A$
- *s*<sub>*pj*</sub> supply/demand of product *p* at location *j*, for each *p* ∈ *P*, *j* ∈ *N* > 0 implies supply, < 0 implies demand
- $c_{pij}$  cost per unit to ship product *p* on link (*i*, *j*), for each *p* ∈ *P*, (*i*, *j*) ∈ *A*

#### Supply-Chain Optimization Model-Based Formulation (cont'd)

#### Determine

 $\begin{aligned} X_{pij} & \text{amount of product } p \text{ to be shipped from location } i \text{ to location } j, \\ & \text{for each } p \in P, (i, j) \in A \end{aligned}$ 

#### to minimize

 $\sum_{p \in \mathbb{P}} \sum_{(i,j) \in \mathbb{A}} c_{pij} X_{pij}$ 

total cost of shipments

subject to

 $\sum_{p \in P} X_{pij} \le u_{ij}$ , for all  $(i, j) \in A$ 

on each link, total shipped must not exceed capacity

$$\sum_{(i,j)\in A} X_{pij} + s_{pj} = \sum_{(j,i)\in A} X_{pji}, \text{ for all } p \in P, j \in N$$

at each location, shipments in plus supply/demand must equal shipments out

## **Complications:** Supply Chain Optimization

#### Additional restrictions imposed by the user

- Cost has fixed and variable parts
  To ab link in such a set if it is used for abian
  - \* Each link incurs a cost if it is *used* for shipping
- Shipments cannot be too small
- Not too many links can be used

#### Additional data for the problem

- $d_{ij}$  fixed cost for using the link from *i* to *j*, for each  $(i, j) \in A$
- *m* smallest total that may be shipped on any link used
- *n* largest number of links that may be used

## *Complications* **Method-Based** (cont'd)

#### What has to be done?

- Revise or re-think the solution approach
- Update or re-implement the method

#### What are the challenges?

- ✤ In this example,
  - \* Shipments have become more interdependent
  - \* Good routes are harder to identify
  - \* Improvements are harder to find
- ✤ In general,
  - Even small changes to a problem can necessitate major changes to the method and its implementation
  - \* Each problem change requires more method development

... and problem changes are frequent!

#### Complications Model-Based (cont'd)

#### What has to be done?

- Update the objective expression
- Formulate additional constraint equations
- Send back to the solver

#### What are the challenges?

- ✤ In this example,
  - \* New variables and expressions to represent fixed costs
  - \* New constraints to impose shipment and arc-use limits

#### ✤ In general,

- \* The formulation tends to get more complicated
- \* A new solver type or solver options may be needed

... but it's easier to update formulations than methods ... and a few solver types handle many formulations

#### Complications Model-Based Formulation (revised)

#### Determine

- $\begin{aligned} X_{pij} & \text{amount of commodity } p \text{ to be shipped on link } (i,j), \\ & \text{for each } p \in P, (i,j) \in A \end{aligned}$
- $\begin{array}{ll} Y_{ij} & 1 \text{ if any amount is shipped from location } i \text{ to location } j, \\ & 0 \text{ otherwise, for each } (i,j) \in A \end{array}$

#### to minimize

$$\sum_{p \in P} \sum_{(i,j) \in A} c_{pij} X_{pij} + \sum_{(i,j) \in A} d_{ij} Y_{ij}$$

total varying plus fixed cost of shipments

#### Complications Model-Based Formulation (revised)

#### Subject to

$$\begin{split} \sum_{p \in P} X_{pij} &\leq u_{ij} Y_{ij}, & \text{for all } (i,j) \in A \\ \text{when the link from location } i \text{ to location } j \text{ is used,} \\ \text{total shipments must not exceed capacity, and } Y_{ij} \text{ must be 1} \\ \sum_{(i,j)\in A} X_{pij} + s_{pj} &= \sum_{(j,i)\in A} X_{pji}, & \text{for all } p \in P, j \in N \\ \text{shipments in plus supply/demand must equal shipments out} \\ \sum_{p \in P} X_{pij} &\geq m Y_{ij}, & \text{for all } (i,j) \in A \\ \text{when the link from node } i \text{ to node } j \text{ is used,} \\ \text{total shipments from } i \text{ to } j \text{ must be at least } m \end{split}$$

