

Discrete Optimization

(at IBM's Mathematical Sciences Department)

Sanjeeb Dash
IBM Research

Lecture, ORF 363
Princeton University, Dec 13, 2016

Outline

- ▷ Real-world optimization (and at IBM)
 - Application areas
 - Recent job postings

- ▷ Discrete Optimization basics
 - Problems
 - Computational Complexity
 - Formulations

- ▷ Solution techniques: integer programming
 - Branch-and-bound
 - Cutting planes

- ▷ Applications
 - Steel industry
 - Pipelines + more

Real-world Optimization

IBM Research

IBM: 377,757 employees (end of 2015)

IBM Research: 12 labs, 3000+ researchers



IBM's Math. Sciences Dept.

IBM Mathematical Sciences Department:

- ◇ 50+ years old
 - ◇ 50+ people
 - ◇ 50 % funding from contracts, 50% from IBM grants
-
- 40% of time spent on applied work \equiv need to publish 2-3 papers (or perish)
 - 100% of time spent on applied work \equiv need to publish 0 papers

Discrete Optimization

Discrete optimization is the study of problems where the goal is to select a minimum cost alternative from a finite (or countable) set of alternatives.

Application areas

Airlines	route planning, crew scheduling revenue management	American, United Air New Zealand, British Airways
Package Delivery	vehicle routing	UPS, Fedex, USPS
Trucking	route planning, vehicle routing	Schnieder
Transportation	network optimization	Amazon
Telecommunication	network design	AT&T
Shipping	route planning	Maersk
Pipelines	batch scheduling, network flows	CLC, CNPC
Steel Industry	cutting stock	Posco
Paper Industry	cutting stock	GSE mbH
Finance	portfolio management	Axioma
Oil & Gas	pooling	ExxonMobil
Petrochemicals		SK Innovation
Power generation	unit commitment, resource management	BC Hydro
Railways	Timetabling, crew-scheduling	BNSF, CSX, Belgian Railways, Deutsche Bahn, Trenitalia

Recent jobs in optimization

2016

Amazon - *Operations Research Scientist*

Network optimization, Linear and Integer programming - AMPL, Mosel, R, Matlab (Ph.D.)

Amazon - *Applied Scientist- Operations Research, Devices*

Linear Programming, Combinatorial optimization, Integer programming - CPLEX, Gurobi, XPRESS (M.S.)

BAE Systems - *Research Engineer Planning and Control*

Vehicle Routing, Network Optimization - Mathematical Programming, Control Theory (B.S./M.S./Ph.D.)

BNSF - *OR & Advanced Analytics Specialist I*

Railroad logistics - CPLEX, Gurobi, ProModel, ARENA, Frontline Solver (M.S./Ph.D.)

Facebook - *Operations Research Scientist*

Supply chain optimization, Inventory planning - Mathematical Programming (M.S./Ph.D.)

FedEx - *Operations Research Analyst*

Schedule optimization, network planning, truck routing, crew planning, facility location (M.S.)

GE - *Operations Research Specialist*

Optimize railroad operations - CPLEX or Gurobi (M.S./Ph.D.)

LG Electronics USA - *Applied Operations Research Lead*

Demand/Inventory planning, Logistics optimization - AMPL, CPLEX (B.S.)

Modular mining - *Operations Researcher*

“Optimization of operational aspects of mining” - CPLEX, Gurobi, GAMS, AMPL (M.S./Ph.D.)

Walt Disney World Resort - *Decision Science Consultant*

Mixed-integer, non-linear, stochastic optimization or Simulation (M.S./Ph.D.)

Uber - *Operations Research Scientist*

Optimize matching of riders to drivers, schedule optimization (Ph.D.)

IBM, SAS, Gurobi, Mosek, ORTEC

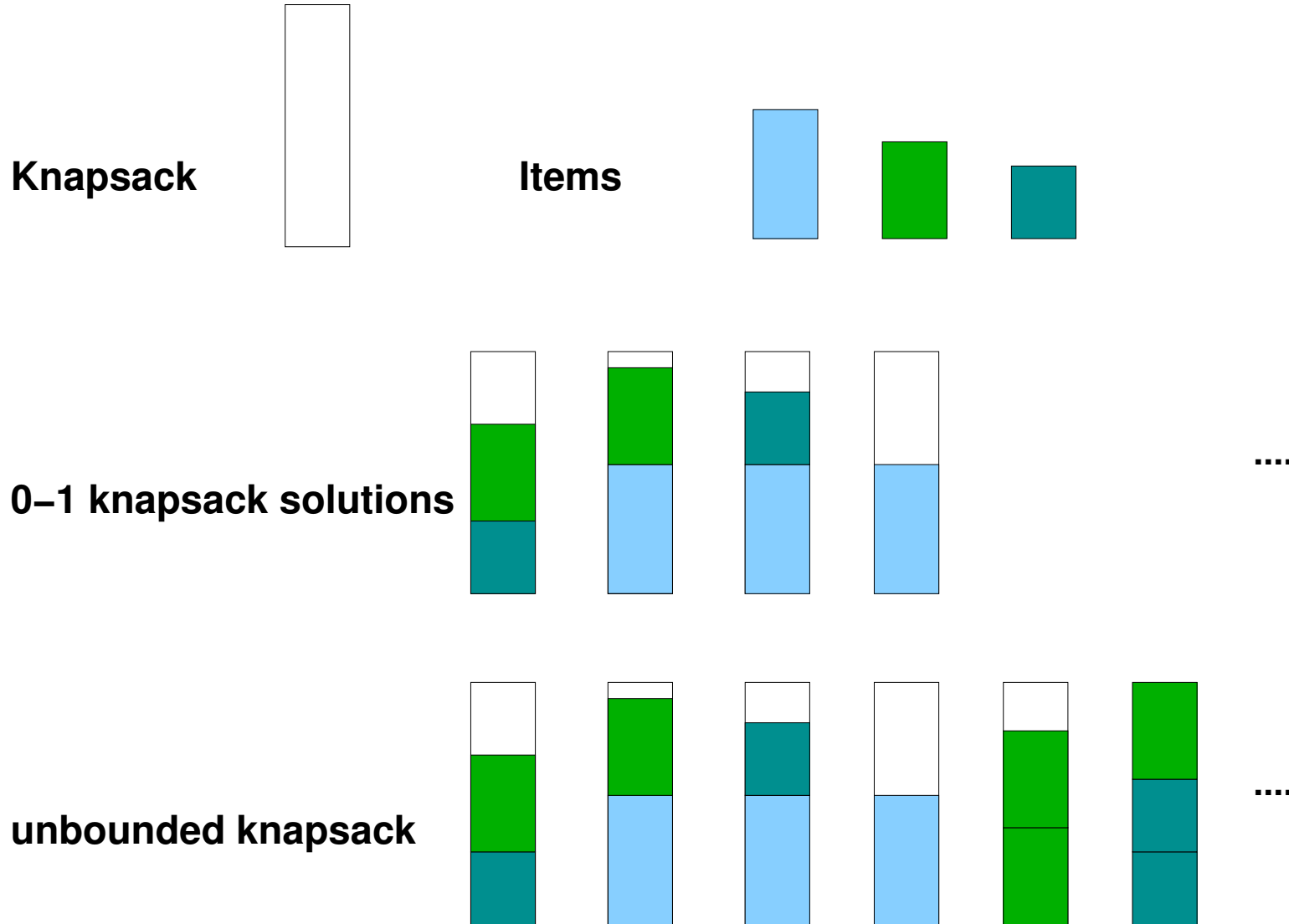
Problems

Knapsack Problem



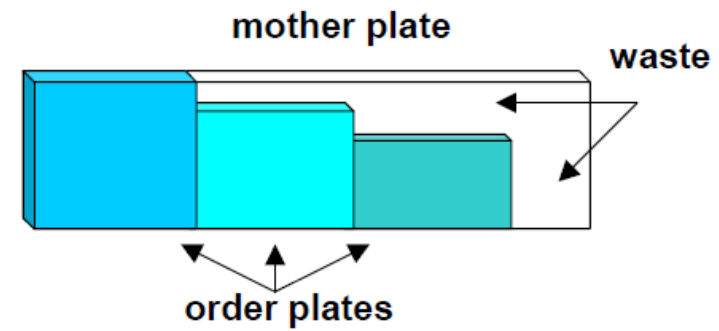
Maximize the value of items packed in a knapsack while not exceeding its capacity

Knapsack Problem



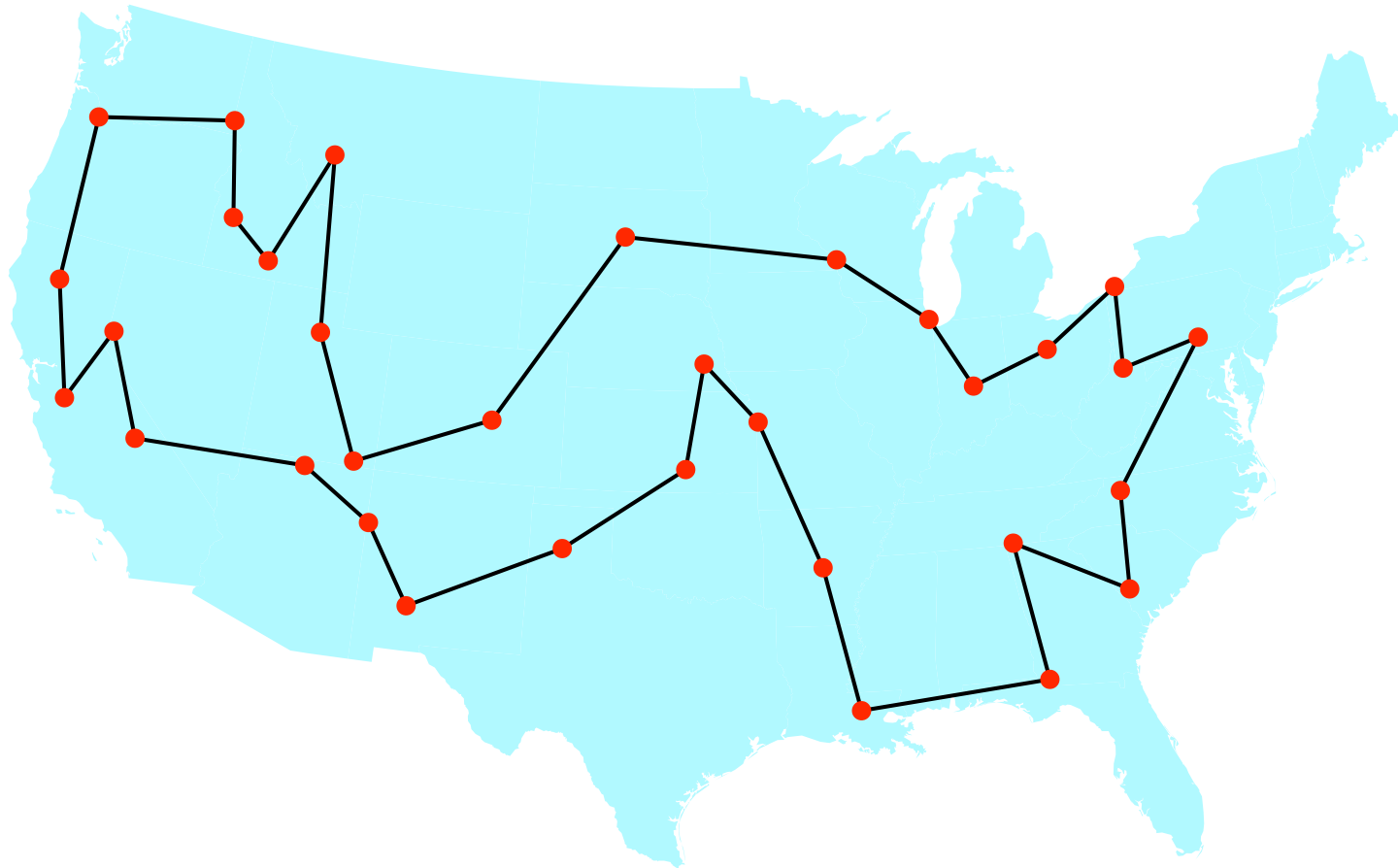
Cutting stock

Pack items into as few identical knapsacks as possible:
(Used in steel, paper industry)



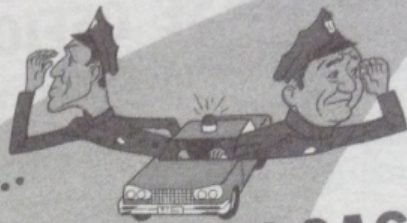
Traveling Salesman Problem

TSP: Minimize distance traveled while visiting a collection of cities and returning to the starting point.



