### Introductory Mathematical Programming for EC

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The Genetic and Evolutionary Computation Conference, GECCO-2025: Introductory Tutorial

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https://doi.org/10.1145/3712255.3716515



### about the presenter

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#### Previously:

- IBM-Research
- Princeton University: Postdoctoral Research Associate
- PhD in CS: Leiden-U adv.: Th. Bäck & M. Vrakking; BSc in CS&Phys at Hebrew-U









### why are we here?

- Global optimization has been for several decades addressed by algorithms and Mathematical Programming (MP) branded as Operations Research (OR), yet rooted at Theoretical CS [1].
- Also it has been treated by dedicated heuristics ("Soft Computing") where EC resides (!)
- These two branches complement each other, yet practically studied under two independent CS disciplines

#### further motivation

EC scholars become stronger, better-equipped researchers when obtaining knowledge on this so-called "optimization complement"

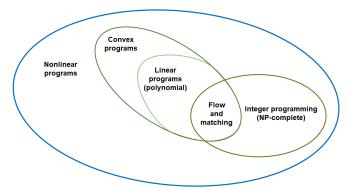
#### Commonly-encountered misbeliefs:

- "if the problem is non-linear, there is no choice but to employ a Randomized Search Heuristic"
- "if it's a combinatorial  $\mathcal{NP}$ -complete problem, EAs are the most reasonable option to approach it"
- "neither Pareto optimization nor uncertainty is/are addressed by OR"
- "OR is the art of giving bad answers to problems, to which, otherwise worse answers are given"

#### outline

- 1 MP fundamentals LP and polyhedra simplex and duality the ellipsoid algorithm discrete optimization
- 2 MP in practice solving an LP basic modeling using OPL QP and the Markowitz model CSP and the N-Queens TSP as an ILP
- 3 extended topic: multiobjective exact optimization
- 4 demo
- 5 discussion





### Mathematical Programming: fundamentals

based on (i) MIT's "Optimization Methods" course material by D. Bertsimas, (ii) "Combinatorial Optimization" by Ch. Papadimitriou & K. Steiglitz, (iii) "The Nature of Computation" by C. Moore and S. Mertens, and (iv) IBM's ILOG/OPL tutorials and documentation.

### the field of operations research

- Developed during WW-II: mathematicians assisted the US-army to solve hard strategical and logistical problems; mainly planning of operations and deployment of military resources. Due to the strong link to military operations, the term Operations Research was coined.
- Post-war: knowledge transfer into industry
- Roots: linear programming (LP), pioneered by George B. Dantzig
- Dantzig worked for the US-government, formulating the generalized LP problem, and devising the Simplex algorithm for tackling it. He also pursued an academic career (Berkeley, Stanford).

### mathematical optimization: $CP \cup MP$

- Partitioning into 2 main approaches: constraints programming (CP) versus mathematical programming (MP). CP is concerned with constraints satisfaction problems (CSPs), which possess no objective functions (sometimes because impossible to model). CP is usually of little interest to us, but it is super important for Formal Verification, where tasks can be modeled as CSPs.
- MP includes the following techniques:
  - 1 linear programming (LP)
  - 2 integer programming (IP)
  - 3 mixed-integer programming (MIP)
  - 4 quadratic programming (QP) and mixed-integer QP (MIQP)
  - 5 nonlinear programming (NLP)

### the canonical optimization problem

The general nonlinear problem formulated in the canonical form [2]:

minimize 
$$\vec{x}$$
  $f(\vec{x})$   $\vec{x} \in \mathbb{R}^d$   
subject to:  $g_1(\vec{x}) \ge 0$   
 $\vdots$   
 $g_m(\vec{x}) \ge 0$   
 $h_1(\vec{x}) = 0$   
 $\vdots$   
 $h_{\ell}(\vec{x}) = 0$ 

# solving the general problem

- Convexity:
  - 1  $f: \mathcal{S} \to \mathbb{R}$
  - 2 The function is convex **iff**  $\forall s_1, s_2 \in \mathcal{S}, \ 0 < \lambda < 1$

$$f(\lambda s_1 + (1 - \lambda) s_2) \le \lambda f(s_1) + (1 - \lambda) f(s_2)$$

- 3 f is concave if -f is convex.
- The problem is called a convex programming problem when i f is convex ii  $g_i$  are all concave
  - iii  $h_j$  are all linear
- Strongest property: local optimality implies global optimality
- Sufficient conditions for optimality exist (Kuhn-Tucker)



# linear programming: standard form

When f and the constraints are all linear, LP is formed by the **standard form** (minimization, equality constraints, non-negative variables) to search over a d-dimensional space,  $\vec{x} \in \mathbb{R}^d$ :

minimize
$$\vec{x}$$
  $\vec{c}^T \vec{x}$  subject to:  $\mathbf{A}\vec{x} = \vec{b}$  (2)

with  $\mathbf{A} \in \mathbb{R}^{m \times d}$  and  $\vec{b} \in \mathbb{R}^m$  describing the constraints.