 $\sum_{(i,j)\in A} Y_{ij} \le n$ 

At most *n* links can be used

## Approaches to Model-Based Optimization

#### Translate between two forms of the problem

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

#### Programming language approach

✤ Write a *computer program* to generate the solver's form

#### Modeling language approach

 Write the *model formulation* in a form that a computer can read and translate

## **Approaches to Modeling Languages**

#### Algebraic modeling languages

- Designed for "algebraic" formulations as seen in our model-based examples
- ✤ Good fit to many applications and many solvers

#### Executable approach

- ✤ Write a computer program . . .
  - \* that resembles an optimization model
  - \* that can be executed to drive a solver

#### Declarative approach

- ✤ Write a model description . . .
  - **\*** in a language specialized for optimization
  - \* that can be translated to the solver's form

## **Example:** Supply Chain Optimization

### Executable approach: 🛋 gurobipy

- Based on the Python programming language
  Designed to look like algebraic notation
- ✤ Generates problems for the Gurobi solver

### Declarative approach: AMPL

- ✤ Based directly on algebraic notation
  - \* Designed specifically for optimization
- ✤ Generates problems for Gurobi and other solvers



## Multi-Product Flow Formulation: Data

#### Given

- *P* set of products
- *N* set of network nodes
- $A \subseteq N \times N$  set of arcs connecting nodes

#### and

- $u_{ij}$  capacity of arc from *i* to *j*, for each  $(i, j) \in A$
- $s_{pj}$  supply/demand of product *p* at node *j*, for each *p* ∈ *P*, *j* ∈ *N* > 0 implies supply, < 0 implies demand
- $c_{pij}$  cost per unit to ship product *p* on arc (*i*, *j*), for each *p* ∈ *P*, (*i*, *j*) ∈ *A*

## Multi-Product Flow Statements: Data

#### gurobipy

 Assign values to Python lists and dictionaries

in a separate file

#### AMPL

 Define symbolic model sets and parameters

set PRODUCTS;
set NODES;

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



## Multi-Product Flow Formulation: Model

#### Determine

 $\begin{aligned} X_{pij} & \text{amount of commodity } p \text{ to be shipped from node } i \text{ to node } j, \\ & \text{for each } p \in P, (i,j) \in A \end{aligned}$ 

#### to minimize

 $\sum_{p \in \mathbb{P}} \sum_{(i,j) \in \mathbb{A}} c_{pij} X_{pij}$ 

total cost of shipping

subject to

 $\sum_{p \in P} X_{pij} \le u_{ij}$ , for all  $(i, j) \in A$ 

total shipped on each arc must not exceed capacity

 $\sum_{(i,j)\in A} X_{pij} + s_{pj} = \sum_{(j,i)\in A} X_{pji}, \text{ for all } p \in P, j \in N$ 

shipments in plus supply/demand must equal shipments out

## Multi-Product Flow Statements: Model

#### gurobipy

```
m = Model('netflow')
flow = m.addVars(products, arcs, obj=cost, name="flow")
m.addConstrs(
  (flow.sum('*',i,j) <= capacity[i,j] for i,j in arcs), "cap")
m.addConstrs(
  (flow.sum(p,'*',j) + inflow[p,j] == flow.sum(p,j,'*')
      for p in products for j in nodes), "node")</pre>
```

```
\sum_{(i,j)\in A} X_{pij} + s_{pj} = \sum_{(j,i)\in A} X_{pji}, \text{ for all } p \in P, j \in N
```

#### *Multi-Product Flow* **Statements: Model** (cont'd)

AMPL

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

 $\sum_{(i,j)\in A} X_{pij} + s_{pj} = \sum_{(j,i)\in A} X_{pji}, \text{ for all } p \in P, j \in N$ 

## Multi-Product Flow Solution

#### gurobipy

```
m.optimize()
if m.status == GRB.Status.OPTIMAL:
    solution = m.getAttr('x', flow)
    for p in products:
        print('\nOptimal flows for %s:' % p)
        for i,j in arcs:
            if solution[p,i,j] > 0:
                print('%s -> %s: %g' % (i, j, solution[p,i,j]))
```

Solved in 0 iterations and 0.00 seconds Optimal objective 5.50000000e+03

```
Optimal flows for Pencils:
Detroit -> Boston: 50
Denver -> New York: 50
Denver -> Seattle: 10
Optimal flows for Pens: ...
```