33-city TSP instance from a 1962 Procter and Gamble competition (\$10,000 prize won by Gerald Thompson of CMU)

HELP! WE'RE LOST!



HELP "CAR 54" ... AND WIN CASH

54...\$1,000 PRIZES
ONE...\$10,000 GRAND PRIZE



Map by Rand McNally



Help Toody and Muldoon find the shortest round trip route to visit all 33 locations shown on the map. All you do is draw connecting straight lines from location to location to show the shortest round trip route.

HERE'S THE CORRECT START ...

Begin at Chicago, Illinois. From there, lines show correct route as far as Erie, Pennsylvania. Next, do you go to Carlisle, Pennsylvania or Wana, West Virginia? Check the easy instructions on back of this entry blank for details.

10-city instance



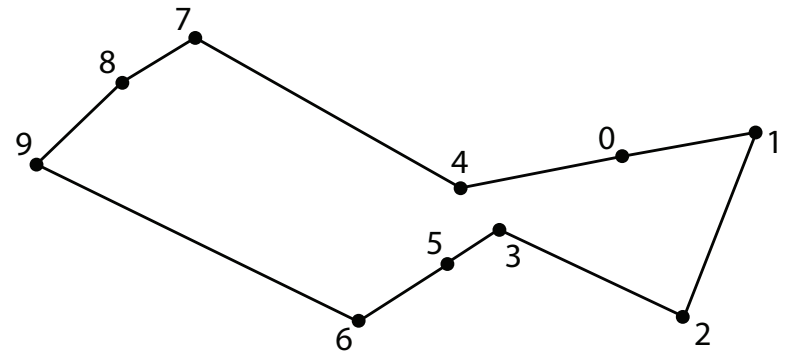
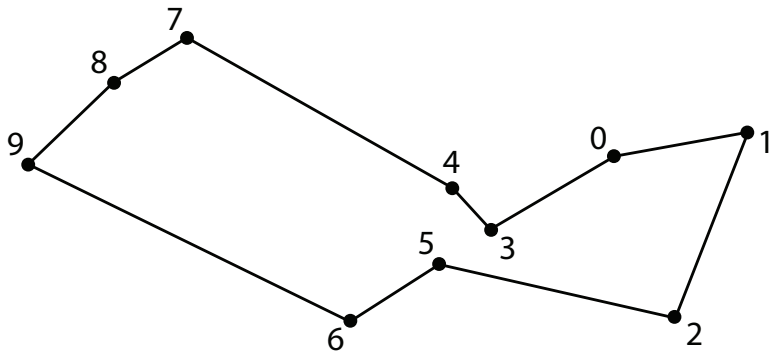
$(n - 1)! = 362,880$ possible tours

10-city instance

	0	1	2	3	4	5	6	7	8	9
0 Chicago	0									
1 Erie	449	0								
2 Chattanooga	618	787	0							
3 Kansas City	504	937	722	0						
4 Lincoln	529	1004	950	219	0					
5 Wichita	805	1132	842	195	256	0				
6 Amarillo	1181	1441	1080	563	624	368	0			
7 Butte	1538	2045	2078	1378	1229	1382	1319	0		
8 Boise	1716	2165	2217	1422	1244	1375	1262	483	0	
9 Reno	2065	2514	2355	1673	1570	1507	1320	842	432	0

