Optimization in Your Toolchain: How AMPL is Making it Faster and Easier

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Optimization in Your Toolchain: How AMPL is Making it Faster and Easier

Optimization has been fundamental to Analytics for as long as there have been computers, yet we are still finding ways to make optimization software more natural to use, faster to run, and easier to integrate with enterprise systems. In this presentation, you'll learn how AMPL's modeling framework has been enhanced to support optimization in today's challenging applications. Topics include:

- Expressing constraint logic more directly and understandably
- Exchanging data and results directly and efficiently with spreadsheets and database systems
- Interfacing to business systems through APIs for popular programming languages
- Deploying optimization in cloud environments and containers

To round out the presentation, the theme of adding optimization to applications will be illustrated by several varied case studies.

Outline

Optimization

- Optimization in practice
- Model-based optimization
- Model-based optimization in AMPL

Developments in AMPL

- * *more natural:* Writing models more like you think about them
- *faster, easier:* Exchanging data and results directly and efficiently with spreadsheets and database systems
- *faster:* Interfacing to enterprise systems through APIs for popular programming languages
- * *easier*: Deploying optimization in containers and in the cloud

Optimization in Practice

Given a recurring need to make many interrelated decisions

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

Consistently make highly desirable choices

By applying ideas from mathematical optimization

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

Optimization in Practice

Large numbers of decision variables

Thousands to millions

An objective function

✤ Minimize or maximize

Various constraint types

✤ 10-20 distinct types

- * Thousands to millions of each type
- Few variables involved in each constraint

Solved many times with different data

✤ Simple rules can't capture all possibilities in advance

Solvable only by a series of computational steps

Number of steps not predictable

Example: Multi-Product Network Flow

Motivation

Ship products efficiently to meet demands

Context

- a transportation network
 nodes O representing cities
 - * arcs \longrightarrow representing roads
- ✤ supplies ---> at nodes
- ♦ demands ---> at nodes
- ✤ capacities on arcs
- ✤ shipping costs on arcs



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Example: Multi-Product Network Flow

Decide

✤ how much of each product to ship on each arc

So that

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



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Example with complications: Multi-Product Network Flow

Decide also

✤ whether to use each arc

So that

- variable plus fixed shipping costs are kept low
- shipments are not too small
- ✤ not too many arcs are used



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Model-Based Optimization

Formulate a minimum shipping cost model

- *decision variables:* What arcs are used and how much is shipped
- * *objective:* Total fixed and variable costs
- *constraints:* Equations that the variables must satisfy to meet the requirements of the problem

Apply model-based optimization software

- *modeling language:* Write a formulation that a computer system can read
- *data:* Read costs, capacities, supplies, demands, and limits that define a specific case to be solved
- *solver:* Send to an off-the-shelf optimization engine that accepts a broad class of problems

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

Multi-Product Flow

Linearized Formulation (variables, objective)

Determine

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

to minimize

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

total cost of shipments

Multi-Product Flow Linearized Formulation (constraints)

Subject to

 $\sum_{p \in \mathbf{P}} X_{pij} \le u_{ij} Y_{ij},$

for all $(i, j) \in A$

when the arc from node *i* to node *j* is used for shipping, total shipments must not exceed capacity, and Y_{ij} must be 1

$$\sum_{p \in P} X_{pij} \ge m Y_{ij}$$

for all $(i, j) \in A$

when the arc from node i to node j is used for shipping, total shipments from i to j must be at least m

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

shipments in plus supply/demand must equal shipments out

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

At most *n* arcs can be used

Multi-Product Flow Linearized Model in AMPL

Symbolic data, variables, objective

```
set PRODUCTS;
set NODES;
set ARCS within {NODES, NODES};
param capacity {ARCS} >= 0;
param inflow {PRODUCTS, NODES};
param min_ship >= 0;
param max_arcs >= 0;
param var_cost {PRODUCTS,ARCS} >= 0;
var Flow {PRODUCTS,ARCS} >= 0;
param fix_cost {ARCS} >= 0;
var Use {ARCS} binary;
minimize TotalCost:
   sum {p in PRODUCTS, (i,j) in ARCS} var_cost[p,i,j] * Flow[p,i,j] +
   sum {(i,j) in ARCS} fix_cost[i,j] * Use[i,j];
```