# polyhedra

• A hyperplane is defined by the set

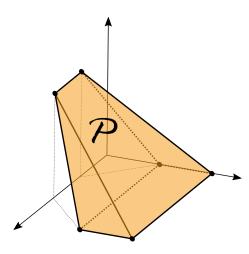
$$\left\{ \vec{x} \in \mathbb{R}^d : \vec{a}^T \vec{x} = b_0 \right\}$$

• A halfspace is defined by the set

$$\left\{ \vec{x} \in \mathbb{R}^d : \vec{a}^T \vec{x} \ge b_0 \right\}$$

- A **polyhedron** is constructed by the intersection of many halfspaces.
- The finite set of candidate solutions is the set of vertices of the convex polyhedron (polytope) defined by the linear constraints!
- Thus, solving any LP reduces to selecting a solution from a finite set of candidates 

  the problem is combinatorial in nature.



# geometry of LP

Given a polytope

$$\mathcal{P} := \left\{ \vec{x} \in \mathbb{R}^d : \mathbf{A}\vec{x} \le \vec{b} \right\}$$

- The point  $\vec{x}$  is a vertex of  $\mathcal{P}$
- $\vec{x} \in \mathcal{P}$  is an extreme point of  $\mathcal{P}$  if

$$\nexists \vec{y}, \vec{z} \in \mathcal{P} \left( \vec{y} \neq \vec{x}, \vec{z} \neq \vec{x} \right) : \quad \vec{x} = \lambda \vec{y} + \left( 1 - \lambda \right) \vec{z}, \ 0 < \lambda < 1$$

- $\vec{x} > \vec{0} \in \mathbb{R}^d$  is a basic feasible solution (BFS) iff  $A\vec{x} = \vec{b}$  and exist indices  $\mathcal{B}_1, \ldots, \mathcal{B}_m$  such that:
  - (i) the columns  $\mathbf{A}_{\mathcal{B}_1}, \dots, \mathbf{A}_{\mathcal{B}_m}$  are linearly independent
  - (ii) if  $j \neq \mathcal{B}_1, \dots, \mathcal{B}_m$  then  $x_j = 0$

# polytopes and LP

#### "Corners" definitions: equivalence theorem

$$\mathcal{P} := \left\{ \vec{x} \in \mathbb{R}^d : \mathbf{A} \vec{x} \leq \vec{b} \right\} ; \, \mathrm{let} \,\, \vec{x} \in \mathcal{P}.$$

 $\vec{x}$  is a vertex  $\iff \vec{x}$  is an extreme point  $\iff \vec{x}$  is a BFS See, e.g., [3] for the proof.

#### Conceptual LP search:

- begin at any "corner"
- while "corner" is not optimal hop to its neighbouring "corner" as long as it improves the objective function value

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### the basic simplex

```
1 t \leftarrow 0; opt, unbounded \leftarrow false, false
 2 \vec{x}_t \leftarrow \text{constructBFS}(), \quad \mathbf{B} \leftarrow [\mathbf{A}_{\mathcal{B}_1}, \dots, \mathbf{A}_{\mathcal{B}_m}]
 3 while !opt && !unbounded do
          if \bar{c}_i := c_i - \bar{c}_R^T \mathbf{B}^{-1} \mathbf{A}_i > 0 \ \forall i \text{ then } opt \leftarrow \text{true}
          else
 5
                select any j such that \bar{c}_i < 0
 6
                if \vec{u} := \mathbf{B}^{-1} \mathbf{A}_i \leq \vec{0} then unbounded \leftarrow \mathsf{true}
 7
                else
 8
                      \vec{x}_{t+1} \leftarrow \text{pivot on } \vec{x}_t \text{ /* see [4] for details */}
 9
                      set new basis A_i /* see [4] for details */
10
                     t \leftarrow t + 1
11
                end
12
          end
13
14 end
    output: \vec{x}_t
```