10-city instance: solutions

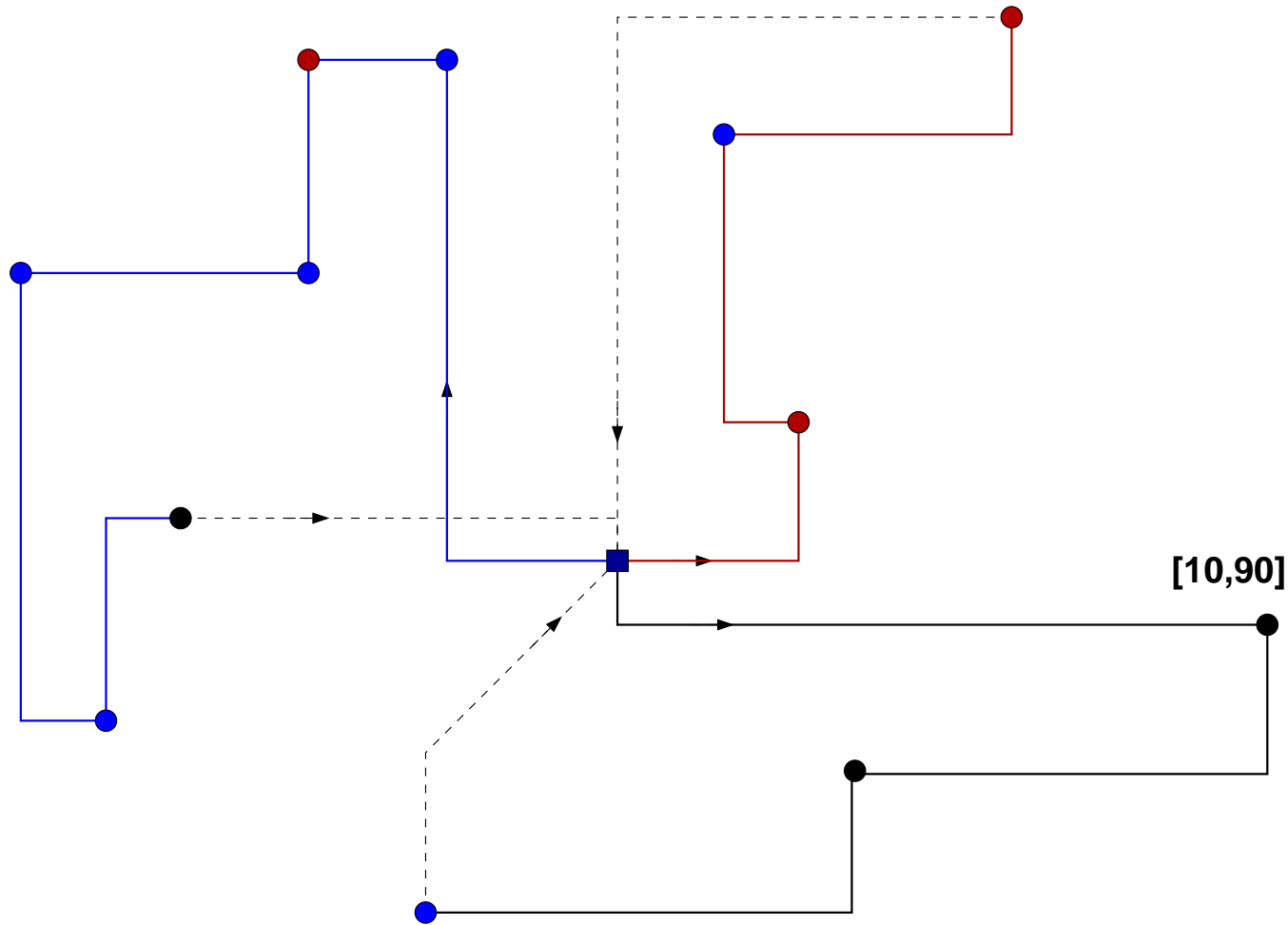
Tours of length 6633 and 6514 miles



Shortest tour: 0, 1, 2, 3, 5, 6, 9, 8, 7, 4

Shortest tour length: 6514

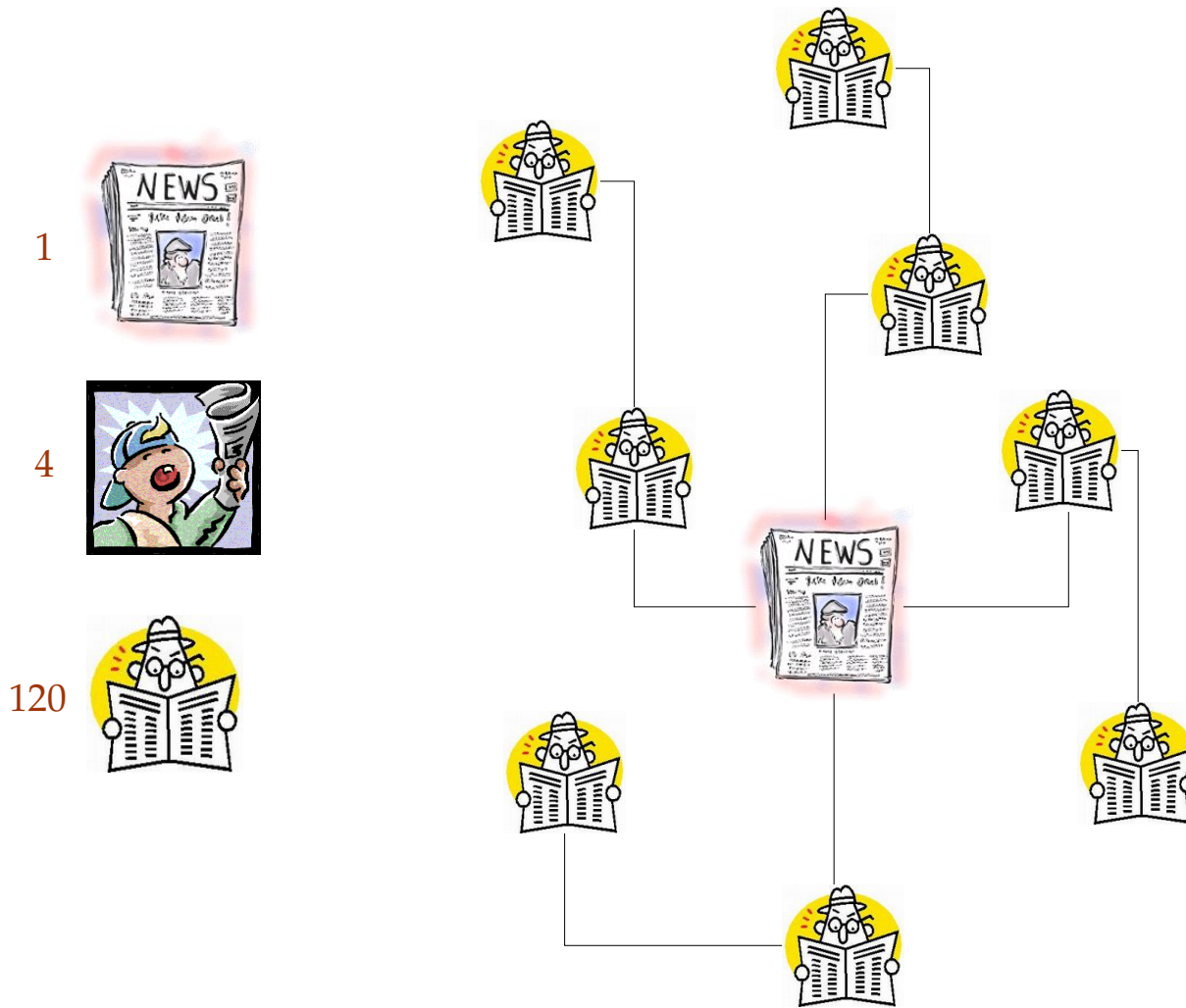
Vehicle Routing



Minimize distance traveled by trucks at a depot delivering to a set of customers within prescribed time windows (used in package delivery by Fedex, USPS etc.)

2014 survey in OR-MS Magazine lists 15+ vendors of VRP software.

Min-max vehicle routing



1996 Whizzkids challenge

- ▷ 5000 Dutch Guilders prize sponsored by CMG
- ▷ Winners: Hemel, van Erk, Jenniskens (U. Eindhoven students)
- ▷ Max path length of 1183
- ▷ Local search techniques, 15,000 hours of computing time.

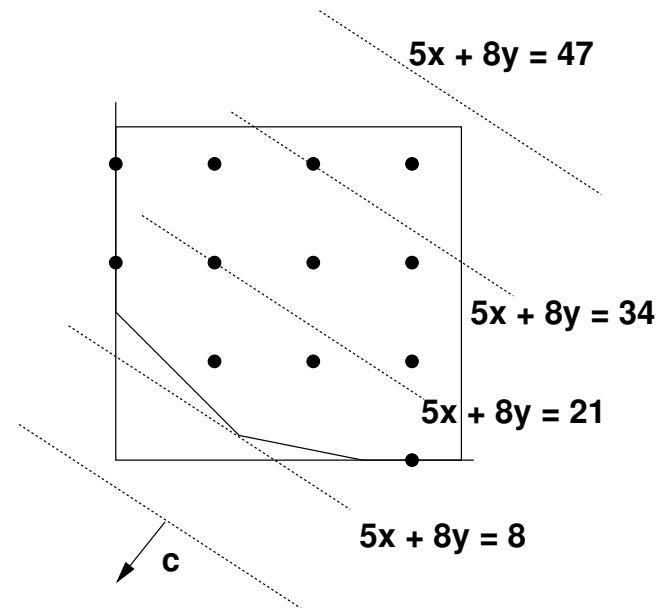
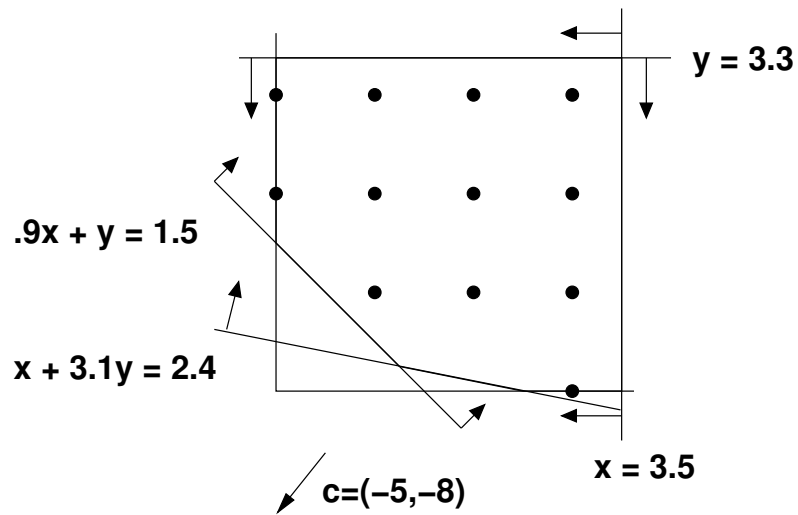
Optimal solution? Lower bound of 1160 given by Hurkens '97.

Integer programming

min $5x + 8y$ subject to

$.9x + y \geq 1.5$, $x + 3.1y \geq 2.4$

$0 \leq x \leq 3.5$, $0 \leq y \leq 3.3$, x, y integral

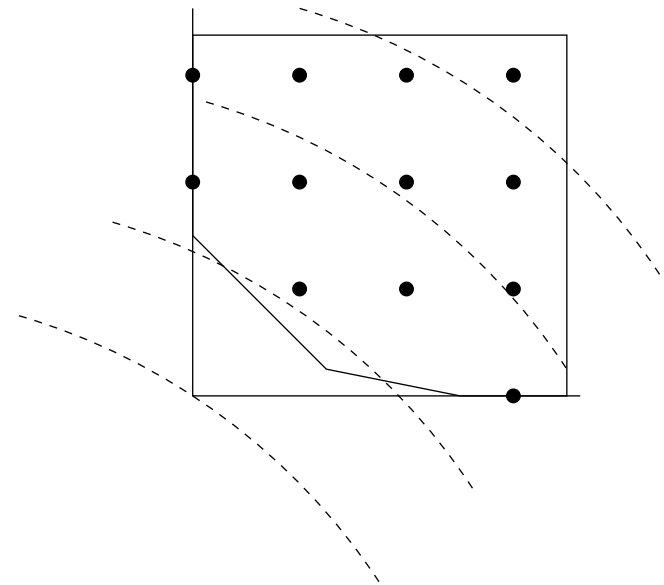
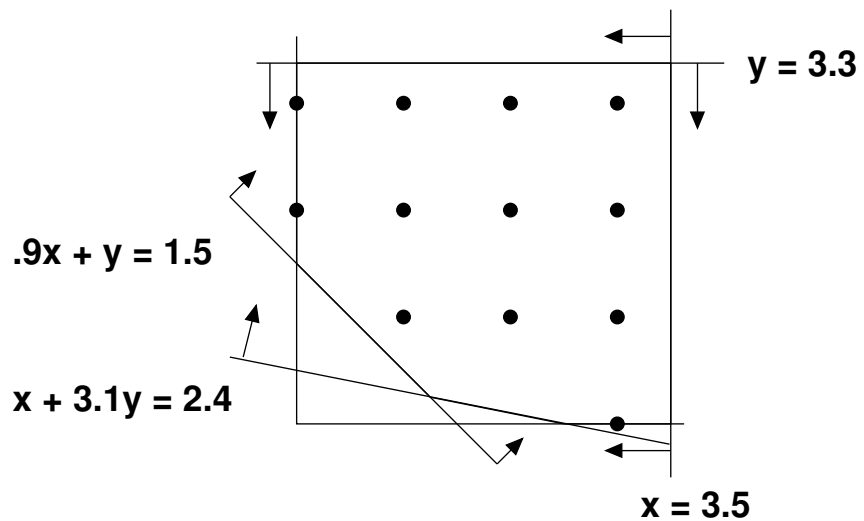


Integer Quadratic programming

$\min 2x^2 + 5y^2 + 6xy + 3x$ subject to

$.9x + y \geq 1.5, x + 3.1y \geq 2.4$

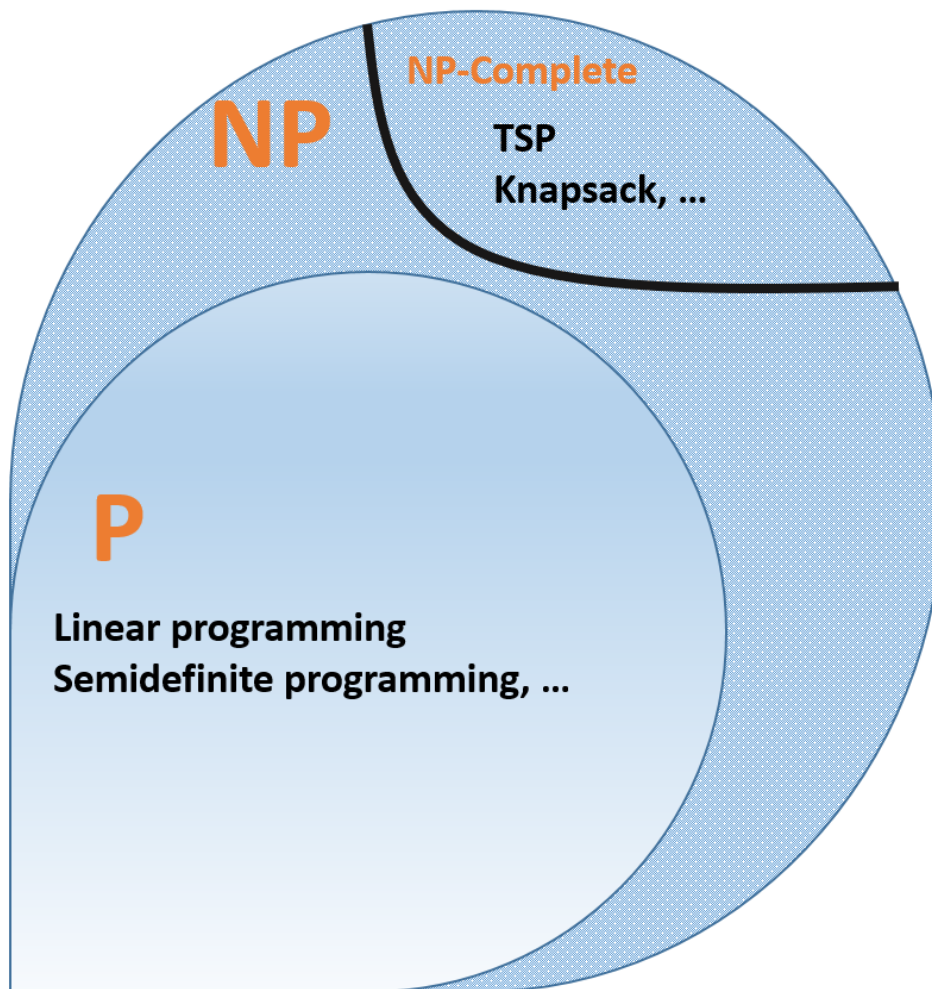
$0 \leq x \leq 3.5, 0 \leq y \leq 3.3, x, y$ integral



Computational Complexity

NP-completeness

The problem of determining if there exists a TSP tour of length less than k is NP-complete.



