DM826 – Spring 2012

Modeling and Solving Constrained Optimization Problems

Lecture 1
Course Introduction
Hybrid Modeling

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[*Partly based on slides by Stefano Gualandi, Politecnico di Milano*]

Outline

Outline

Schedule and Material

- Schedule (28 lecture hours):
  - Monday 16.15-18
  - Wednesday 12.15-14
  - Friday 10.15-12
  - Last lecture: Friday, 16th March, 2012
- Communication tools
  - Public Course Webpage (Wp) http://www.imada.sdu.dk/~marco/DM826/
  - In Blackboard (Bb):
    - Announcements
    - Assignments Hand In
    - Documents (Photocopies)
    - Discussion Board (subscribe)
  - Personal email
  - You are welcome to visit me in my office in working hours.

Evaluation

- Two obligatory assignments (50% of final grade)
  - Model
  - Implementation
  - Report (3 pages)
- Third final assignment (50% of final grade)
  - Model
  - Implement
  - Report (Max 10 pages)

References

- Main References:

  B1 F. Rossi, P. van Beek and T. Walsh (ed.), Handbook of Constraint Programming, Elsevier, 2006
  B2 J.N. Hooker, Integrated Methods for Optimization. Springer, 2007
  B3 C. Schulte, G. Tack, M.Z. Lagerkvist, Modelling and Programming with Gecode 2010

- Photocopies (Bb)
- Articles from the Webpage
- Lecture slides
- Assignments

- ...but take notes in class!

Outline

Computational Model

We basically have three Computational Model to solve (combinatorial) optimization problems:

- Mathematical Programming (LP, ILP, QP, SDP, ...)
- Constraint Programming (SAT as a very special case)
- Local Search (... and Meta-heuristics)

Constraint Programming

- In MILP we formulate problems as a set of linear inequalities
- In CP we describe substructures (so-called global constraints) and combine them with various combinators.
- Substructures capture building blocks often (but not always) comptuationally tractable by special-purpose algorithms
- CP models can:
  - be linearized and solved by their MIP solvers;
  - be translated in CNF and sovled by SAT solvers;
  - be handled by local search
- In MILP the solver is often seen as a black-box
  In CP and LS solvers leave the user the task of programming the search.
- CP = model + propagation + search
  constraint propagation by domain filtering $\rightsquigarrow$ inference
  search = backtracking, branch and bound, local search

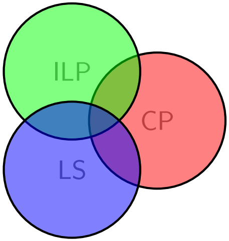
Hybrid Methods

Strengths:

- CP is excellent to explore highly constrained combinatorial spaces quickly
- Math programming is particulary good at deriving lower bounds
- LS is particualry good at derving upper bounds

How to combine them to get better "solvers"?

- Exploiting OR algorithms for filtering
- Exploiting LP (and SDP) relaxation into CP
- Hybrid decompositions:
  1. Logical Benders decomposition
  2. Column generation
  3. Large-scale neigbhrohood search



Outline

Modeling

Modeling:

1. identify variables, domains, constraints and objective functions that formulate the problem
2. express what in point 1) in a way that allows the solution by available software

Integrated Modeling

Models interact with solution process hence models in CP and IP are different.

To integrate one needs:

- to know both sides
- to have available a modelling language that allow integration (Comet)

There are typcially alternative ways to formulate a problem. Some may yield faster solutions.

Typical procedure:

- begin with a strightforward model to solve a small problem instance
- alter and refine the model while scaling up the instances to maintain tractability

Linear Programming

Linear Programming

Given A matrix $A \in \mathbb{R}^{m \times n}$ and column vectors $b \in \mathbb{R}^m, c \in \mathbb{R}^n$.

Task Find a column vector $x \in \mathbb{R}^n$ such that $Ax \leq b$ and $c^T x$ is maximum, decide that $\{x \in \mathbb{R}^n \mid Ax \leq b\}$ is empty, or decide that for all $\alpha \in \mathbb{R}$ there is an $x \in \mathbb{R}^n$ with $Ax \leq b$ and $c^T x > \alpha$.