# duality

i. Every LP has an associated problem known as its **dual**; min turns into max, each constraint in the primal has an associated dual variable:

$$\begin{aligned} & \text{minimize}_{\vec{x}} \quad \vec{c}^T \vec{x} \quad \vec{x} \in \mathbb{R}^d \\ & \text{subject to: } \mathbf{A} \vec{x} = \vec{b} \\ & \quad \vec{x} \ge 0 \end{aligned}$$

maximize
$$\vec{p}$$
  $\vec{p}^T \vec{b}$   $\vec{p} \in \mathbb{R}^m$  subject to:  $\vec{p}^T \mathbf{A} \leq \vec{c}^T$ 

$$\begin{aligned} & \text{minimize}_{\vec{x}} \quad \vec{c}^T \vec{x} \quad \vec{x} \in \mathbb{R}^d \\ & \text{subject to: } \mathbf{A} \vec{x} \geq \vec{b} \end{aligned}$$

$$\begin{aligned} & \text{maximize}_{\vec{p}} \quad \vec{p}^T \vec{b} \quad \vec{p} \in \mathbb{R}^m \\ & \text{subject to: } \vec{p}^T \mathbf{A} = \vec{c}^T \\ & \vec{p} \geq 0 \end{aligned}$$

ii. The dual of the dual is the primal.

# • Weak duality theorem

If  $\vec{x} \in \mathbb{R}^d$  is primal feasible and  $\vec{p} \in \mathbb{R}^m$  is dual feasible then

$$\vec{p}^T \vec{b} \le \vec{c}^T \vec{x}$$

• Corollary: If  $\vec{x}$  is primal feasible,  $\vec{p}$  is dual feasible, and  $\vec{p}^T \vec{b} = \vec{c}^T \vec{x}$ , then  $\vec{x}$  is optimal in the primal and  $\vec{p}$  is optimal in the dual.

#### • Strong duality theorem

Given an LP, if it has an optimal solution – then so does its dual – having equal objective functions' values.

 $\Rightarrow$  The dual provides a bound that in the best case equals the optimal solution to the primal – and thus can help solve difficult primal problems.

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### dual simplex

- Simplex is a primal algorithm: maintaining primal feasibility while working on dual feasibility
- Dual-simplex: maintaining dual feasibility while working on primal feasibility –
  - Implicitly use the dual to obtain an optimal solution to the primal as early as possible, regardless of feasibility; then hop from one vertex to another, while gradually decreasing the infeasibility while maintaining optimality
- Dual-simplex is the first practical choice for most LPs.

R. Vanderbei, Linear Programming: Foundations and Extensions. Springer,  $5^{th}$  ed., 2020, ISBN: 978-3-030-39414-1.

# simplex: convergence

- Dantzig's simplex finds an optimal solution to any LP in a finite number of steps (avoiding cycles is easy, but excluded here).
- Over half-century of improvements, its robust forms are very effective in treating very large LPs.
- However, simplex is not a polynomial-time algorithm, even if it is fast in practice over the majority of cases.
- Pathological LP-cases exist (e.g., the Klee-Minty cube [5]) where an **exponential number of steps** is needed for convergence.
- An ellipsoid algorithm [5], devised by Soviet mathematicians in the late 1970's, is guaranteed to solve every LP in a polynomial number of steps.

# "high-level" ellipsoid [Shor-Nemirovsky-Yudin]

### **input**: a bounded convex set $\mathcal{P} \in \mathbb{R}^d$

- 1  $t \leftarrow 0$
- 2  $\mathcal{E}_t \leftarrow \text{ellipsoid containing } \mathcal{P}$
- 3 while center  $\vec{\xi_t}$  of  $\mathcal{E}_t$  is not in  $\mathcal{P}$  do
- let  $\vec{c}^T \vec{x} \leq \vec{c}^T \vec{\xi_t}$  be such that  $\left\{ \vec{x} : \vec{c}^T \vec{x} \leq \vec{c}^T \vec{\xi_t} \right\} \supseteq \mathcal{P}$
- 5 update to the ellipsoid with minimal volume containing the intersected subspace:

$$\mathcal{E}_{t+1} \leftarrow \mathcal{E}_t \cap \left\{ \vec{x} : \vec{c}^T \vec{x} \le \vec{c}^T \vec{\xi_t} \right\}$$

6 
$$t \leftarrow t+1$$

7 end

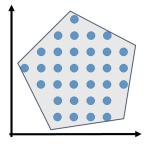
output: center  $\vec{\xi}_t \in \mathcal{P}$ 

### ellipsoid aftermath

bounded convex set

• Polynomial-time algorithm for obtaining  $\vec{x}^*$  within any given

- Khachian first used it (1979) to show polynomial solvability of LPs
- **Theorem**: if there exists a polynomial-time algorithm for solving a strict linear inequalities problem, then there exists a polynomial-time algorithm for solving LPs (see [3] for the proof).
- Conceptual novelty: disregarding the combinatorial nature of LPs
- In practice, unlike simplex, the ellipsoid is slow yet steady.
- However, its theoretical "polynomiality" has strong implications also for discrete optimization.



discrete optimization

# Integer Programming

Integer Programming (IP) involves optimization problems with discrete decision variables and is central to both practical computation and the theoretical foundations of Computer Science.

