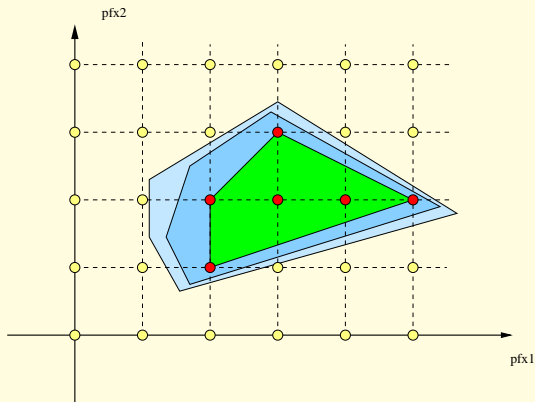


(2/5/2024)

Recap: Formulating IPs



There are different ways to formulate the same integer program:

$$P^1 \supsetneq P^2 \supsetneq P^3 \quad \text{where as} \quad K^1 = K^2 = K^3$$

where $K^i = P^i \cap \mathbb{Z}^n$ for $i = 1, 2, 3$

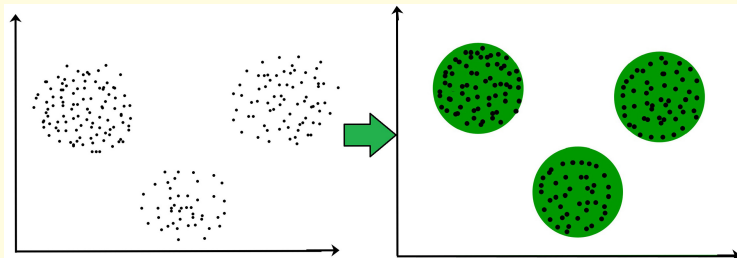
Recap: Clustering problem

Given: An integer $k > 1$ and a collection of points $X = \{x^1, x^2, \dots\}$ together with distances between pairs of these points.

Goal: Partition X into k clusters C_1, \dots, C_k , such that minimum distance between pairs of points in different clusters:

$$\min_{i \in C_p, j \in C_q, p \neq q} d(i, j)$$

is **maximized**. ($d(i, j)$ measures the distance between points i and j)



Lloyd's algorithm: K-Means clustering

Clustering problem: Partition X into clusters C_1, \dots, C_k so as to maximize minimum distance between clusters :

$$d^* = \max_{C_1, \dots, C_k \text{ is a partition}} \left(\min_{i \in C_p, j \in C_q, p \neq q} d(i, j) \right)$$

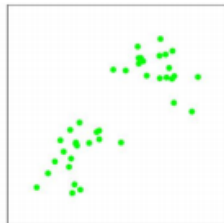
- K-Means is the most popular clustering algorithm (it is a **heuristic**).
 1. Randomly pick k seed points (one for each cluster).
 2. Assign points to the closest seed to form the clusters.
 3. Change the seed points to a "central" point in each cluster
 4. Repeat until clusters do not change much.
 5. Return the best solution found during the search
- Easy to understand and implement.
- It is a good heuristic for the clustering problem (practical performance).

K-Means example

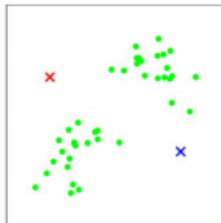
Data points

Initial seeds

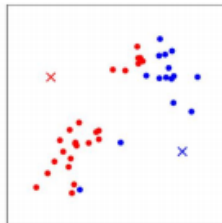
A clustering



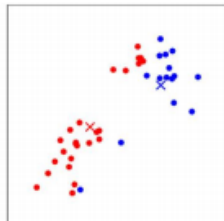
(a)



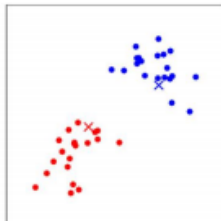
(b)



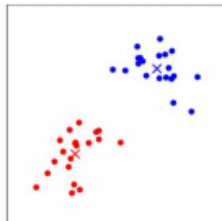
(c)