Running time growth

- ▷ Traveling salesman problem: $O(n^2 2^n)$ algorithm by Held and Karp
- ▷ Shortest path problem: $O(n^2)$ algorithm by Dijkstra

function	5	10	30	64
n^2	25	100	900	4096
$n^2 \log n$	58.0	332.2	4,416.2	24,576
2^n	32	1024	1,073,741,824	18,446,744,073,709,551,616
1.1^n	1.6	2.6	17.4	445.8

Important: For real-life applications, the data/problem size are restricted.

Time taken by Pisinger's MINKNAP algorithm on knapsack instances with n items and item weights chosen uniformly at random from $1, \dots, R$.

	uncorrelated			strongly correlated		
n/R	100	1000	10000	100	1000	10000
100	.002	.002	.002	.002	.002	.076
1000	.002	.002	.003	.019	.078	.172
10000	.004	.005	.010	.050	1.19	25.2

Formulations

0-1 Knapsack formulations

Profits p_i and weights w_i are assumed to nonnegative

integer program:

$$\begin{aligned} \text{Maximize} \quad & p_1x_1 + p_2x_2 + \dots + p_nx_n \\ \text{s.t.} \quad & w_1x_1 + w_2x_2 + \dots + w_nx_n \leq c \\ & x_1, x_2, \dots, x_n \in \{0, 1\}. \end{aligned}$$

For *unbounded knapsack* replace $\{0, 1\}$ by $\{\text{integers}\}$ above.

nonlinear integer program:

$$\begin{aligned} \text{Maximize} \quad & p_1x_1 + p_2x_2 + \dots + p_nx_n \\ \text{s.t.} \quad & w_1x_1^2 + w_2x_2^2 + \dots + w_nx_n^2 \leq c \\ & x_1, x_2, \dots, x_n \in \{0, 1\}. \end{aligned}$$

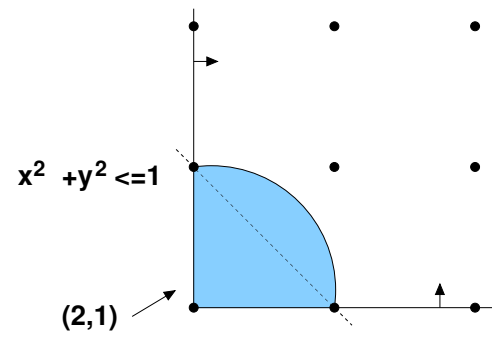
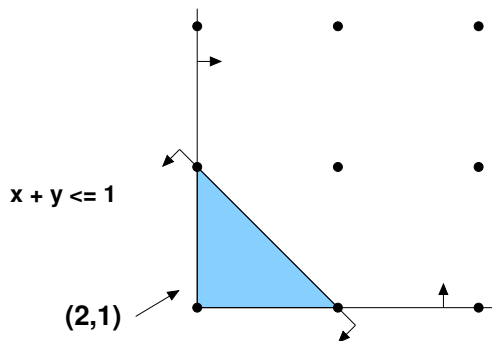
0-1 Knapsack relaxations

Maximize $2x_1 + x_2$
s.t. $x_1 + x_2 \leq 1$
 $x_1, x_2 \in \{0, 1\}$.

Maximize $2x_1 + x_2$
s.t. $x_1^2 + x_2^2 \leq 1$
 $x_1, x_2 \in \{0, 1\}$.

Maximize $2x_1 + x_2$
s.t. $x_1 + x_2 \leq 1$
 $x_1, x_2 \in [0, 1]$.

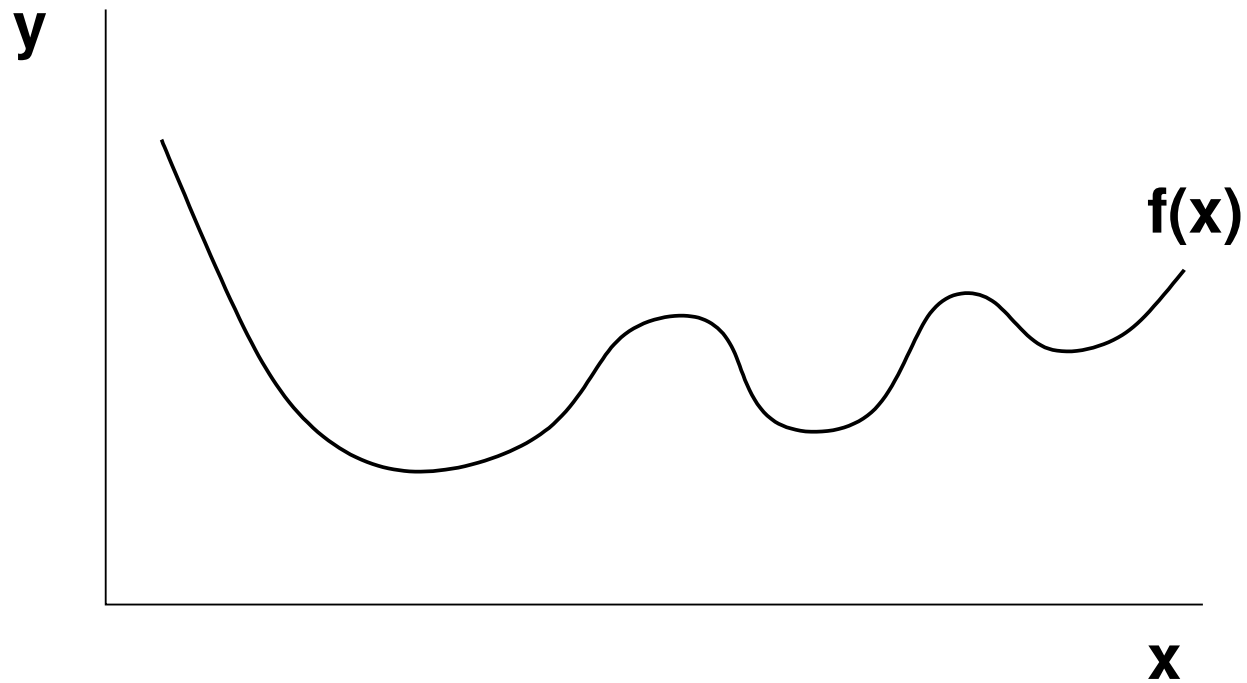
Maximize $2x_1 + x_2$
s.t. $x_1^2 + x_2^2 \leq 1$
 $x_1, x_2 \in [0, 1]$.



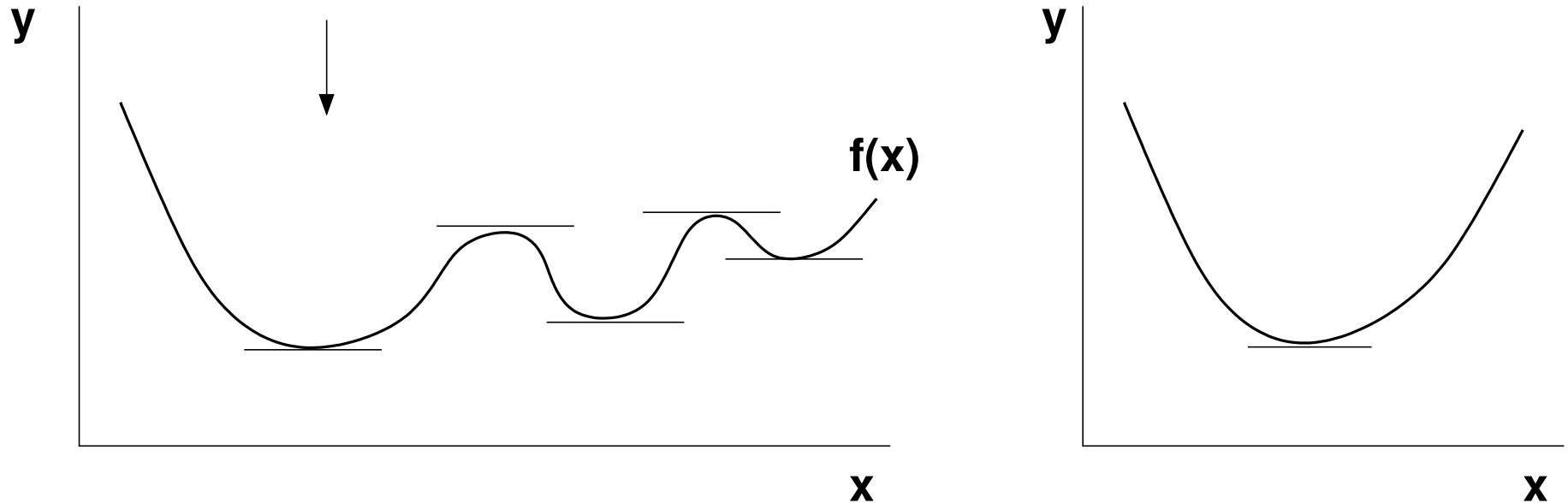
Solution techniques

Basic optimization

Minimize $f(x)$ for x in some domain



Optimality conditions



Necessary condition for optimality of x is $f'(x) = 0$. $f''(x) > 0$ is sufficient condition for local optimality. For convex functions, first condition is sufficient.

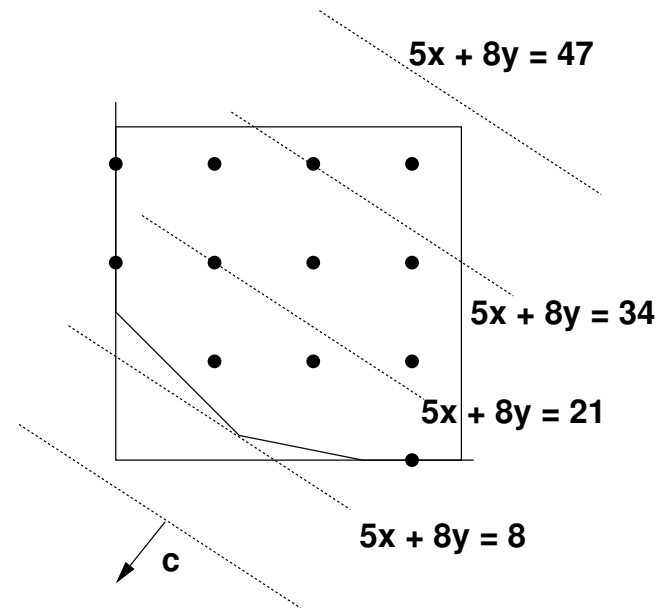
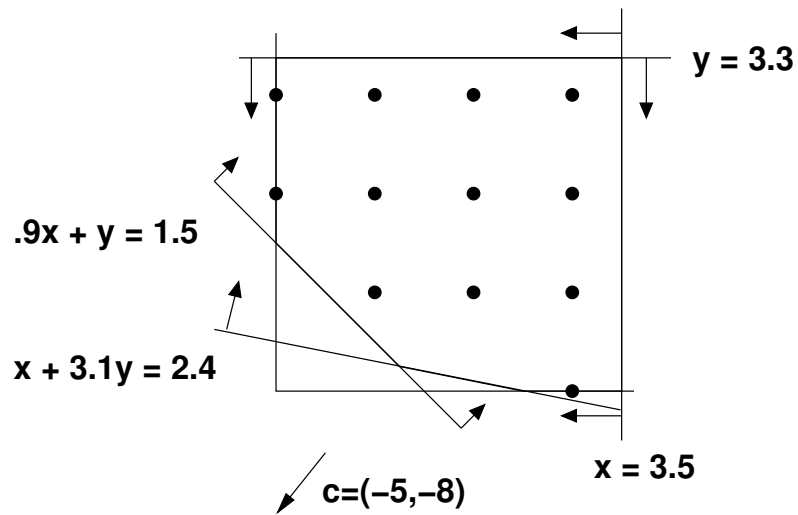
For constrained optimization, KKT conditions are necessary (Kuhn, Tucker '54, Karush '39).