- The decision version of IP is  $\mathcal{NP}$ -hard.
- For decades, the fastest exact algorithm was due to Kannan, with a running time of: poly(d)  $2^{\mathcal{O}(d)}$  for an instance with d variables.
- A recent breakthrough by Rothvoss & Reis tightened this bound [6] by providing a randomized algorithm that solves any IP in:

$$(\log(2d))^{\mathcal{O}(d)}$$
 steps.

• Nevertheless, heuristics remain the primary problem-solvers.

- The introduction of integer decision variables into a linear optimization problem yields a so-called (mixed)-integer linear program ((M)ILP) [7].
- A powerful modeling framework with much flexibility in describing discrete optimization problems.
- The general ILP is itself  $\mathcal{NP}$ -complete and yet, there are subsets of "very easy" versus "very hard" problems.
- p2p shortest path over a graph with d nodes has an algorithm with  $\mathcal{O}(d^2)$  complexity, versus the traveling salesman problem...
- Unlike "pure-LP", whose complexity is dictated by d+m(variables+constraints), the choice of formulation in ILP is critical!
- Direction what if the **constraints matrix** is **unimodular** [8] ?

### integer linear optimization

• Pure integer:

maximize
$$\vec{x}$$
  $\vec{c}^T \vec{x}$  subject to:  $\mathbf{A} \vec{x} \leq \vec{b}$   $\vec{x} \in \mathbb{Z}_+^d$  (3)

• Binary optimization (**important special case**):

The above pure integer model with  $\vec{x} \in \{0, 1\}^d$ 

Mixed-integer:

maximize<sub>$$\vec{x}$$</sub>  $\vec{c}^T \vec{x} + \vec{h}^T \vec{y}$   
subject to:  $\mathbf{A}\vec{x} + \mathbf{B}\vec{y} \le \vec{b}$   
 $\vec{x} \in \mathbb{Z}_+^d, \ \vec{y} \in \mathbb{R}_+^\ell$  (4)

#### LP relaxations and the convex hull

• Given a discrete optimization problem, its consideration as a "pure" (continuous) LP is called its **LP relaxation**; e.g., each binary variable becomes continuous within the interval [0, 1]:

$$x_i \in \{0, 1\} \quad \leadsto \quad 0 \le x_i \le 1$$

- Formally, given a valid ILP formulation  $\left\{\vec{x} \in \mathbb{Z}_+^d \mid \mathbf{A}\vec{x} \leq \vec{b}\right\}$ , the polytope  $\left\{\vec{x} \in \mathbb{R}^d \mid \mathbf{A}\vec{x} \leq \vec{b}\right\}$  constitutes its LP relaxation.
- The **convex hull** of a set of points is defined as the "smallest polytope" that contains all of the points in the set; given a finite set  $S := \{p^{(1)}, \dots, p^{(N)}\}$ , it is defined as

$$C(S) := \left\{ q \middle| q = \sum_{k=1}^{N} \lambda_k p^{(k)}, \sum_{k=1}^{N} \lambda_k = 1, \ \lambda_k \ge 0, \ p^{(k)} \in S \right\}$$
 (5)

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### quality of formulations

• The **integral hull** is the convex hull of the set of integer solutions:

$$\widetilde{\mathcal{P}} := \mathcal{C}(X), \quad X \subset \mathbb{Z}^d \text{ solution points}$$

- The quality of an ILP formulation for a problem having a feasible solution set X, is governed by the **closeness** of the feasible set of its LP relaxation to C(X).
- Given an ILP with two formulations,  $\{P_1, P_2\}$ , you may formally determine, e.g., that  $P_1$  is as strong as  $P_2$ , in terms of the feasible sets of their LP relaxations.
- Explicit knowledge of  $\mathcal{C}(X)$  is thus very valuable!

# "Easy Polyhedra"

- If the integral hull is attainable as  $\widetilde{\mathcal{P}} = \left\{ \vec{x} \in \mathbb{R}^d \mid \widetilde{\mathbf{A}} \vec{x} \leq \widetilde{\vec{b}} \right\}$ , the problem is polynomially solvable (all vertices are integers!) [7]
- Another perspective: an LP relaxation of an ILP with a totally unimodular constraint matrix has only integer solutions! [8]
- MILPs with fully-understood integral hulls assignment, min-cost flow, matching, spanning tree, et cetera.

#### branch-and-bound

One of the common approaches to address integer programming, relying on the ability to bound a given problem.