(d)



(e)



(f)

Clustering when $d(i, j) \in \{0, 1\}$

(points are either similar or dissimilar)

Clustering Problem

Consider the following clustering problem:

- There are n objects $N = \{1, \dots, n\}$.
 - Any pair of objects $i, j \in N$ is either similar or dissimilar
[$d(i, j)$ is either 0 (if similar) or 1 (if dissimilar)]
 - We are given a set D that contains pairs of dissimilar objects (the other pairs are similar)
 - We want to cluster the objects in exactly k clusters so that each cluster C_1, \dots, C_k consists of items that are mostly similar to each other. $K = \{1, \dots, k\}$
 - In addition, each cluster must contain at least ℓ objects.
-
- Model this as an IP where the objective is to minimize the total number of pairs of dissimilar objects put in the same cluster.

Clustering problem

Input:

- n objects numbered $1, 2, \dots, n$
- Desired number of clusters k , and a lower bound ℓ on the number of objects in a cluster
- A set D of pairs of dissimilar objects
(i.e. $\{i, j\} \in D$ means that objects i and j are dissimilar)

Output:

- A partitioning of the objects into cluster C_1, C_2, \dots, C_k

Partitioning means:

- (i) $C_1 \cup C_2 \cup \dots \cup C_k = \{1, 2, \dots, n\}$, and
- (ii) $C_s \cap C_t = \emptyset$ for all $s \neq t$.

Goal:

- Minimize the total number of pairs $\{i, j\}$ where i and j are clustered in the same cluster, but are dissimilar (meaning, $\{i, j\} \in D$)

Clustering Problem

Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{ijs} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if both objects } i \text{ and } j \text{ are put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases} \quad (\text{only for } i < j)$$

IP Formulation:

$$\min \quad \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \quad \longleftarrow \quad \text{dissimilar pairs in the same cluster}$$

$$\text{s.t.} \quad \sum_{s \in K} y_{is} = 1 \quad \forall i \in N \quad \longleftarrow \quad \text{objects}$$

$$\sum_{i \in N} y_{is} \geq \ell \quad \forall s \in K \quad \longleftarrow \quad \text{clusters}$$

$$x_{ijs} \in \{0, 1\} \quad \forall i < j \in N, \forall s \in K$$

$$y_{is} \in \{0, 1\} \quad \forall i \in N, \forall s \in K$$

Clustering Problem

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$$\text{How do we say: } x_{ijs} = \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{ijs} \in \{0, 1\} \quad \forall i < j \in N, \forall s \in K$$

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- How do we say:

$$x_{ijs} = \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

using the fact that x and y take $\{0, 1\}$ values?

- First idea: We can write

$$x_{ijs} \geq y_{is} + y_{js} - 1$$

and

$$x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js})$$

- When both $y_{is} = 1$ and $y_{js} = 1$ the we have

$$x_{ijs} \geq 1 + 1 - 1 = 1 \quad \text{and} \quad x_{ijs} \leq \frac{1}{2}(1 + 1) = 1 \implies x_{ijs} = 1$$

- If not, then we must have $y_{is} + y_{js} \leq 1$ and

$$\underbrace{x_{ijs} \geq y_{is} + y_{js} - 1}_{x_{ijs} \geq 0} \quad \text{and} \quad \underbrace{x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js})}_{x_{ijs} \leq 1/2} \implies x_{ijs} = 0$$

- It works! (because $x_{ijs} \in \{0, 1\}$)

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- It works! (because $x_{ijs} \in \{0, 1\}$)

Clustering Problem: Formulation 0

Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{ijs} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if both objects } i \text{ and } j \text{ are put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases} \quad (\text{only for } i < j)$$