Theory vs. Practice

In theory the Simplex algorithm is exponential, in practice it works.

In theory the Ellipsoid algorithm is polynomial, in practice it is not better than the Simplex.

Integer Programming

Integer Programming

Given A matrix $A \in \mathbb{Z}^{m \times n}$ and vectors $b \in \mathbb{Z}^m, c \in \mathbb{Z}^n$.

Task Find a vector $x \in \mathbb{Z}^n$ such that $Ax \leq b$ and cx is maximum,
or decide that $\{x \in \mathbb{Z}^n \mid Ax \leq b\} = \emptyset$,
or decide that $\sup\{cx \mid x \in \mathbb{Z}^n,\ Ax \leq b\} = \infty$.

Theory vs. Practice

In theory, IP problems can be solved efficiently by exploiting (if you can find-/approximate) the convex hull of the problem.
In practice, we heavily rely on branch&bound search tree algorithms, that solve LP relaxations at every node.
Logical Statements Frequently (but not always) the integer variables are restricted to be in {0,1} representing Yes/No decisions.

Quadratic Programming

Quadratic Programming

Given Matrices $A, Q_i \in \mathbb{R}^{n \times n}$, with $i = 0, \ldots, q$, and column vectors $a_i, b, c \in \mathbb{R}^n$.

Task Find a column vector $x \in \mathbb{R}^n$ such that $x^T Q_i x + a_i^T x \leq b$ and $x^T Q_0 X + c^T x$ is maximum,
or decide that $\{x \in \mathbb{R}^n \mid x^T Q_i x + a_i^T x \leq b\}$ is empty,
or decide that it is unbounded.

Theory vs. Practice

In theory, this is a richer modeling language (quadratic constraints and/or objective functions).
In practice, we linearize all the time, relying on (most of the time linear) cutting plane algorithms.

Example
Quadratic programming (QP), quadratically-constrained programming (QCP), mixed integer quadratic programming (MIQP), and mixed-integer quadratically-constrained programming (MIQCP).
Conventionally, a quadratic program is formulated this way:

$$\begin{aligned} \min \quad & 1/2x^T Qx + cTx \\ s.t. \quad & Ax \sim b \\ & lb \leq x \leq ub \end{aligned}$$

Q is a matrix of coefficients. That is, the elements Q_{jj} are the coefficients of the quadratic terms x_j^2, and the elements Q_{ij} and Q_{ji} are summed to make the coefficient of the term $x_i x_j$.

$$
\begin{aligned}
\min\ & x_1 + 2x_2 + 3x_3 + \frac{1}{2}(-33x_1^2 + 12x_1x_2 - 22x_2^2 + 23x_2x_3 - 11x_3) \\
& -x_1 + x_2 + x_3 \leq 20 \\
& x_1 - 3x_2 + x_3 \leq 30 \\
& +x_1^2 + x_2^2 + x_3^2 \leq 1
\end{aligned}
$$

Example `qpex1.py` and `qpex1.lp`
Example `qcpex1.py` and `qcpex1.lp`

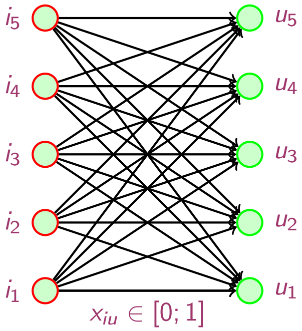
Example: Quadratic Assignment Problem

- **Given:**
  n units with a matrix $F = [f_{ij}] \in \mathbf{R}^{n \times n}$ of flows between them and
  n locations with a matrix $D = [d_{uv}] \in \mathbf{R}^{n \times n}$ of distances
- **Task:** Find the assignment σ of units to locations that minimizes the sum of product between flows and distances, ie,

$$\min_{\sigma \in \Sigma} \sum_{i,j} f_{ij} d_{\sigma(i)\sigma(j)}$$

Applications: hospital layout; keyboard layout

Quadratic Programming Formulation



indices i, j for units and u, v for locations:
Quadratic 0-1 problem:

$$\min \sum_i \sum_u \sum_j \sum_v f_{uv} d_{ij} x_{iu} x_{jv}$$

$$\sum_i x_{iu} = 1 \qquad \forall u$$

$$\sum_u x_{ui} = 1 \qquad \forall i$$

$$x_{iu} \in \{0, 1\}$$

Largest instances solvable exactly $n = 30$

Example: QAP

$$D = \begin{pmatrix} 0 & 4 & 3 & 2 & 1 \\ 4 & 0 & 3 & 2 & 1 \\ 3 & 3 & 0 & 2 & 1 \\ 2 & 2 & 2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix} \qquad F = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 1 & 0 & 2 & 3 & 4 \\ 2 & 2 & 0 & 3 & 4 \\ 3 & 3 & 3 & 0 & 4 \\ 4 & 4 & 4 & 4 & 0 \end{pmatrix}$$

The optimal solution is $\sigma = (1, 2, 3, 4, 5)$, that is,
facility 1 is assigned to location 1,
facility 2 is assigned to location 2, etc.

The value of $f(\sigma)$ is 100.

A possible linearization with $y_{iujv} = x_{iu}x_{jv}$ (Adams-Johnson model)

$$
\begin{aligned}
\min \sum_{i,u,j,v} a_{uv} b_{ij} y_{iujv} & & \\
\sum_{i} x_{iu} &= 1 & \forall u \\
\sum_{u} x_{ui} &= 1 & \forall i \\
\sum_{v} y_{iujv} &= x_{iu} & \forall i, u, j \\
\sum_{j} y_{iujv} &= x_{iu} & \forall i, u, v \\
y_{iujv} &= y_{jviu} & \forall i, u, j, v \\
x_{iu} &\geq 0 & \forall i, u \\
y_{iujv} &\geq 0 & \forall i, u, j, v
\end{aligned}
$$

The symmetry constraints $\Rightarrow y_{iujv}, i \leq k$.

$y_{ijij} = x_{ij}$ for all i and j,
$y_{iuiv} = 0$ for all i and $u \neq v$,
and $y_{iuju} = 0$ for all $i \neq j$
$\rightsquigarrow n^2 + n^2(n-1)/2$ variables.

Constraints
$2n(n-1)2-(n-1)(n-2), n \geq 3$.

In practice

Modeling Languages (e.g., AMPL, Mosel, AIMMS, ZIMPL, Comet, OPL,...)

Write your problem as:

$$\min\{\mathbf{c}^T\mathbf{z} + \mathbf{d}^T\mathbf{y} \mid A\mathbf{z} + B\mathbf{y} \geq b, z \in \mathbb{R}^n, y \in \mathbb{Z}\}$$

push the button solve, and ... cross your fingers!

Theory vs. Practice

In theory, plenty of optimization problem solved in this manner.
In practice, for many real-life discrete (optimization) problems this approach is not suitable (typically, it does not scale well).

The case of Integer Programming

The problem with Integer Programming [Williams, 2010]

IP is essentially concerned with the intersection of two structures:

- Linear inequalities giving rise to polytopes.
- Lattices of integer points.

Mathematical and computational methods and results exist for both these structures on their own. *However mixing them is like mixing oil and water*. Problems arise in both the computation of optimal solutions and the economic interpretation of the results.

Example:

How many times do we really have (an approximation of) the convex hull in our integer problem?

Example: Send More Money

Send + More = Money

You are asked to replace each letter by a different digit so that

$$\begin{array}{cccccc} & S & E & N & D & + \\ & M & O & R & E & = \\ \hline M & O & N & E & Y & \end{array}$$

is correct. Because S and M are the leading digits, they cannot be equal to the 0 digit.

Can you model this problem as an IP?