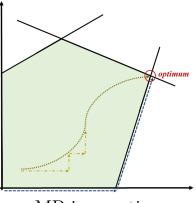
It is a tree-search, adhering to the principle of divide-and-conquer:

- (i) **branch**: select an active subproblem  $\hat{\mathcal{F}}$
- (ii) **prune**: if  $\hat{\mathcal{F}}$  is infeasible discard it
- (iii) **bound**: otherwise, compute its lower bound  $L(\hat{\mathcal{F}})$
- (iv) **prune**: if  $L(\hat{\mathcal{F}}) \geq U$ , the current best upper bound, discard  $\hat{\mathcal{F}}$
- (v) **partition**: if  $L(\hat{\mathcal{F}}) < U$ , either completely solve  $\hat{\mathcal{F}}$ , or further break it to subproblems added to the list of active problems

# "high-level" LP-based branch-and-bound

**input**: a linear integer program  $\mathcal{F}$ 

```
1 \Omega \leftarrow \{\mathcal{F}\}; \ U \leftarrow \infty /* active problems' set; global upper bound */
 2 while \Omega is not empty do
           let \hat{\mathcal{F}} be a active subproblem, \hat{\mathcal{F}} \in \Omega; \Omega \leftarrow \Omega \setminus \left\{ \hat{\mathcal{F}} \right\}
 3
           compute its lower bound L(\hat{\mathcal{F}}) by solving its LP relaxation
 4
           if L(\hat{\mathcal{F}}) < U then
 5
                 U \leftarrow L(\hat{\mathcal{F}})
 6
                 if exists heuristic solution \vec{\psi} for \hat{\mathcal{F}} then \vec{x}^* \leftarrow \vec{\psi}
 7
                 else given the LP relaxation's optimizer, \vec{\xi}, if it contains a
 8
                   fractional decision variable \xi_i, construct 2 subproblems
                   \{\dot{\mathcal{F}}, \ddot{\mathcal{F}}\} by imposing either one of the new constraints
                   x_i \leq \lfloor \xi_i \rfloor or x_i \geq \lceil \xi_i \rceil — and add them \Omega \leftarrow \Omega \cup \{\dot{\mathcal{F}}, \ddot{\mathcal{F}}\}\
                 /* selection rules needed if #fractional \xi_i > 2*/
 9
           end
10
11 end
    output: \vec{x}^*
```



MP in practice

### obtaining an LP standard form

• LP's **standard form** (minimization, equality constraints, non-negative variables):

$$\begin{aligned} & \text{minimize}_{\vec{x}} \ \vec{c}^T \vec{x} \\ & \text{subject to: } \mathbf{A} \vec{x} = \vec{b} \\ & \vec{x} \geq 0 \end{aligned}$$

• Applicable transformations to obtain standard form (introducing slack/surplus variables and accounting for unrestricted variables):

(a) 
$$\max \vec{c}^T \vec{x}$$
  $\Leftrightarrow$   $-\min \left(-\vec{c}^T \vec{x}\right)$ 

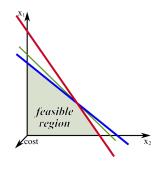
(b) 
$$\vec{a}_i^T \vec{x} \le b_i$$
  $\Leftrightarrow$   $\vec{a}_i^T \vec{x} + s_i = b_i, \ s_i \ge 0$ 

(c) 
$$\vec{a}_i^T \vec{x} \ge b_i$$
  $\Leftrightarrow$   $\vec{a}_i^T \vec{x} - s_i = b_i, \ s_i \ge 0$ 

(a) 
$$\max \vec{c}^T \vec{x}$$
  $\Leftrightarrow -\min \left( -\vec{c}^T \vec{x} \right)$   
(b)  $\vec{a}_i^T \vec{x} \le b_i$   $\Leftrightarrow \vec{a}_i^T \vec{x} + s_i = b_i, \ s_i \ge 0$   
(c)  $\vec{a}_i^T \vec{x} \ge b_i$   $\Leftrightarrow \vec{a}_i^T \vec{x} - s_i = b_i, \ s_i \ge 0$   
(d)  $-\infty < x_j < \infty$   $\Leftrightarrow x_j := x_j^+ - x_j^-, \ x_j^+ \ge 0, \ x_j^- \ge 0$ 

### linear programming: solutions

minimize 
$$-x_1 - x_2$$
  
subject to:  $x_1 + 2x_2 \le 3$   
 $2x_1 + x_2 \le 3$   
 $x_1, x_2 \ge 0$ 



```
dvar float+ x1,x2,s1,s2;
minimize
    -x1 - x2;
subject to {
    x1 + 2x2 + s1 == 3;
    2x1 + x2 + s2 == 3;
}
```

# the fractional (continuous) knapsack problem

n items to be picked in a fractional way,  $i = 1, \ldots, n$ :

- $v_i$ : value of each item
- $w_i$ : weight of each item

Target: **maximize the total value** within a knapsack of capacity C.