Integer programming

min $5x + 8y$ subject to

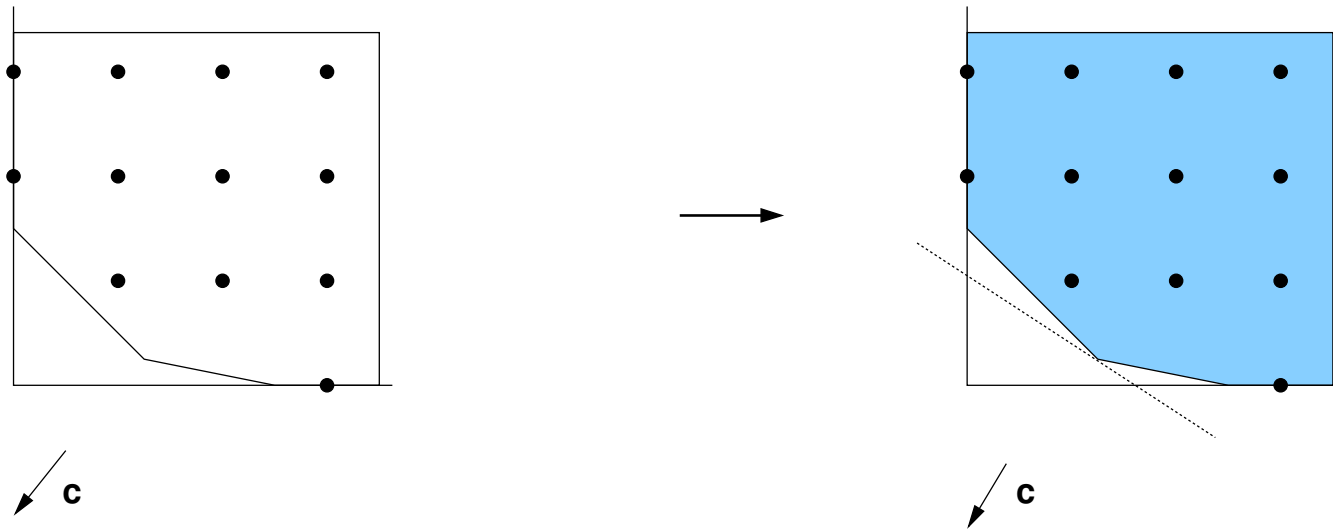
$.9x + y \geq 1.5$, $x + 3.1y \geq 2.4$

$0 \leq x \leq 3.5$, $0 \leq y \leq 3.3$, x, y integral



LP relaxation

min $5x + 8y$ subject to
 $.9x + y \geq 1.5$, $x + 3.1y \geq 2.4$
 $0 \leq x \leq 3.5$, $0 \leq y \leq 3.3$



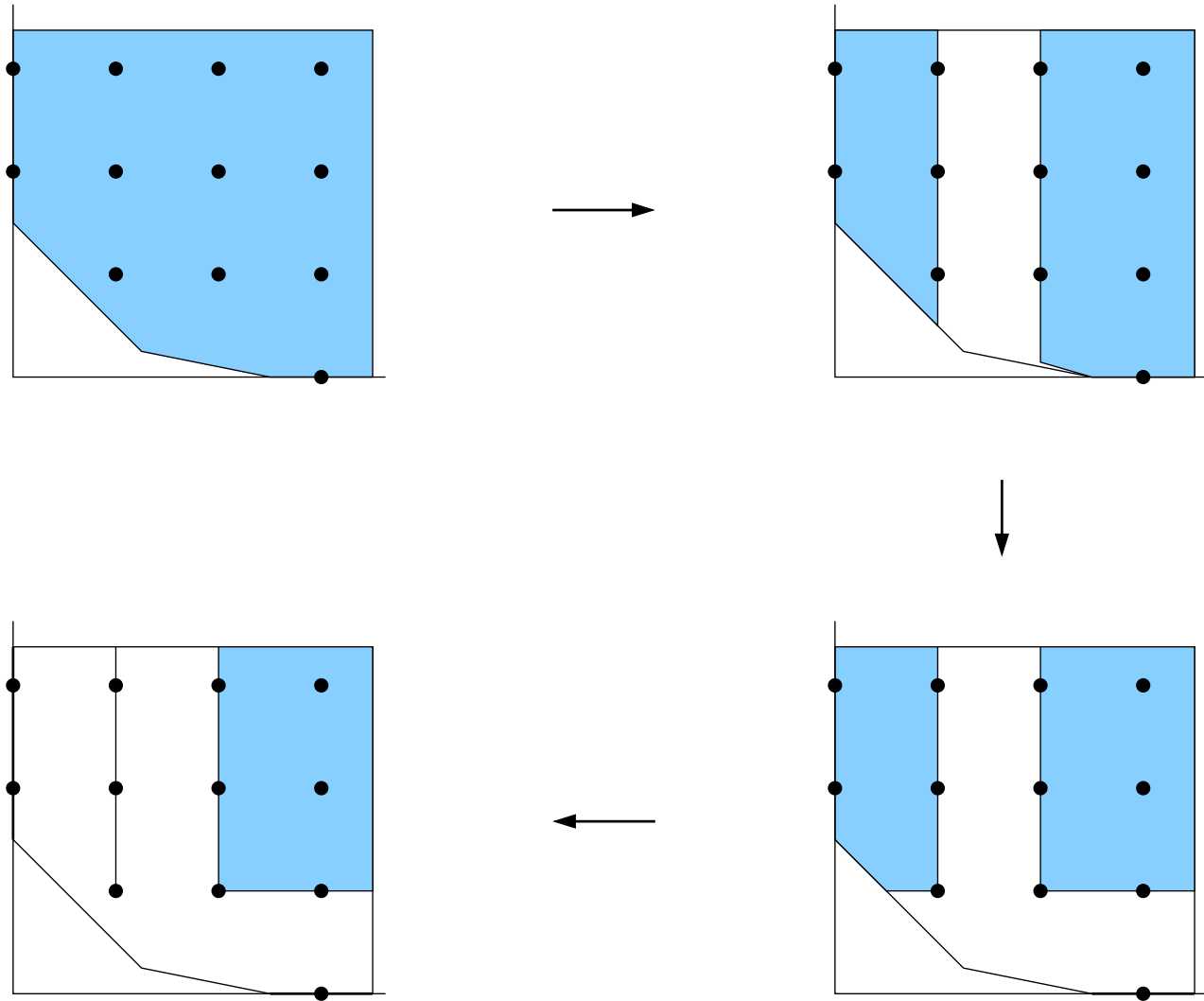
LP relaxation + branching

$$\begin{aligned} &\min 5x + 8y \text{ subject to} \\ &.9x + y \geq 1.5, \quad x + 3.1y \geq 2.4 \\ &0 \leq x \leq 3.5, \quad 0 \leq y \leq 3.3 \end{aligned}$$

$$\begin{aligned} &\min 5x + 8y \text{ subject to} \\ &.9x + y \geq 1.5, \quad x + 3.1y \geq 2.4 \\ &0 \leq x \leq 1, \quad 0 \leq y \leq 3.3 \end{aligned}$$

$$\begin{aligned} &\min 5x + 8y \text{ subject to} \\ &.9x + y \geq 1.5, \quad x + 3.1y \geq 2.4 \\ &2 \leq x \leq 3.5, \quad 0 \leq y \leq 3.3 \end{aligned}$$

Branch and bound



cplex-log2.txt

Problem 'pp08a' read.

.....
 Reduced MIP has 133 rows, 234 columns, and 468 nonzeros.
 Reduced MIP has 64 binaries, 0 generals, 0 SOSs, and 0 indicators.

	Nodes		Objective	IInf	Best Integer	Cuts/ Best Bound	ItCnt	Gap
	Node	Left						
*	0+	0			27080.0000		77	---
	0	0	2748.3452	51	27080.0000	2748.3452	77	89.85%
*	0+	0			14300.0000	2748.3452	77	80.78%
*	0+	0			7950.0000	2748.3452	77	65.43%
	0	2	2748.3452	51	7950.0000	2748.3452	77	65.43%
Elapsed real time = 0.03 sec. (tree size = 0.00 MB, solutions = 3)								
*	100+	94			7860.0000	2848.3452	428	63.76%
*	100+	90			7640.0000	2848.3452	428	62.72%
	2862	2111	6556.5595	28	7640.0000	3981.3452	9387	47.89%
	6557	5339	6788.4524	21	7640.0000	4254.2976	20447	44.32%
*	10017+	8320			7630.0000	4369.3452	30879	42.73%
*	10017+	8067			7520.0000	4369.3452	30879	41.90%
*	10017+	8047			7510.0000	4369.3452	30879	41.82%
*	10017+	7947			7480.0000	4369.3452	30879	41.59%
	10017	7949	7152.1667	16	7480.0000	4369.3452	30879	41.59%
.....								
	467260	381944	6279.9524	23	7480.0000	5330.2500	1336479	28.74%
Elapsed real time = 76.80 sec. (tree size = 86.82 MB, solutions = 9)								
	488008	398616	6870.4881	16	7480.0000	5340.1310	1393871	28.61%
	508767	415262	7018.3810	21	7480.0000	5350.3452	1451784	28.47%
	529510	431893	5359.7738	26	7480.0000	5359.7738	1509653	28.35%
	550267	448498	5819.7024	30	7480.0000	5368.3929	1567040	28.23%
	570955	465047	7091.7738	13	7480.0000	5377.4405	1624524	28.11%
.....								
	760995	616110	6726.4405	24	7480.0000	5445.6548	2152219	27.20%
	778020	629628	6542.1548	30	7480.0000	5451.3214	2199840	27.12%
	794094	642371	6215.4881	25	7480.0000	5456.2024	2244463	27.06%
	811975	656559	cutoff		7480.0000	5461.4405	2294026	26.99%
	829297	670288	6740.9167	28	7480.0000	5466.6786	2342402	26.92%
	846366	683716	6716.6786	22	7480.0000	5471.6786	2389544	26.85%
Elapsed real time = 143.55 sec. (tree size = 155.11 MB, solutions = 9)								