Multi-Product Flow Linearized Model in AMPL

Constraints

```
subject to Capacity {(i,j) in ARCS}:
    sum {p in PRODUCTS} Flow[p,i,j] <= capacity[i,j] * Use[i,j];
    subject to Min_Shipment {(i,j) in ARCS}:
        sum {p in PRODUCTS} Flow[p,i,j] >= min_ship * Use[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];
    subject to Max_Used:
        sum {(i,j) in ARCS} Use[i,j] <= max_arcs;</pre>
```

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

Multi-Product Flow Data Instance in AMPL Text Format

Limits

```
set PRODUCTS := Bands Coils :
set NODES := Detroit Denver Boston 'New York' Seattle ;
param: ARCS: capacity:
      Boston 'New York' Seattle :=
Detroit
         100
                 80
                        120
Denver 120 120
                        120 ;
param inflow:
       Detroit Denver Boston 'New York' Seattle :=
 Bands
          50
                60
                   -50 -50
                                     -10
 Coils 60 40 -40 -30
                                     -30;
param min_ship := 15 ;
param max_arcs := 4 ;
```

Multi-Product Flow Data Instance in AMPL Text Format

Costs

param var_cost: [Bands,*,*] Boston 'New York' Seattle := Detroit 10 20 60 40 Denver 40 30 [Coils,*,*] Boston 'New York' Seattle := Detroit 20 20 80 Denver 60 70 30; param fix_cost default 75 ;

Multi-Product Flow Optimization by a "MIP" Solver (gurobi)

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Formulating Models More Like You Think About Them

Describe an optimization problem

- * In a form *you find natural or convenient*
- Using readily recognized expressions

Send it to a solver

- ✤ In a form the solver will accept
- Relying on the modeling software to translate

Get back a result

✤ In the form you originally used

Formulating Positive Shipments Incur Fixed Costs

Linearized formulation

sum {(i,j) in ARCS} fix_cost[i,j] * Use[i,j];

Natural formulation

sum {(i,j) in ARCS}
if exists {p in PRODUCTS} Flow[p,i,j] > 0 then fix_cost[i,j]

Formulating Shipments Can't Be Too Small

Linearized formulation

```
sum {p in PRODUCTS} Flow[p,i,j] >= min_ship * Use[i,j];
sum {p in PRODUCTS} Flow[p,i,j] <= capacity[i,j] * Use[i,j];</pre>
```

Natural formulation

sum {p in PRODUCTS} Flow[p,i,j] = 0 or min_ship <= sum {p in PRODUCTS} Flow[p,i,j] <= capacity[i,j]</pre>

Formulating Can't Use Too Many Arcs

Linearized formulation

sum {(i,j) in ARCS} Use[i,j] <= max_arcs;</pre>

Natural formulation

count {(i,j) in ARCS} (sum {p in PRODUCTS} Flow[p,i,j] > 0) <= max_arcs;</pre>

Formulating Optimization by Same MIP Solver (x-gurobi)

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	< >>	<	>

Formulating Supported Model Expressions

Arithmetic operators

✤ iterated sum, prod

Logical operators

- ✤ if-then, if-then-else; ==> (implies)
- $\boldsymbol{\ast}$ or, and, not
- ✤ iterated exists, forall, count

Almost-linear functions

- ✤ min, max, abs

Univarite nonlinear functions

- ✤ sin, cos, tan; sinh, cosh, tanh; asin, acos, ...
- \bullet log, log10

Formulating **Supported Model Expressions** (cont'd)

Relational constraints

- ✤ =, >=, <=</p>
- \diamond double >=, <=

Logical constraints

- ✤ <, >, !=
- ✤ atleast, atmost, exactly
- ✤ alldiff
- complements

Variable domains

- ♦ >=, <=</p>
- ✤ integer, binary
- ✤ in set

Formulating Interface to MIP Solvers

Read objectives & constraints from AMPL

- ✤ Store initially as expression trees
 - * (except for linear ones)
- ✤ Analyze to determine which are linearizable

Generate linearizations

- Walk trees to build linearizations (flatten)
- Define auxiliary variables (often zero-one)
- ✤ Generate equivalent constraints

Solve

- Send to solver through its API
- Convert optimal solution back to the original AMPL variables
- ✤ Write solution to AMPL

Formulating Interface Options for Gurobi

Apply our linearization (count)

✤ Use Gurobi's linear API

Have Gurobi do simple linearizations (or, abs)