Send More Money: ILP model 1

- $x_i \in \{0, \ldots, 9\}$ for all $i \in I = \{S, E, N, D, M, O, R, Y\}$
- $\delta_{ij} \begin{cases} 0 & \text{if } x_i < x_j \\ 1 & \text{if } x_j < x_i \end{cases}$
- Crypto constraint:

$$\begin{array}{cccccc} & 10^3 x_1 & +10^2 x_2 & +10 x_3 & +x_4 & + \\ & 10^3 x_5 & +10^2 x_6 & +10 x_7 & +x_2 & = \\ \hline 10^4 x_5 & +10^3 x_6 & +10^2 x_3 & +10 x_2 & +x_8 & \end{array}$$

- Each letter takes a different digit:

$$\begin{array}{ll} x_i - x_j - 10\delta_{ij} \leq -1, & \text{for all } i, j,\ i < j \\ x_j - x_i + 10\delta_{ij} \leq 9, & \text{for all } i, j,\ i < j \end{array}$$

Send More Money: ILP model 2

- $x_i \in \{0,\dots,9\}$ for all $i \in I = \{S,E,N,D,M,O,R,Y\}$
- $y_{ij} \in \{0,1\}$ for all $i \in I$, $j \in J = \{0,\dots,9\}$
- Crypto constraint:

$$\begin{array}{cccccc} & 10^3x_1 & +10^2x_2 & +10x_3 & +x_4 & + \\ & 10^3x_5 & +10^2x_6 & +10x_7 & +x_2 & = \\ \hline 10^4x_5 & +10^3x_6 & +10^2x_3 & +10x_2 & +x_8 & \end{array}$$

- Each letter takes a different digit:

$$\sum_{j\in J} y_{ij} = 1, \qquad \forall i \in I,$$
$$\sum_{i\in I} y_{ij} \le 1, \qquad \forall j \in J,$$
$$x_i = \sum_{j\in J} j y_{ij}, \qquad \forall i \in I.$$

Send More Money: ILP model

The quality of these formulations depends on both the tightness of the LP relaxations and the number of constraints and variables (compactness)

- Which of the two models is tighter?
  project out all extra variables in the LP so that the polytope for LP is in the space of the x variables. By linear comb. of constraints:

Model 1

$$-1 \leq x_i - x_j \leq 10 - 1$$

Model 2

$$\sum_{j \in J} x_j \geq \frac{|J|\,(|J|-1)}{2}, \qquad \forall J \subset I,$$

$$\sum_{j \in J} x_j \leq \frac{|J|\,(2k-|J|)+1}{2}, \qquad \forall J \subset I.$$

- Can you find the convex hull of this problem?
  Williams and Yan [2001] prove that model 2 is facet defining

Suppose we want to maximize MONEY, how strong is the upper bound obtained with this formulation? How to obtain a stronger upper bound?

Send More Money: ILP model (revisited)

- $x_i \in \{0, \dots, 9\}$ for all $i \in I = \{S, E, N, D, M, O, R, Y\}$
- Crypto constraint:

$$\begin{array}{cccccc} & 10^3 x_1 & +10^2 x_2 & +10 x_3 & +x_4 & + \\ & 10^3 x_5 & +10^2 x_6 & +10 x_7 & +x_2 & = \\ \hline 10^4 x_5 & +10^3 x_6 & +10^2 x_3 & +10 x_2 & +x_8 & \end{array}$$

- Each letter takes a different digit:

$$\sum_{j \in J} x_j \geq \frac{|J|\,(|J|-1)}{2}, \qquad \forall J \subset I,$$

$$\sum_{j \in J} x_j \leq \frac{|J|\,(2k-|J|)+1}{2}, \qquad \forall J \subset I.$$

But exponentially many!

Constraint Programming

The **domain** of a variable x, denoted $D(x)$, is a finite set of elements that can be assigned to x.

A **constraint** C on X is a subset of the Cartesian product of the domains of the variables in X, i.e., $C \subseteq D(x_1) \times \cdots \times D(x_k)$. A tuple $(d_1, \ldots, d_k) \in C$ is called a solution to C.
Equivalently, we say that a solution $(d_1, ..., d_k) \in C$ is an assignment of the value d_i to the variable $x_i, \forall 1 \leq i \leq k$, and that this assignment satisfies C.
If $C = \emptyset$, we say that it is inconsistent.