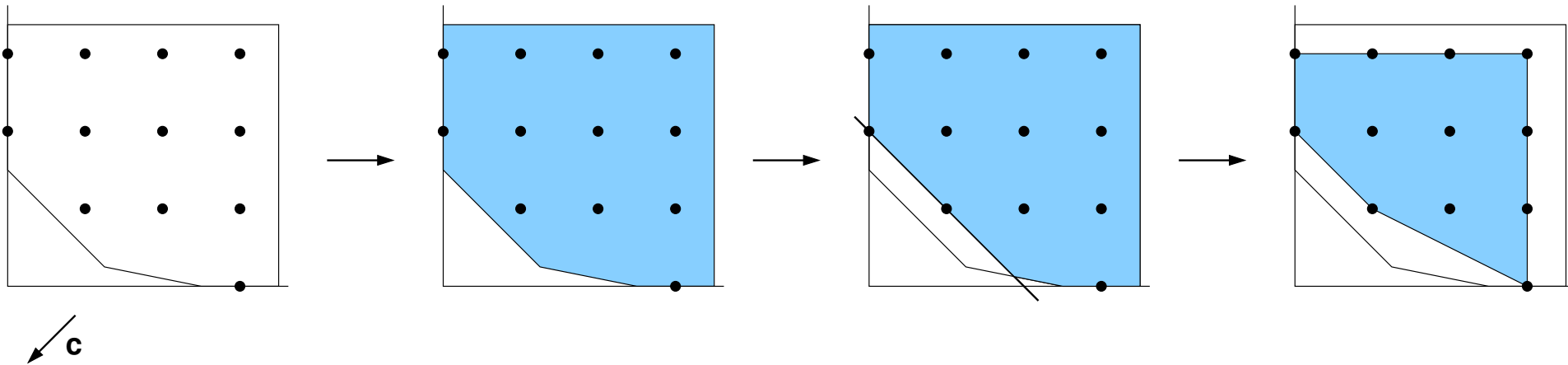
Cutting planes

cutting plane: an inequality satisfied by integral solutions of linear inequalities.

min $5x + 8y$ subject to

$.9x + y \geq 1.5$, $x + 3.1y \geq 2.4$

$0 \leq x \leq 3.5$, $0 \leq y \leq 3.3$, x, y integral



Gomory-Chvátal cutting planes (cuts)

$$x \leq 3.5 \Rightarrow x \leq 3$$

$$y \leq 3.3 \Rightarrow y \leq 3$$

$$(.9x + y \geq 1.5) + (.1x \geq 0) \rightarrow$$

$$x + y \geq 1.5 \Rightarrow x + y \geq 2$$

$$(x + y \geq 2) \times .6 + (x + 3.1y \geq 2.4) \times .4 \rightarrow$$

$$x + 1.84y \geq 2.16 \rightarrow$$

$$x + 2y \geq 2.16 \Rightarrow x + 2y \geq 3.$$

Every integer program can be solved by Gomory-Chvátal cuts (Gomory '60), though it may take exponential time in the worst case (Pudlák '97).

cplex-log.txt

Problem 'pp08a' read.

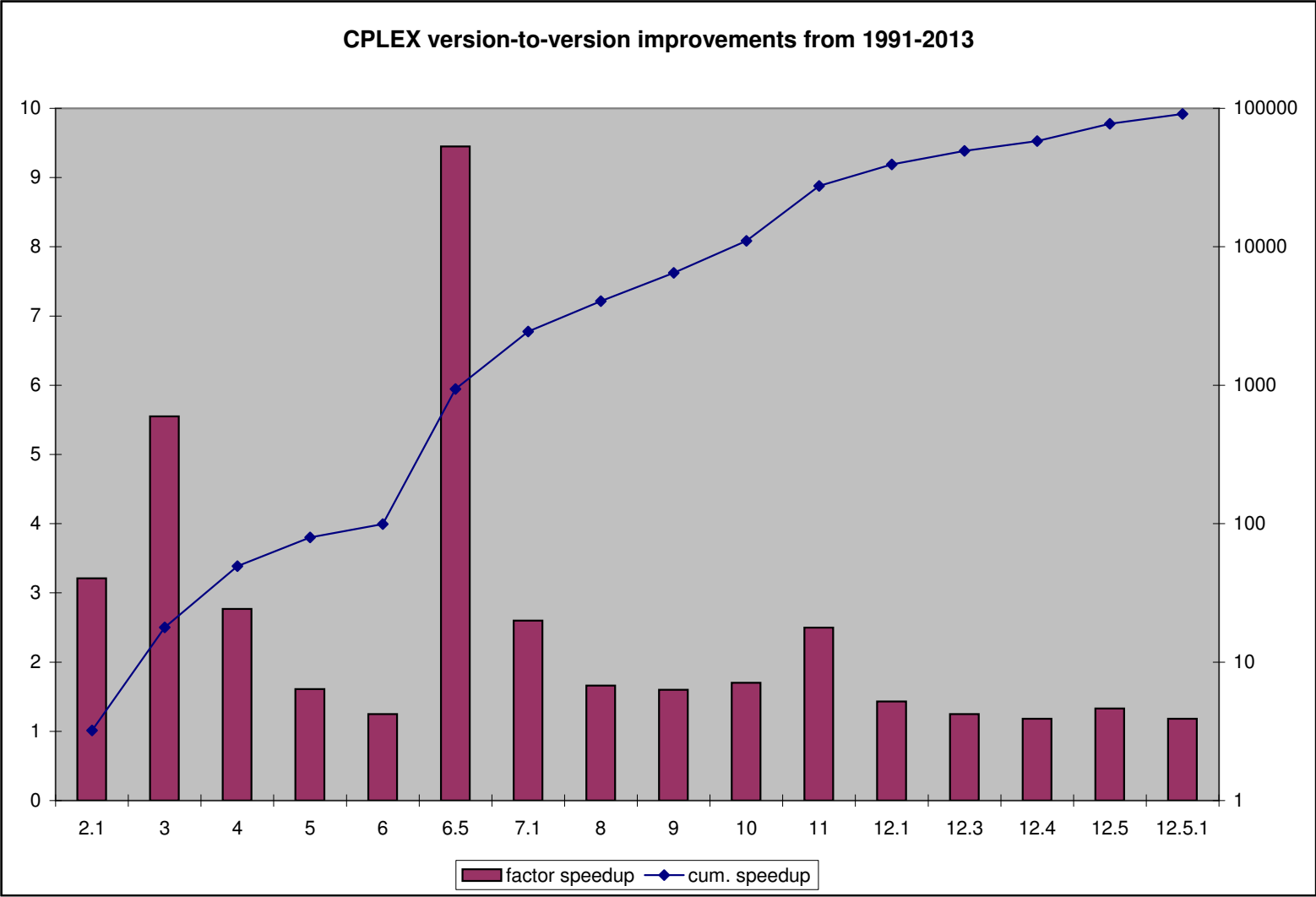
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*	0+	0			27080.0000		77	---
	0	0	2748.3452	51	27080.0000	2748.3452	77	89.85%
*	0+	0			14300.0000	2748.3452	77	80.78%
	0	0	5046.0422	48	14300.0000	Cuts: 133	153	64.71%
	0	0	6749.5837	24	14300.0000	Cuts: 130	265	52.80%
*	0+	0			10650.0000	6749.5837	265	36.62%
	0	0	7099.1233	27	10650.0000	Cuts: 53	327	33.34%
	0	0	7171.1837	28	10650.0000	Cuts: 35	356	32.66%
*	0+	0			7540.0000	7171.1837	356	4.89%
	0	0	7176.2716	31	7540.0000	Cuts: 19	370	4.82%
	0	0	7187.8155	33	7540.0000	Cuts: 20	388	4.67%
	0	0	7188.4198	28	7540.0000	Cuts: 4	398	4.66%
	0	0	7189.5182	30	7540.0000	Cuts: 9	409	4.65%
	0	0	7189.5877	30	7540.0000	Flowcuts: 5	413	4.65%
	0	0	7189.9535	26	7540.0000	Flowcuts: 2	420	4.64%
	0	2	7189.9535	26	7540.0000	7190.0161	420	4.64%
Elapsed real time = 0.27 sec. (tree size = 0.00 MB, solutions = 4)								
*	50+	40			7530.0000	7218.8496	1733	4.13%
*	55	44	integral	0	7520.0000	7218.8496	1783	4.00%
*	60+	45			7490.0000	7218.8496	1892	3.62%
*	60+	38			7420.0000	7218.8496	1892	2.71%
*	110+	53			7400.0000	7238.6753	2712	2.18%
*	210	64	integral	0	7350.0000	7255.3139	4760	1.29%

Implied bound cuts applied: 1
 Flow cuts applied: 149
 Flow path cuts applied: 23
 Multi commodity flow cuts applied: 5
 Gomory fractional cuts applied: 34

.....
 Total (root+branch&cut) = 0.95 sec.

cplex_speedups Chart 4



Applications

Steel industry application

Context: Large steel plant (3 million tons of plates/year \approx 10,000 tons/day) in East Asia moving from a producer-centric model to a customer-centric model

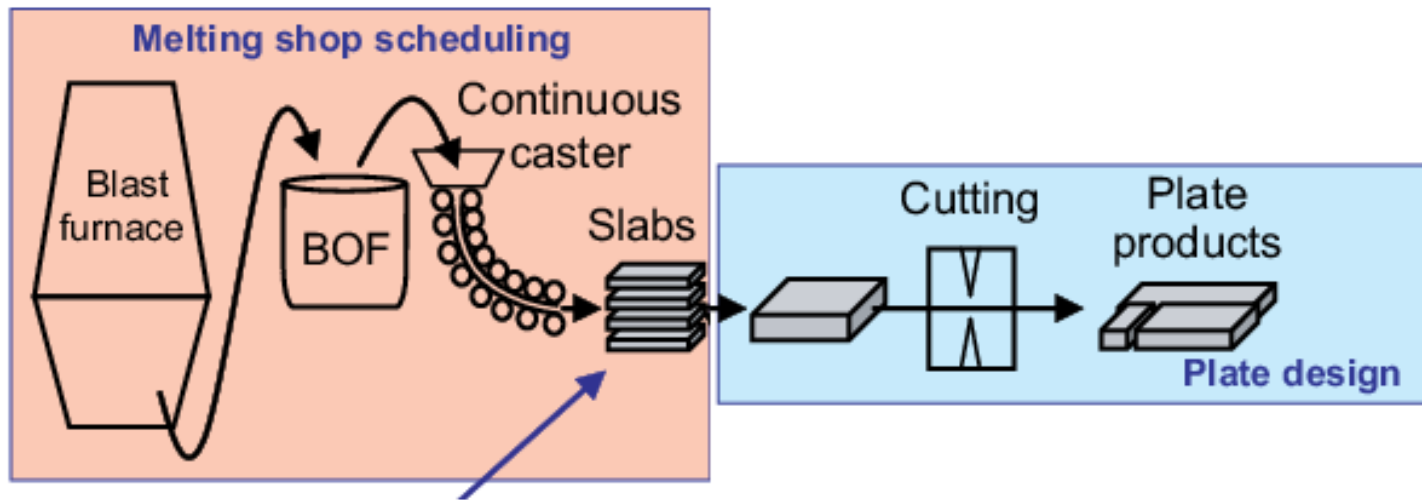
Goal: Optimization tool to generate a production design – a detailed description of production steps and related intermediate products