- Simplify and "flatten" the expression tree
- ✤ Use Gurobi's "general constraint" API
 - * addGenConstrOr (resbinvar, [binvars])
 tells Gurobi: resbinvar = 1 iff at least one item in [binvars] = 1
 - * addGenConstrAbs (resvar, argvar)
 tells Gurobi: resvar = |argvar|

Have Gurobi piecewise-linearize (log)

- Replace univariate nonlinear functions by p-l approximations
- ✤ Use Gurobi's "function constraint" API
 - * addGenContstrLog (xvar, yvar)
 tells Gurobi: yvar = a piecewise-linear approximation of log(xvar)

Formulating Implementation Issues

Is an expression repeated?

Detect common subexpressions

```
subject to Shipment_Limits {(i,j) in ARCS}:
sum {p in PRODUCTS} Flow[p,i,j] = 0 or
min_ship <= sum {p in PRODUCTS} Flow[p,i,j] <= capacity[i,j];</pre>
```

Is there a simplified formulation?

✤ Yes for min-max, no for max-min

```
minimize Max_Cost:
    max {i in PEOPLE} sum {j in PROJECTS} cost[i,j] * Assign[i,j];
```

```
maximize Max_Value:
    sum {t in T} max {n in N} weight[t,n] * Value[n];
```

Formulating Implementation Issues (cont'd)

Does an exact linearization exist?

- ✤ Yes if constraint set is "closed"
- ✤ No if constraint set is "open"

```
var Flow {ARCS} >= 0;
var Use {ARCS} binary;
subj to Use_Definition {(i,j) in ARCS}:
    Use[i,j] = 0 ==> Flow[i,j] = 0;
```

```
subj to Use_Definition {(i,j) in ARCS}:
    Flow[i,j] = 0 ==> Use[i,j] = 0 else Use[i,j] = 1;
```

Formulating Implementation Issues (cont'd)

Does an exact linearization exist?

- ✤ Yes if constraint set is "closed"
- ✤ No if constraint set is "open"

```
var Flow {ARCS} >= 0;
var Use {ARCS} binary;
subj to Use_Definition {(i,j) in ARCS}:
    Use[i,j] = 0 ==> Flow[i,j] = 0 else Flow[i,j] >= 0;
```

```
subj to Use_Definition {(i,j) in ARCS}:
    Use[i,j] = 0 ==> Flow[i,j] = 0 else Flow[i,j] > 0;
```

Exchanging data and results with spreadsheets and database systems

Direct spreadsheet (.xlsx) file interface

- ✤ Works with all .xlsx files on Windows, Linux, macOS
- Supports "two-dimensional" spreadsheet tables

Direct comma-separated value (.csv) file interface

New ODBC interface for database systems

- Support for Microsoft ODBC, unixODBC, iODBC
- ✤ Faster operation
- Extended update features

Direct Spreadsheet Interface

"1D" spreadsheet ranges

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5			Detroit	Seattle	120		Bands	Detroit	Seattle	60		
6			Denver	Boston	120		Bands	Denver	Boston	40		
7	NODES		Denver	New York	120		Bands	Denver	New York	40		
8	Detroit		Denver	Seattle	120		Bands	Denver	Seattle	30		
9	Denver						Coils	Detroit	Boston	20		
10	Boston						Coils	Detroit	New York	20		
11	New York		ITEMS	NODES	inflow		Coils	Detroit	Seattle	80		
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Direct Spreadsheet Interface

"2D" spreadsheet ranges

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Direct spreadsheet interface Data Handling

Script (input)

```
model netflow1.mod;
```

```
table Products IN "amplxl" "netflow2.xlsx" "Items":
     PRODUCTS <- [ITEMS];</pre>
```

```
table Nodes IN "amplxl" "netflow2.xlsx":
    NODES <- [NODES];</pre>
```

```
table Capacity IN "amplxl" "netflow2.xlsx":
    ARCS <- [FROM,TO], capacity;</pre>
```

```
table Inflow IN "amplxl" "netflow2.xlsx":
    [ITEMS,NODES], inflow;
```

```
table Cost IN "amplxl" "netflow2.xlsx":
    [ITEMS,FROM,TO], cost;
```

```
load amplxl.dll;
```

```
read table Products; read table Nodes;
read table Capacity; read table Inflow; read table Cost;
```