[FKP] maximize 
$$\sum_{i=1}^{n} v_i \cdot x_i$$
  
subject to:  
$$\sum_{i=1}^{n} x_i \leq C$$
$$w_i \geq x_i \in \mathbb{R} \quad \forall i \in 1 \dots n$$
 (6)

# basic f-knapsack in OPL

```
// Data reading from external database (or sheet or flat file)
\{int\}\ N = \ldots;
{float} CAPACITY = ...;
{float[N]} Values = ...;
{float[N]} Weights = ...;
dvar float+ select ind[N] in 0..CAPACITY ;
maximize
   sum (n in N) (select ind[n] * Values[n]);
subject to {
     forall (n in N) select ind[n] <= Weights[n] ;</pre>
```

# integer knapsack in OPL

```
// Data reading from external database
\{int\}\ N = \ldots;
{int} CAPACITY = ...;
{int[N]} Values = ...;
{int[N]} Weights = ...;
dvar int select ind[N] in 0..1;
maximize
   sum (n in N) (select ind[n] * Values[n]);
subject to {
     sum (n in N) select ind[n]*Weights[n] <= CAPACITY;</pre>
```

#### solver operations

• Modern solvers allow the user to choose/tune their core algorithms:

```
cplex.startalg = 1; //primal simplex; for LP relaxation
cplex.lpmethod = 2; //dual simplex
cplex.epgap = 0.001; //relative MIP optimality gap
cplex.IntSolLim = 100; //number of integer solutions to stop
cplex.polishtime = 1800; //polishing time; see text below
cplex.tilim = 1800; //computation time limit
```

• Some MILP solvers actually employ *evolutionary operators* in their heuristic components, such as CPLEX's polish subroutine [9].

## quadratic programming (QP)

• The simplest formulation of a QP has a *quadratic* objective function and *linear* constraints:

minimize<sub>$$\vec{x}$$</sub>  $\frac{1}{2}\vec{x}^T\mathbf{Q}\vec{x} + \vec{c}^T\vec{x}$   
subject to:  $\mathbf{A}\vec{x} \leq \vec{b}$   $\vec{\ell} \leq \vec{x} \leq \vec{u}$  (7)

• Renowned QP: the Markowitz portfolio – minimizing risk while ensuring minimal ROI, subject to a bounded portfolio investment:

 $\mathbf{Q}$ : portfolio's covariance matrix, representing RISK  $\vec{c} = \vec{0}$   $\vec{\rho}$ : stochastic return, representing ROI (8) constraints:  $\vec{\rho}^T \vec{x} \geq \mathrm{ROI}_{min}$ 

$$\sum_{i} x_{i} = \text{INVEST}_{total}$$

# Markowitz: OPL implementation

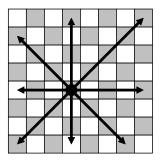
```
{string} Investments = ...;
float Return[Investments] = ...;
float Covariance[Investments] [Investments] = ...;
float BUDGET = ...;
float alpha = ...;
range float FloatRange = 0..BUDGET;
dvar float Allocation[Investments] in FloatRange;
maximize (sum(i in Investments) Return[i]*Allocation[i])
   - alpha*(sum(i, j in Investments)
       Covariance[i][j]*Allocation[i]*Allocation[j]);
subject to {
  // SPEND-IT-ALL: sum of allocations equals the given budget
  allocate: (sum (i in Investments) (Allocation[i])) == BUDGET;
```

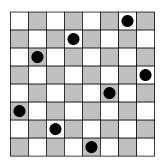
# QCP, (M)IQP/(M)IQCP and QUBO

- A Quadratically-Constrained Program (QCP) has quadratic terms in its constraints (possibly no quadratic terms in the objective)
- (Mixed-)Integer QP and QCP involve integer decision variables (partially or entirely)
- Renowned MIQP: the quadratic assignment problem (QAP)
- QUBO: Quadratic Unconstrained Binary Optimization special case of IQP with only binary variables and without constraints.
- Highly relevant to the emerging Quantum Optimization field due to the inherent link to the Ising model.
- Intrigued? Visit the Quantum Optimization Tutorial and Workshop @gecco2025!

#### CSP: the N-queens problem

The N-queens problem (NQP) [10] is defined as the task to place N queens on an  $N \times N$  chessboard in such a way that they cannot attack each other.