## Multi-Product Flow **Solution** (cont'd)

#### AMPL

```
ampl: model netflow.mod;
ampl: data netflow.dat;
ampl: option solver gurobi;
ampl: solve;
Gurobi 9.0.3: optimal solution; objective 5500
2 simplex iterations
ampl: display Flow;
Flow [Pencils,*,*]
       Boston 'New York' Seattle
                                    :=
Denver
           0
                   50
                            10
Detroit 50
                    0
                             0
 [Pens,*,*]
       Boston 'New York' Seattle
                                    :=
Denver
          10
                    0
                            30
Detroit 30
                   30
                             0
;
```

#### Multi-Product Flow Solution (cont'd)

#### AMPL

```
ampl: model netflow.mod;
ampl: data netflow.dat;
ampl: option solver cplex;
ampl: solve;
CPLEX 12.10.0.0: optimal solution; objective 5500
0 dual simplex iterations (0 in phase I)
ampl: display Flow;
Flow [Pencils,*,*]
       Boston 'New York' Seattle
                                     :=
Denver
           0
                    50
                             10
Detroit 50
                     0
                              0
 [Pens,*,*]
       Boston 'New York' Seattle
                                     :=
Denver
           10
                    0
                             30
Detroit 30
                    30
                              0
;
```

Algebraic Modeling Languages

## Executable

#### Concept

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

#### Advantages

- Complete application development in one language
- Direct access to advanced solver features

#### Disadvantages

- Programming languages are not designed for describing models
  - \* Constraint descriptions can be awkward
  - \* Special methods may be required for efficiency
- Modeling and programming bugs are hard to separate

Algebraic Modeling Languages

## Declarative

#### Concept

- Design a language for describing optimization models
- ✤ Connect to external applications via . . .
  - \* extensions for scripting and data transfer
  - \* APIs for programming languages

#### Disadvantages

✤ Adds a system between application and solver

#### Advantages

- Designed for building and using optimization models
  - \* Streamlines model building and processing
  - \* Promotes validation and maintenance of models
- Not specific to one programming language or solver

#### Algebraic Modeling Languages Integration with Applications

#### gurobipy

- Everything can be developed in Python
- ✤ Part of the Gurobi package
  - \* Free solver-independent alternatives (Pyomo, PuLP, Python-MIP)

#### AMPL

- Prototypes can be developed in AMPL
  - \* Modeling language extended with loops, tests, assignments
- Application programming interfaces (APIs) for integrating AMPL with popular programming languages
   \* C++, C#, Java, MATLAB, Python, R

#### Algebraic Modeling Languages Integration with Solvers

#### gurobipy

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

#### AMPL

- 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
  - \* Connects to global optimization and constraint programming solvers

### **Case Studies**

#### Young's Plant Farm

Packing shipments

#### Motion Robotics

✤ Designing aircraft

#### ABB

Managing power grids

#### New York Education Department

Assigning students to classes

# *Case:* Young's Plant Farm *Packing Shipments*



## Packing

#### Situation

- ✤ Grows plants of many kinds and sizes
- Ships to retailers on their own trucks
  \* Large customers include Walmart, Lowe's
- ✤ Plants are packed on special rolling racks
  - \* 3 feet wide, 4 feet long, 7 feet tall
  - **\*** 4 to 12 shelves



#### Goal

- ✤ Generate good packing plans for a day's orders
  - Don't use more racks than needed
- ✤ Finish in time to get the orders out

## Packing Evaluation

#### Approaches considered

- Spreadsheet "by hand"
- Algebraic modeling language + integer linear solver

#### Choice of AMPL

- Dramatically better solutions
- Numerous economies
  - ✤ Faster solutions using many fewer people
  - ✤ Faster loading of racks
  - ✤ Fewer trucks required
- Selection of solvers

#### Packing Implementation

#### Development

- ✤ Original model built by Prof. Rafay Ishfaq of Auburn University
- Extended to handle larger orders by AMPL Optimization

#### **Optimization**

- Implemented using AMPL model, data, and scripts
- Minimum size: low 100s of thousands of variables & constraints Maximum size: 100 *million* variables & constraints
- Solve time: 10 to 45 minutes

#### Deployment

- VBA-modified spreadsheet for data prep and result reporting
- One replenishment specialist uses the tool multiple times a day

... considering adaptations to new use cases

## **Case:** Motion Robotics Designing Aircraft



## Design

#### Situation

- Develops and sells electric flying vehicles
  - \* Drones and related infrastructure (such as docking stations)
  - \* Electric motors using a highly efficient radial (vs. traditional axial) design
- Designs drones for specific applications

#### Goal

- ✤ Create new electric aircraft
- Evaluate over many possibilities
  - \* Design: propulsion, aerodynamics, structures
  - \* Architecture: rotor size, battery capacity, etc.
  - \* Flight path: initial & final position, velocity, etc.