Timeline: 1.5 years

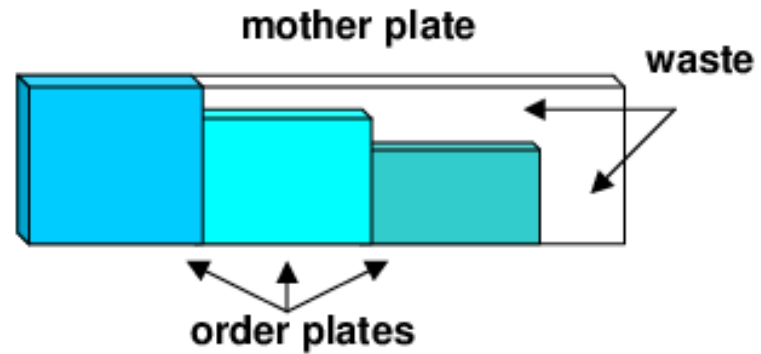
(5 man years on optimization, 25 man years on databases/GUI/analysis)

(joint work with J. Kalagnanam, C. Reddy, M. Trumbo)

Manufacturing process



Slab design



Consulting Issues

- ◇ 2+ research man years spent defining problem (high complexity)
 - Very large number of constraints including objectives masked as constraints
 - 500+ pages of specifications: scope of problem not known at contract signing
- ◇ High level problem has non-linearities
- ◇ Software/data issues - 1000+ files
- ◇ 30 minutes of computing time allowed
 - 100+ complex cutting stock problems with up to 2000 orders solved via integer programming column generation

Pipeline management

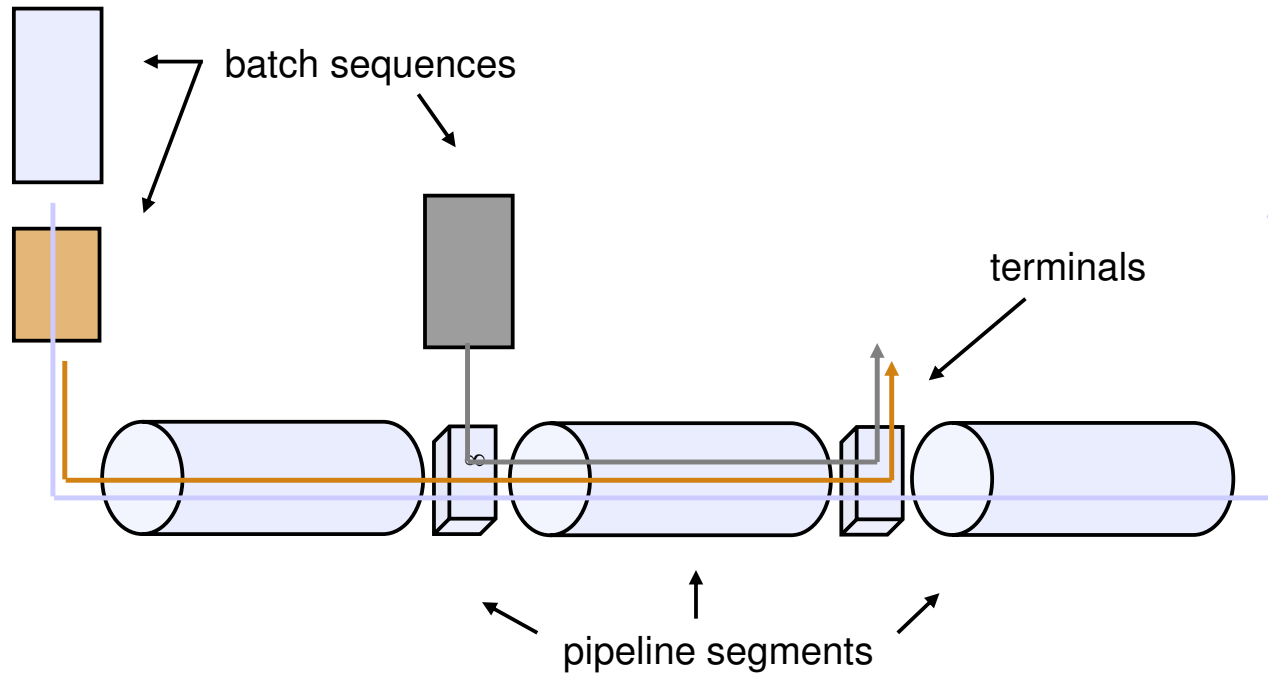
Schedule injections of batches of oil on a pipeline network while minimizing interface costs, delays, and power costs and satisfying tank constraints

(joint work with V. Austel, O. Günlük, P. Rimshnick, B. Schieber)

A pipeline network has many pipelines, each with multiple segments, each of which can run at multiple 'natural rates'.

Timeline: 2.5 years (10+ man years on optimization)

Inputs to Batch Sequencing Problem



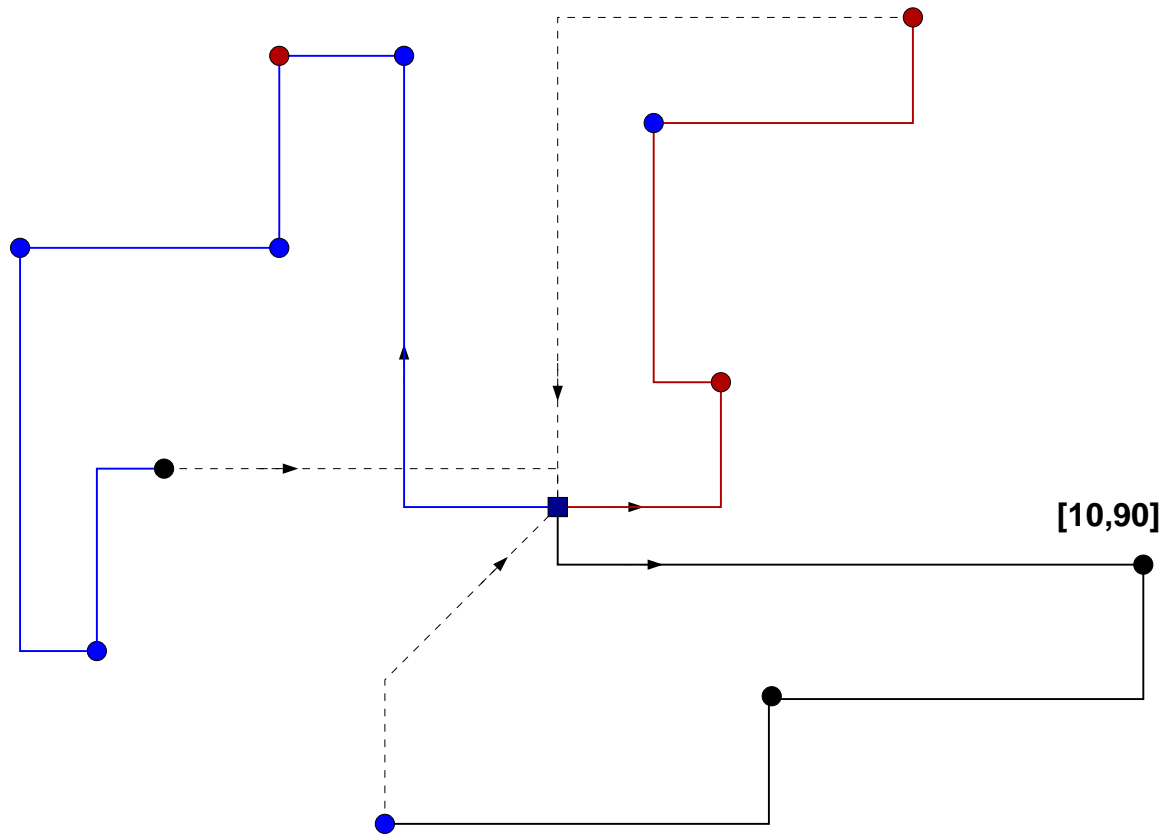
Interface cost table

	Grey	Blue	Brown
Grey	0	0.9	∞
Blue	1.5	0	2.5
Brown	2.7		0

Vehicle routing application

Context: Food distribution company in North America trying to improve delivery to customers within desired time windows, while minimizing travel costs.

VRPTW with driver preferences

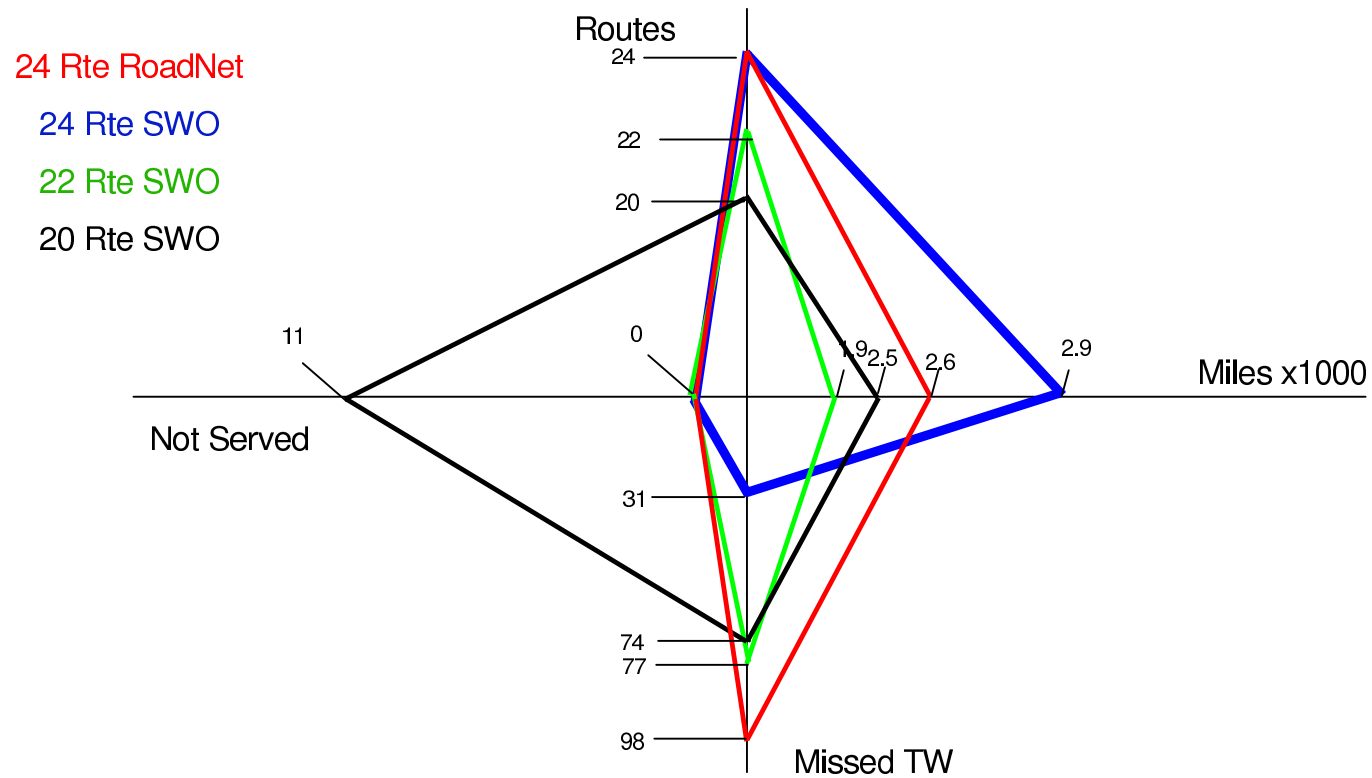


Customers have preferred drivers; penalize for delivery by non-preferred driver.