Direct spreadsheet interface Data Handling

Script (input)

```
model netflow1.mod;
table Products IN "amplxl" "netflow2.xlsx" "Items":
    PRODUCTS <- [ITEMS];
table Nodes IN "amplxl" "netflow2.xlsx":
    NODES <- [NODES];
table Capacity IN "amplxl" "netflow2.xlsx" "2D":
    ARCS <- [FROM,TO], capacity;
table Inflow IN "amplxl" "netflow2.xlsx" "2D":
    [ITEMS, NODES], inflow;
table Cost IN "amplxl" "netflow2.xlsx" "2D":
    [ITEMS, FROM, TO], cost;
load amplxl.dll;
read table Products; read table Nodes;
```

```
read table Capacity; read table Inflow; read table Cost;
```

Direct spreadsheet interface Data Handling

Script (output)

```
option solver gurobi;
solve;
table Results OUT "amplxl" "netflow1.xlsx" "2D":
   [ITEMS,FROM,TO], Flow;
table Summary OUT "amplxl" "netflow1.xlsx":
   {(i,j) in ARCS} -> [FROM,TO],
   sum {p in PRODUCTS} Flow[p,i,j] ~ TotFlow,
   sum {p in PRODUCTS} Flow[p,i,j] / capacity[i,j] ~ "%Used";
write table Results;
write table Results;
write table Summary;
```

Direct spreadsheet interface **Data Results**

"2D" spreadsheet range

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6	Detroit	Seattle	0	0	De	etroit	Seattle	0	0.0%				
7	Denver	Boston	0	10	De	enver	Boston	10	8.3%				
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New ODBC Interface

Open Database Connectivity

- Standard API for accessing database management systems
- Many database systems have ODBC drivers
- Supported by AMPL table statements
 - * Can include SQL queries

Enhancements

- ✤ Faster writes
- ✤ Table rewrite support
 - * Preserve the column data types
- Table update support
 - * Modify only selected records of a large table
- Table "upsert" support (experimental)
 - * Update a record if it already exists, otherwise insert it
 - * Requires a database-specific SQL statement

Reading Efficiency



Writing Efficiency



Updating Efficiency



Interfacing to Enterprise Systems through AMPL APIs

Embed AMPL in applications

- Program in C++, C#, Java, MATLAB, Python, R
- Call AMPL to do optimization, via API (application programming interface) library routines
 - * Import data and export solutions
 - * Read AMPL models & execute AMPL commands
 - ***** Invoke solvers

Recent enhancements

- Snapshots
- ✤ AMPL Colaboratory

Snapshots

Save & restore an AMPL session

- ✤ Save key state information in a text file
 - * Model declaration, data, current solution, options, ...
- Restore the state as a starting point for later sessions

Valuable in API programming

- Avoid repeating expensive setups
 - * Set up once and record a snapshot
 - * Create many containers and restore the snapshot in each
- Debug API programs
 - * Check correctness of model and data setup
 - * Move to interactive environment for troubleshooting

Snapshot Command Listing

###snapshot-version: 0.1.1 ###model-start set PRODUCTS: set NODES: set ARCS within {NODES, NODES}; param capacity{ARCS} >= 0; param inflow{PRODUCTS, NODES}; param cost{PRODUCTS, ARCS} >= 0; var Flow{PRODUCTS, ARCS} >= 0; minimize TotalCost: sum{p in PRODUCTS, (i,j) in ARCS} cost[p,i,j subject to Capacity{(i,j) in ARCS} : sum{p in PRODUCTS} Flow[p,I,j] <= capacity[i,j];</pre> subject to Conservation{p in PRODUCTS, j in NODES} : sum{(i,j) i Flow[p,i,j] + inflow[p,j] == sum{(j,i) in ARCS} Flow[p,j,i]; ###model-end ###options-start option AMPLFUNC 'C:\Users\AMPL\Desktop\Solvers\ampltabl_64.dll'; option ampl_Include 'C:\Users\AMPL\Desktop\Analytics\Netflow'; option ampl_include 'C:\Users\AMPL\Desktop\Analytics\Netflow'; ###options-end ###data-start data: set PRODUCTS := 'Pencils' 'Pens': set NODES := 'Detroit' 'Denver' 'Boston' 'New York' 'Seattle': set ARCS := ('Detroit', 'Boston') ('Detroit', 'New York') ('Detroit','Seattle') ('Denver', 'Boston') ('Denver', 'New York') ('Denver','Seattle'); param capacity := ['Detroit', 'Boston'] 100