## N-queens as maximization

maximize 
$$\sum_{i,j} x_{ij}$$
  
subject to:  

$$\sum_{i} x_{ij} \leq 1 \quad \forall j \in \{1..., N\}$$

$$\sum_{i} x_{ij} \leq 1 \quad \forall i \in \{1..., N\}$$

$$\sum_{j-i=k} x_{ij} \leq 1 \quad \forall k \in \{-N+2, -N+3, ..., N-3, N-2\}$$

$$\sum_{i+j=\ell} x_{ij} \leq 1 \quad \forall \ell \in \{3, 4, ..., 2N-3, 2N-1\}$$

$$x_{ij} \in \{0, 1\} \quad \forall i, j \in \{1, ..., N\}$$

# N-queens: OPL implementation [CSP]

```
int N = \dots;
range R = 1..N;
dvar boolean queen [R][R];
// NO OBJECTIVE FUNCTION !
subject to {
  forall (s in R) {
     sum (t in R) queen[s][t] == 1;
    sum (t in R) queen[t][s] == 1;
  }
  forall (k in (-N+2)..(N-2)) {
     sum(s1 in R, t1 in R: t1-s1==k) queen[s1][t1] <= 1;</pre>
  forall (k in 3..(2*N-1)) {
     sum(s1 in R, t1 in R: s1+t1==k) queen[s1][t1] <= 1;</pre>
```

## the traveling salesman problem

• The archetypical Traveling Salesman Problem (TSP) is posed as finding a Hamilton cycle of minimal total cost. Explicitly, given a directed graph G, with a vertex set  $V = \{1, \ldots, d\}$  and an edge set  $E = \{\langle i, j \rangle\}$ , each edge has cost information  $c_{ij} \in \mathbb{R}^+$ .

#### • Black-box formulation: cyclic permutations

[TSP-perm] minimize 
$$\sum_{i=0}^{d-1} c_{\pi(i),\pi((i+1)_{\text{mod}d})}$$
subject to:  

$$\pi \in P_{\pi}^{(d)}$$
(9)

• But this is clearly not an MP, since it does not adhere to the canonical form!

## ILP formulation [Miller-Tucker-Zemlin]

TSP as an ILP utilizes  $d^2$  binary decision variables  $\mathbf{x}_{ij}$ :

[TSP-ILP] minimize 
$$\sum_{\langle i,j\rangle \in E} c_{ij} \cdot \mathbf{x}_{ij}$$
subject to:
$$\sum_{j \in V} \mathbf{x}_{ij} = 1 \quad \forall i \in V$$
$$\sum_{i \in V} \mathbf{x}_{ij} = 1 \quad \forall j \in V$$
$$\mathbf{x}_{ij} \in \{0,1\} \quad \forall i,j \in V$$

But is this enough? What about inner-circles?

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d integers  $u_i$  are needed as decision variables to prevent inner-circles:

## the EC perspective

- Unlike GAs, which require dedicated mutation and crossover operators for cyclic permutations, the challenge here is mostly about obtaining an effective formulation
- Perhaps counter-intuitively, increasing the order of magnitude of constraints does not necessarily render the problem harder to be solved as MP.
- The given MTZ formulation for TSP is itself of a polynomial size; an alternative formulation possesses  $\mathcal{O}\left(2^{d}\right)$  subtour elimination constraints, though impractical for large graphs.
- In any case, TSP's integral hull is unknown; an  $\mathcal{NP}$ -hard problem.
- Note that EC researchers have started looking at TSP and other problems in a gray-box perspective: Darrell Whitley's tutorial on "Graybox Optimization and Next Generation Genetic Algorithms".

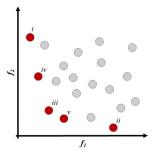
#### TSP on undirected graphs: OPL implementation

Addressing the undirected TSP by means of "node labeling" – assuming a single visit per node:

```
// Data preparation
tuple Raw_Edge {int point1; int point2; int dist; int active;}
{Raw_Edge} raw_edges = ...;
//Every edge is taken in both directions due to the graph
   nature, using 'union':
tuple Edge {int point1; int point2; int dist;}
{Edge} edges = {<e.point1, e.point2, e.dist> | e in raw edges :
   e.active == 1
     union {<e.point2, e.point1, e.dist> | e in raw edges :
         e.active == 1}:
{int} points = {e.point1 | e in edges};
int d = card (points); //set cardinality, i.e., number of cities
```