## Design **Evaluation**

#### Approaches considered

- Spreadsheet (not realistic)
- Simulation and machine learning
- Python-based design optimization system
- Algebraic modeling language + nonlinear solver

#### Choice of AMPL

- Formal optimization model
  - ✤ Generality to implement complex physics equations
  - ✤ Best results within a reasonable time frame
- Variety of solvers
- ✤ Ability to deploy via API
  - \* Import data
  - \* Run many optimizations in parallel

## Design Implementation

#### Development

- Suggested by a professor at a local university
- Implemented by two analysts at Motion Robotics
- ✤ 1D prototypes built within months
- Expanded to 2D with many complicating factors

#### **Optimization**

- ✤ 7 minutes for a solve
  - \* Tested five nonlinear solvers, chose LOQO
- ✤ AMPL scripts for core application
- Python API for data & results

#### Deployment

- Parallel runs on 2,000 nodes in a cluster
- ✤ Connections to MATLAB, TensorFlow, etc.

## Case: ABB Managing Power Grids



## Case: ABB Power Grid Management

## GridView

For studies within the Western Electric Coordinating Council territory, GridView provides an industry-accepted simulation approach. The advanced analysis methodology combines generation, transmission, loads, fuels, and market economics into one integrated framework to

deliver location dependent market indicators, transmission system utilization measures and power system reliability and market performance indices. It provides invaluable information for both generation and transmission planning, operational decision making and risk management.

GridView uses state-of-the-art modeling technology to simulate security-constrained unit commitment and economic dispatch. It produces unit commitment and economic dispatch that respect the physical laws of power flow and transmission reliability requirements. As such, the generation dispatch and market clearing price are feasible market solutions within real power transmission networks.

## **Power Grid Management**

#### Situation

- \* A power grid operator providing electrical service
- ✤ Two kinds of decisions
  - \* *Unit commitment:* When to turn power plants on and off
  - \* *Network flow:* How to transmit power over the grid to meet demand

#### Goal

- Simulate optimal decisions to support planning
  - \* Transmission network expansion
  - \* Plant addition and retirement
  - \* Integration of renewable energy sources

#### Power Evaluation

#### Approaches considered

- ✤ C++ for entire GridView system
- Modeling language for optimization, C++ for user interfaces

#### Choice of AMPL

- ✤ Ease of modeling
  - \* ABB can formulate complex and powerful models
  - \* Customers can understand the AMPL formulations
  - \* Customers can customize models for their particular situations
- ✤ Ease of embedding
  - \* AMPL has an API (application programming interface) for C++
  - \* ABB can easily build AMPL into the GridView product

#### Power Implementation

#### Development

- ✤ Prototype at University of Tennessee, Knoxville
- ✤ Full AMPL implementation by three analysts at ABB

#### **Optimization**

- Mixed-integer linear solver
- Millions of variables
- Tens of thousands of integer variables
- ✤ 10 minutes to solve

#### Deployment

- ✤ 30+ customer companies
- Hundreds of customer-side users

## Case: New York Education Department Assigning Students to Classes



## Assignment

#### Situation

- Covid-19 closed New York State public schools in Spring 2020
- ✤ Now the schools want to reopen for Fall
- ✤ To limit the spread of the virus . . .
  - classrooms can hold only a limited number of students
  - state is offering "blended" instruction:
    "cohorts" of students can attend only 1-3 days each week

#### Goal

- Create a tool for making workable assignments
- ✤ Make the tool usable by school principals, on short notice
- ✤ Support many simultaneous users . . .

## Assignment



## Assignment Evaluation

#### Approaches considered

- Every principal figures out how to make their own assignment
- Algebraic modeling language + integer linear solver

#### Choice of AMPL

- ✤ Fast prototyping and development
- Flexibility of solver choice
- Python API for deployment in easy-to-use web tool

#### Assignment Implementation

#### Development

- Dr. Howard Karloff, Vice President, Goldman Sachs
  - \* model completed in a few days
- ✤ Caleb Ren, Harvard University student
- Filipe Brandão, AMPL Optimization

#### **Optimization**

- Tens of thousands of variables
- ✤ 1 to 4 minutes to solve

#### Deployment

- Easy-to-use web tool for data input and result reporting
  click "submit" to run
- Python application parses data, runs AMPL and Gurobi
  - $\star$  new AWS container spawned for each submission
  - **\*** application built in 2 weeks