IP Formulation:

$$\min \quad \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs}$$

$$\text{s.t.} \quad \sum_{s \in K} y_{is} = 1 \quad \forall i \in N \quad \longleftarrow \quad \text{objects}$$

$$\sum_{i \in N} y_{is} \geq \ell \quad \forall s \in K \quad \longleftarrow \quad \text{clusters}$$

$$x_{ijs} \geq y_{is} + y_{js} - 1 \quad \forall i < j \in N, s \in K$$

$$x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js}) \quad \forall i < j \in N, s \in K$$

$$x_{ijs} \in \{0, 1\} \quad \forall i < j \in N, \forall s \in K$$

$$y_{is} \in \{0, 1\} \quad \forall i \in N, \forall s \in K$$

- We want to say:

$$x_{ijs} = \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

using the fact that x and y take $\{0, 1\}$ values?

- This is same as

$$x_{ijs} = y_{is}y_{js}$$

- But we cannot write this in a **linear** integer program.
- So instead we wrote 2 linear inequalities

$$x_{ijs} \geq y_{is} + y_{js} - 1$$

and

$$x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js})$$

- **Question:** Can we do better?

Taking a step back: Multiplying binary variables

- Let $y_1 \in \{0, 1\}$ and $y_2 \in \{0, 1\}$ be two binary variables.
- Assume we are interested in their product $y_1 \cdot y_2$.
- How can we express their product $x = y_1 y_2$ using linear inequalities?

$$x = \begin{cases} 1 & \text{if } y_1 = 1 \text{ and } y_2 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

- Consider the following inequalities:

$$x \leq y_1$$

$$x \leq y_2$$

$$x \geq 0$$

$$x \geq y_1 + y_2 - 1$$

Claim

If $y_1, y_2 \in \{0, 1\}$ and x satisfies the constraints above, then

$$x = y_1 y_2$$

Claim

If x, y_1, y_2 satisfy the McCormick constraints

$$x \leq y_1,$$

$$x \leq y_2,$$

$$x \geq y_1 + y_2 - 1,$$

$$x \geq 0,$$

and

$$y_1, y_2 \in \{0, 1\}$$

then $x = y_1 y_2$.

Proof :

y_1	y_2	constraints		x
0	0	$x \leq y_1,$	$x \geq 0$	0
0	1	$x \leq y_1,$	$x \geq 0$	0
1	0	$x \leq y_2,$	$x \geq 0$	0
1	1	$x \geq y_1 + y_2 - 1,$	$x \leq y_1$	1

Back to Formulation 0 for the Clustering Problem

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \quad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

(Notice that we want x_{ijs} variable to be equal to $y_{is} \cdot y_{js}$)

IP Formulation:

$$\begin{aligned} \min \quad & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ \text{s.t.} \quad & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow \text{clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N, s \in K \\ & x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js}) & \forall i < j \in N, s \in K \\ & x_{ijs} \in \{0, 1\} & \forall i < j \in N, \forall s \in K \\ & y_{is} \in \{0, 1\} & \forall i \in N, \forall s \in K \end{aligned}$$

Clustering Problem: Formulation 1

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \quad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

IP Formulation:

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Comparing formulations 0 and 1

- Size of the formulation for $n = 40$ objects and $k = 3$ clusters:

	variables	constraints	nonzeros
Formulation 0	2,460	4,723	14,280
Formulation 1	2,460	7,063	16,620

- y_{is} variables: $40 \times 3 = 120$
 - x_{ijs} variables: $\binom{40}{2} \times 3 = 780 \times 3 = 2340$
- Solution time:

	B& B nodes	Simplex iterations	Solution time
Formulation 0	40,560	11,210,558	327.78 seconds
Formulation 1	23,050	4,033,965	159.24 seconds

- Form. 1 needs much fewer nodes to solve the IP.
- Surprisingly, Form. 1 is $\approx 20\%$ faster per B&B node (# of LPs)
- In both formulations x and y variables are declared binary
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Why fewer nodes?