#### TSP in OPL continued: core model

```
dvar int edge_selector[edges] in 0..1;
dvar int label[points] in 0..d-1;
minimize sum (e in edges) edge_selector[e]*e.dist;
subject to {
 forall (p in points)
  ct in deg equal one:
   sum (e in edges : e.point2 == p) edge_selector[e] == 1;
 forall (p in points)
  ct out deg equal one:
   sum (e in edges : e.point1 == p)edge selector[e] == 1;
  forall (e in edges : e.point2 != 1)
  ct monotone labeling:
   edge_selector [e] == 1 => label [e.point1] ==
       label[e.point2]-1;
}
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                        Introductory MathProg for EC
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```



extended topic: multiobjective optimization

#### multiobjective exact optimization

Diversity Maximization Approach (DMA) [11] key features:

- Iterative-exact nature: obtains a new **exact non-dominated** solution per each iteration
- Criteria exist for the attainment of the complete Pareto frontier
- Fine distribution of the existing set already found is guaranteed
- Optimality gap is provided what may be gained by continuing constructing the Pareto frontier
- Solves any type of frontier (even if seems as a weighted sum)
- Importantly, DMA is MILP if the original problem is MILP

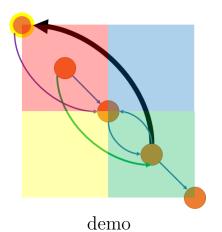
M. Masin and Y. Bukchin, 2008, "Diversity Maximization Approach for Multi-Objective Optimization", *Operations Research*, 56, 411-424.

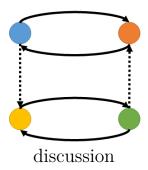
# "high-level" DMA for M-objectives linear problems

#### **input**: a linear program featuring M objectives

- 1 Find an optimal solution for a weighted sum of multiple objectives with any reasonable strictly positive weights. If there is no feasible solution – Stop.
- 2 Set the partial efficient frontier equal to the found optimal solution. Choose optimality gap tolerance and maximal number of iterations.
- 3 If the maximal number of iterations is reached **Stop**, otherwise add M binary variables and (M+1) linear constraints to the previous MILP model.
- 4 Maximize the proposed diversity measure. If the diversity measure is less than the optimality gap tolerance **Stop**, otherwise add the optimal solution to the partial efficient frontier and go to Step 3.

output: Pareto set, Pareto frontier





#### quick summary

- MP is a well-established domain encompassing a variety of algorithms with underlying rigorous theory.
- Broad knowledge of MP is valuable for both EC theoreticians and practitioners
- Given convex problems, MP is most likely the fittest tool
- Given discrete optimization problems that may be formulated as MILP/MIQP – it makes sense to first try MP-solvers
- MP is inherently adjusted to constrained problems (unlike EC...)
- Effective MP formulation lies in the heart of practical problem-solving
- Robustness to uncertainty, Pareto optimization, and hybridization are solid extensions to classical MP

O.M. Shir and M. Emmerich, "Multi-Objective Mixed-Integer Quadratic Models: A Study on Mathematical Programming and Evolutionary Computation". IEEE TEC **29**(3) (2025) 661–675 doi

#### communities and resources

- INFORMS: The Institute for Operations Research and the Management Sciences; https://www.informs.org/
- COIN-OR: Computational Infrastructure for Operations Research

   a project that aims to "create for mathematical software what
   the open literature is for mathematical theory";
   https://www.coin-or.org/

• MATHEURISTICS: model-based metaheuristics, exploiting MP in a metaheuristic framework; http://mh2018.sciencesconf.org/

#### partial list of languages and solvers

- Modeling languages:
  - 1 GAMS
  - 2 AMPL
  - 3 OPL
  - 4 (python (Gurobi-Python, SciPy), MATLAB, ...)
- Environments and modeling systems:
  - 1 OR-Tools Google Developers (open source!)
  - 2 IBM ILOG CPLEX (academia-free)
  - 3 Gurobi
  - 4 sas
  - 5 YALMIP
- Third-party solvers (free and open-source):
  - 1 CBC (via Coin-OR)
  - 2 GLPK (GNU Linear Programming Kit)
  - 3 SoPlex
  - 4 LP\_SOLVE



## benchmarking and competitions

 MIPLIB: the Mixed Integer Programming LIBrary http://miplib.zib.de/

 CSPLib: a problem library for constraints http://csplib.org/

- SAT-LIB: the Satisfiability Library Benchmark Problems http://www.cs.ubc.ca/~hoos/SATLIB/benchm.html
- TSP-LIB: the Traveling Salesman Problem sample instances http://comopt.ifi.uni-heidelberg.de/software/TSPLIB95/

Acknowledgements go to

Dr. Yossi Shiloach (IBM-Research retired)

Dr. Michael Masin (former IBM-Research)

## gracias

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