- ◇ 200-300 customers, 20-30 routes per shift, 3-6 shifts per day
- ◇ Create preference relationships between ≈ 200 drivers and 1000 customers (joint work with O. Günlük, G. Sorkin)



Graphic Route Comparison

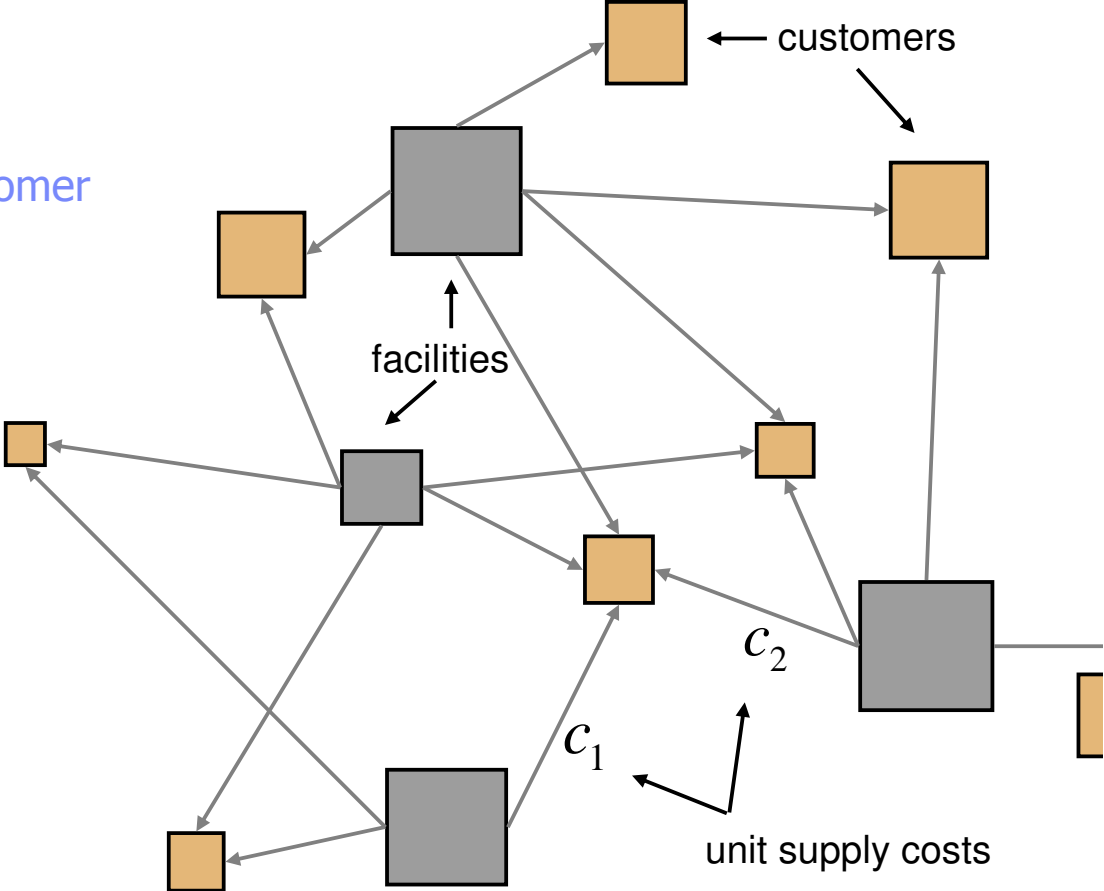


Comparison of route characteristics – Changing Input Parameters and Penalties directly impacts optimizer solution.

Facility location problem

Inputs:
Facilities + capacities
Cost of opening each facility
Customers + demands
Unit cost of supplying a customer from each facility

Goal:
Minimize cost of opening facilities to satisfy demand



Related to Fermat-Weber problem

Machine learning application

▷ Insurance company wants to answer a long list of customer questions, but has a budget for only 500 answers (Dmitry Malioutov).

Does it cost more to insure a red car?

How much liability insurance is required in NJ?

How much liability insurance is required in Princeton?

Will my insurance go up if I let my boyfriend drive my car?

Will my insurance go up if I let my girlfriend drive my car?

- ▷ The problem is an “active learning” problem: try to optimize which questions to answer.
- ▷ Balance “information gain” vs. “diversity” for each answered question.

Inputs:

- 1) Each node/question has a notion of how much additional information it will add by providing a human answer – this is the node cost.
- 2) The similarity of each question to other questions: there is no point in answering the same question 20 times, so it’s great to have a diverse set of questions to ask humans to answer.

DWave Quantum Computer

DWave: An adiabatic quantum computer performing “quantum annealing”.

▷ A special-purpose analog machine employing “flux qubits” arranged in a Chimera graph structure solving the Ising Model Problem. DWave does not guarantee optimality.


DWave experiments

McGeoch and Wang: Experimental Evaluation of an adiabatic quantum system for combinatorial optimization, *ACM Conference on Computing Frontiers* 2013.

In horserace terms, QA dominates on the Chimera-structure QUBO problems: at the largest problem size $n = 439$, CPLEX (best among the software solvers), returns comparable results running about 3600 times slower than the hardware. On the W2SAT problems, Blackbox, AK, and TABU

▷ DWave Two takes half a second versus half an hour for CPLEX 12.3. on quadratic unconstrained boolean optimization (QUBO) problems defined on a Chimera graph

New York Times:

MAY 16, 2013, 5:00 AM |  30 Comments

Google Buys a Quantum Computer

By QUENTIN HARDY

quantum physics. Their quantum computer, which performs complex calculations thousands of times faster than existing supercomputers, is expected to be in active use in the third quarter of this year.

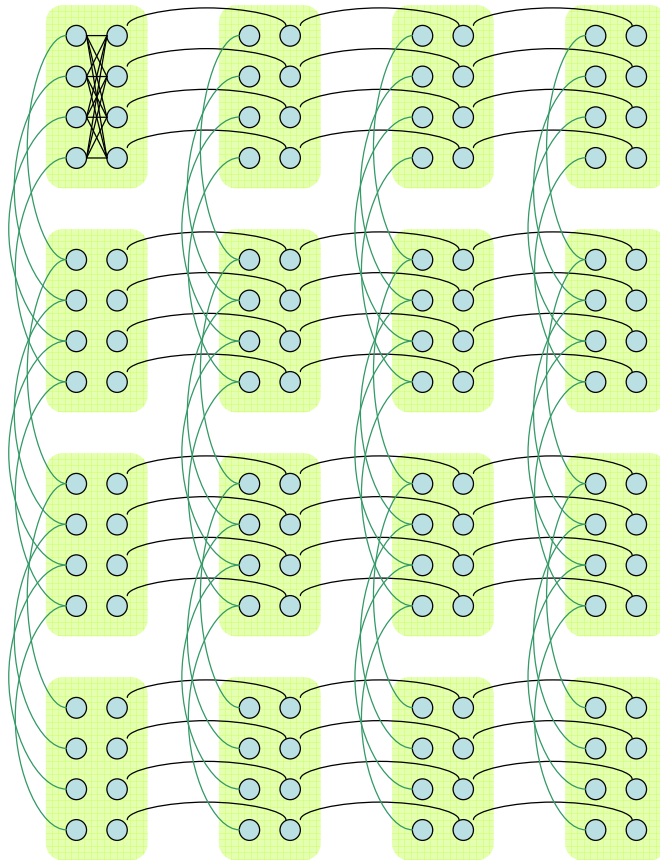
New York Times (Nov 14,2013):

This year, Google and a corporation associated with NASA acquired for study an experimental computer that appears to make use of quantum properties to deliver results sometimes 3,600 times faster than traditional supercomputers. The maker of the quantum computer, D-Wave Systems of Burnaby, British Columbia, counts Mr. Bezos as an investor.

Chimera graphs

Chimera graph C_n : $8n^2$ nodes with n^2 $K_{4,4}$ graphs arranged in a $n \times n$ grid.

C_4



QUBO problem

The Ising model problem is equivalent to the QUBO problem.

▷ The quadratic unconstrained boolean optimization problem (QUBO) problem: Given an $n \times n$ matrix Q :

$$\text{Min } \sum_{i,j} Q_{ij}x_i x_j \text{ subject to } x \in \{0, 1\}^n. \quad (1)$$

QUBO problems

McGeoch and Wang solve QUBO-miqp using the CPLEX MIQP solver

The CPLEX MIQP solver does branch-and-bound based on the QP relaxation:

$$\text{Min } \sum_{i,j} Q_{ij}x_i x_j \text{ subject to } x \in [0, 1]^n. \quad (2)$$

QUBO problems

QUBO-milp: Classical mixed-integer linear programming formulation (assume Q is upper triangular):

$$\text{Min } \sum_{i < j} Q_{ij} z_{ij} + \sum_{i=1}^n Q_{ii} x_i \quad (3)$$

subject to

$$x \in \{0, 1\}^n, \quad (4)$$

$$z_{ij} \leq x_i \quad \forall i < j, \quad (5)$$

$$z_{ij} \leq x_j \quad \forall i < j, \quad (6)$$

$$x_i + x_j - z_{ij} \leq 1 \quad \forall i < j, \quad (7)$$

$$z_{ij} \geq 0 \quad \forall i < j. \quad (8)$$

For any fixed i, j , the constraints (5)-(8) are called Fortet inequalities or McCormick inequalities and force z_{ij} to equal $x_i x_j$ when $x_i, x_j \in \{0, 1\}$.

Experiments

- ▷ CPLEX 12.3/QUBO-MILP takes 93.8 seconds in the worst case and not half an hour: Dash, Puget '14
- ▷ Simulated annealing heuristic takes 0.02 seconds on 512 node instances: Boixo, Ronnow, Isacker, Wang, Wecker, Lidar, Martinis, Troyer '13.
- ▷ Specialized heuristic takes 0.01 seconds on 439 node instances: Selby '13.

Conclusions

- ▷ Many real-life optimization problems can be modeled as instances of NP-hard problems. However, as the data and problem sizes are restricted, such problems can often be solved with customized techniques.
- ▷ Linear-integer programming is the most widely used optimization tool in practical applications, but some important problems (e.g., portfolio optimization) are modeled as nonlinear (quadratic) integer programs.
- ▷ Linear constraints are more common in combinatorial problems, whereas nonlinear constraints are more common in systems where the physics is important.