Extensional: specifies the satisfying tuples
Intensional: specifies the characteristic function

Constraint Programming

Constraint Satisfaction Problem (CSP)

A CSP is a finite set of variables X, together with a finite set of constraints C, each on a subset of X. A **solution** to a CSP is an assignment of a value $d \in D(x)$ to each $x \in X$, such that all constraints are satisfied simultaneously.

Constraint Optimization Problem (COP)

A COP is a CSP P defined on the variables $x_1, \ldots, x_n$, together with an objective function $f : D(x_1) \times \cdots \times D(x_n) \rightarrow Q$ that assigns a value to each assignment of values to the variables. An **optimal solution** to a minimization (maximization) COP is a solution d to P that minimizes (maximizes) the value of $f(d)$.

Global Constraint: `alldifferent`

Global constraint:

set of more elementary constraints that exhibit a special structure when considered together.

`alldifferent` constraint

Let $x_1, x_2, \ldots, x_n$ be variables. Then:

$$\texttt{alldifferent}(x_1, ..., x_n) = \{(d_1, ..., d_n) \mid \forall i, d_i \in D(x_i), \quad \forall i \neq j, \; d_i \neq d_j\}.$$

Note: different notation and names used in the literature

Send More Money
Constraint Programming model

Send + More = Money

- $X_i \in \{0, \ldots, 9\}$ for all $i \in I = \{S, E, N, D, M, O, R, Y\}$
- Crypto constraint:

$$\begin{array}{cccccc} & 10^3 X_1 & +10^2 X_2 & +10 X_3 & +X_4 & + \\ & 10^3 X_5 & +10^2 X_6 & +10 X_7 & +X_2 & = \\ \hline 10^4 X_5 & +10^3 X_6 & +10^2 X_3 & +10 X_2 & +X_8 & \end{array}$$

- Each letter takes a different digit:

$$\texttt{alldifferent}([X_1, X_2, \ldots, X_8]).$$

The convex hull of alldifferent

Convex Hull of of alldifferent

Given a set $I = \{1, \dots, n\}$ (variable indices) and a set $D = \{0, \dots, k\}$ with $k \geq n$, we consider

$$\text{alldifferent}([x_1, \dots, x_n]), \text{ with } 0 \leq x_i \leq k.$$

all the facets of the previous ILP formulation for the alldifferent constraint are

$$\sum_{j \in J} x_j \geq \frac{|J|\,(|J|-1)}{2}, \qquad \forall J \subset I,$$
$$\sum_{j \in J} x_j \leq \frac{|J|\,(2k-|J|)+1}{2}, \qquad \forall J \subset I.$$

[Williams and Yan [2001]]

ILP model + CP propagation

- $x_i \in \{0, \dots, 9\}$ for all $i \in I = \{S, E, N, D, M, O, R, Y\}$
- $y_{ij} \in \{0, 1\}$ for all $i \in I$, $j \in J = \{0, \dots, 9\}$

$$\begin{array}{cccccc}
 & 10^3 x_1 & +10^2 x_2 & +10 x_3 & +x_4 & + \\
 & 10^3 x_5 & +10^2 x_6 & +10 x_7 & +x_2 & = \\
\hline
10^4 x_5 & +10^3 x_6 & +10^2 x_3 & +10 x_2 & +x_8 &
\end{array}$$

- $$\begin{aligned}
\sum_{j \in J} y_{ij} = 1, & \qquad \forall i \in I, \\
\sum_{i \in I} y_{ij} \le 1, & \qquad \forall j \in J, \\
x_i = \sum_{j \in J} j y_{ij}, & \qquad \forall i \in I.
\end{aligned}$$

- Propagation adds valid inequalities:

$$LB(X_i) \le x_i \le UB(X_i) \text{ for all } i \in I$$

.