['Detroit', 'New York'] 80 ['Detroit', 'Seattle'] 120 ['Denver', 'Boston'] 120 ['Denver', 'New York'] 120 ['Denver','Seattle'] 120; param 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', 'New York'] 70 ['Pens', 'Denver', 'Seattle'] 30; model: ###data-end ###current-problem-start problem Initial; environ Initial; ###current-problem-end ###objectives-start objective TotalCost; ###objectives-end ###fixes-start unfix Flow; ###fixes-end ###drop-restore-start restore Capacity; restore Conservation; ###drop-restore-end ###solution-start ###solution-end

Snapshot Usage

For use with an API

snapshot = ampl.get_output('snapshot;')

ampl2.eval(snapshot)

For use in interactive debugging

```
snapshot = ampl.get_output('snapshot;')
```

```
print(snapshot, file=open('snapshot.run', 'w'))
```

include "snapshot.run";

AMPL Colaboratory

Run sample models free in Jupyter notebooks

- Run a short Python cell for setup
- Run AMPL cells for model, data, scripts
 ... execute in Google Colab, Kaggle, etc.

Great for getting started with AMPL

- No local downloads or installation needed
- Try out examples
 - * From the AMPL book
 - * From previous talks and papers
- Copy and modify an example

Deploying optimization in containers and in the cloud

Virtual licensing

- Not a machine-locked license scheme
 - * Doesn't rely on fixed machine characteristics
- Not a traditional floating license scheme
 - * Doesn't rely on a customer's machine for validation
- For clouds containers clusters . . . even physical machines

Container setup

- ✤ Use any base image
- Load needed AMPL and solver modules
- ✤ Initialize virtual licensing

Virtual Licensing

Short-term leases

- ✤ Last 5 minutes
- ✤ Automatically renewed

Renewal procedure

- Sends current license & usage data to our REST API endpoints
 * Hosted across multiple cloud providers (AWS, Azure, . . .)
- ✤ User details and usage data are logged
- New license file is returned

... lease remains active during renewal process

Virtual Licensing

Flexible license limits

- No automatic enforcement
- Short-term use in excess of limits is expected
- ✤ If use exceeds limits in longer term, customer is contacted

Information reported in renewal request

- ✤ CPU cores in the underlying machine
- ✤ CPU threads available

Information tracked

- Total concurrent active leases
- Total CPU threads available across all active leases
- Total different underlying machines with active leases
- ✤ Total CPU cores across all machines with active leases

Container Setup

Install curl, build arguments, get AMPL module

```
# Use any image as base image
FROM python:3.9-slim-buster
```

```
# Install curl in order to download the modules necessary
RUN apt-get update && apt-get install -y curl
```

```
# Build arguments
ARG LICENSE_UUID=f9758f88-b0a3-11eb-9e10-c75c7742e3ae
ARG MODULES_URL=https://ampl.com/dl/modules
```

```
# Download ampl-module.linux64.tgz
RUN cd /opt/ && curl -0 ${MODULES_URL}/ampl-module.linux64.tgz && \
    tar xzvf ampl-module.linux64.tgz && rm ampl-module.linux64.tgz
```

Container Setup (*cont'd*)

Load Gurobi, COIN-OR solvers, license, amplpy API

```
# Download Gurobi solver
RUN cd /opt/ && curl -0 ${MODULES_URL}/gurobi-module.linux64.tgz && \
    tar xzvf gurobi-module.linux64.tgz && rm gurobi-module.linux64.tgz
# Download COIN-OR solvers
RUN cd /opt/ && curl -0 ${MODULES_URL}/coin-module.linux64.tgz && \
    tar xzvf coin-module.linux64.tgz && rm coin-module.linux64.tgz
# Download initial license file
RUN cd /opt/ampl.linux-intel64/ && curl -0 \
    https://portal.ampl.com/download/license/${LICENSE_UUID}/ampl.lic
# Add installation directory to the environment variable PATH
```

ENV PATH="/opt/ampl.linux-intel64/:\${PATH}"

Install amplpy API
RUN pip3 install amplpy

Learn More

https://dev.ampl.com

new AMPL development projects

https://github.com/ampl/

✤ all AMPL open-source projects

https://colab.ampl.com/

✤ AMPL Colaboratory links