- H. Simonis' demo, slides 42-56

Send More Money: CP model (revisited)

- $X_i \in \{0,\dots,9\}$ for all $i \in I = \{S,E,N,D,M,O,R,Y\}$

$$\begin{array}{cccccc} & 10^3X_1 & +10^2X_2 & +10X_3 & +X_4 & + \\ & 10^3X_5 & +10^2X_6 & +10X_7 & +X_2 & = \\ \hline 10^4X_5 & +10^3X_6 & +10^2X_3 & +10X_2 & +X_8 & \end{array}$$

- $$\text{alldifferent}([X_1, X_2, \dots, X_8]).$$

- Redundant constraints

$$\begin{aligned} X_4 + X_2 &= 10\,r_1 + X_8, \\ X_3 + X_7 + r_1 &= 10\,r_2 + X_2, \\ X_2 + X_6 + r_2 &= 10\,r_3 + X_3, \\ X_1 + X_5 + r_3 &= 10\,r_4 + X_6, \\ +r_4 &= X_5. \end{aligned}$$

Can we do better? Can we propagate more?

Send More Money: LP relaxation

Comet

```
Solver<LP> lp();
var<LP>{float} y[Letters, Domain](lp, 0..1);
var<LP>{float} x[Letters](lp, Domain);
var<LP>{float} S = x[1];

maximize<lp>
   10000 * M + 1000 * O + 100 * N + 10 * E + Y
subject to {
  lp.post( S >= 1 );
  lp.post( M >= 1 );
  lp.post(             1000 * S + 100 * E + 10 * N + D +
               1000 * M + 100 * O + 10 * R + E ==
   10000 * M + 1000 * O + 100 * N + 10 * E + Y );

  forall (j in Domain)
    lp.post( sum(i in Letters) y[i,j] <= 1);

  forall (i in Letters) {
    lp.post( sum(j in Domain) y[i,j] == 1 );
    lp.post( x[i] == sum(j in Domain) j*y[i,j] );
  }
}
```

Send More Money: CP model
Comet

```
range Letters = 1..8;
range Domain = 0..9;

Solver<CP> cp();
var<CP>{int} r[1..4](cp, 0..1);
var<CP>{int} x[Letters](cp, Domain);
var<CP>{int} S = x[1];  [...]

solve<cp> {
  cp.post( S != 0 );
  cp.post( M != 0 );
  cp.post(            1000 * S + 100 * E + 10 * N + D +
                      1000 * M + 100 * O + 10 * R + E ==
           10000 * M + 1000 * O + 100 * N + 10 * E + Y );

  cp.post( alldifferent(x) );

  cp.post(  S + M + r[3] == O + 10*r[4] );
  cp.post(  E + O + r[2] == N + 10*r[3] );
  cp.post(  N + R + r[1] == E + 10*r[2] );
  cp.post(  D + E        == Y + 10*r[1] );
}
```

Send More Money: CP model

Gecode-python

```
from gecode import *

s = space()
letters = s.intvars(8,0,9)
S,E,N,D,M,O,R,Y = letters
s.rel(M,IRT_NQ,0)
s.rel(S,IRT_NQ,0)
s.distinct(letters)
C = [1000, 100, 10, 1,
     1000, 100, 10, 1,
     -10000, -1000, -100, -10, -1]
X = [S,E,N,D,
     M,O,R,E,
     M,O,N,E,Y]
s.linear(C,X,IRT_EQ,0)
s.branch(letters,INT_VAR_SIZE_MIN,INT_VAL_MIN)
for s2 in s.search():
    print(s2.val(letters))
```

References

Hooker J.N. (2011). **Hybrid modeling**. In *Hybrid Optimization*, edited by P.M. Pardalos, P. van Hentenryck, and M. Milano, vol. 45 of **Optimization and Its Applications**, pp. 11–62. Springer New York.

Williams H. (2010). **The problem with integer programming**. Tech. Rep. LSE0R 10-118, London School of Economics and Political Science.

Williams H. and Yan H. (2001). **Representations of the all_different predicate of constraint satisfaction in integer programming**. *INFORMS JOURNAL ON COMPUTING*, 13(2), pp. 96–103.