LP relaxation of these two formulations look like:

$$\begin{array}{llll} \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \leftarrow \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \leftarrow \text{clusters} \\ & x_{ijs} \text{ constraints} & \forall i < j \in N, s \in K & \\ & 1 \geq x_{ijs} \geq 0 & 1 \geq y_{is} \geq 0 & \end{array}$$

Formulation 0:

$$x_{ijs} \geq y_{is} + y_{js} - 1$$

$$x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js})$$

Formulation 1:

$$x_{ijs} \geq y_{is} + y_{js} - 1$$

$$x_{ijs} \leq y_{is}$$

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- Now consider a feasible solution to the LP relaxation of F1.

$$\underbrace{(x_{ijs} \leq y_{is}) \text{ AND } (x_{ijs} \leq y_{js})}_{\text{solution feasible for F1}} \Rightarrow \underbrace{(x_{ijs} \leq \frac{1}{2}(y_{is} + y_{js}))}_{\text{also feasible for F0}}$$

- Therefore, Formulation 1 is better as its LP feasible region is smaller.

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- Therefore, Formulation 1 is **better** as its LP feasible region is **smaller**.

Observation 0: If x, y_1, y_2 satisfy the constraints

$$x \geq y_1 + y_2 - 1$$

$$x \leq \frac{1}{2}(y_1 + y_2)$$

$$y_1, y_2 \in \{0, 1\} \text{ and } x \in \{0, 1\}$$

then $x = y_1 y_2$. (i.e., $x = 1$ only when both $y_1 = 1$ and $y_2 = 1$)

Without $x \in \{0, 1\}$, the point $\underbrace{(1, 0, \frac{1}{2})}_{(y_1, y_2, x)}$ is feasible to the system above.

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Clustering Problem: Formulation 1⁺

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \quad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

IP Formulation:

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Comparing formulations 0, 1 and 1⁺

- Size of the formulation for $n = 40$ objects and $k = 3$ clusters:

	variables	constraints	nonzeros
Formulation 0	2,460	4,723	14,280
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Formulation 1 ⁺	2,460	7,063	16,620

- y_{is} variables: $40 \times 3 = 120$ ← binary
- x_{ijs} variables: $\binom{40}{2} \times 3 = 780 \times 3 = 2340$ ← continuous in F 1⁺

- Solution time:

	B& B nodes	Simplex iterations	Solution time
Formulation 0	40,560	11,210,558	327.78 seconds
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Question: Even if we did not have the constraints $x_{ijs} \leq y_{is}$, $x_{ijs} \leq y_{js}$, would $x_{ijs} = 1$ in an optimal sol. if either $y_{is} = 0$ or $y_{js} = 0$?

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Note: This formulation allows $x_{ijs} = 1$ even when items i and j are in different clusters but this would never happen in an opt. solution.

Comparing the Formulations 0, 1, 1⁺ and 1⁺⁺

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- LPs are now much easier to solve (fewer constraints and non-zeroes).

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Clustering Problem: Formulation 2

Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$z_{ij} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if objects } i \text{ and } j \text{ are put in the same cluster} \\ 0 & \text{otherwise.} \end{cases} \quad (\text{only for } i < j)$$

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How to say $z_{ij} = 1$ when both $y_{is}, y_{js} = 1$ for some $s \in K$

$$z_{ij} \geq 0 \quad \forall i < j \in N$$

$$y_{is} \in \{0, 1\} \quad \forall i \in N, s \in K$$

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(Formulation 2 is 35% faster than Formulation 1⁺⁺)

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Gurobi Output for Formulation 2

Gurobi log file for last model:

=====

900 variables, all binary

2383 constraints, all linear; 7260 nonzeros

40 equality constraints

2343 inequality constraints

1 linear objective; 226 nonzeros.

Gurobi 9.1.1: outlev=1

threads=4

Gurobi Optimizer version 9.1.1 build v9.1.1rc0 (linux64)

Thread count: 32 physical cores, 64 logical processors, using up to 64 threads

Optimize a model with 2383 rows, 900 columns and 7260 nonzeros

Model fingerprint: 0xae721739

Variable types: 0 continuous, 900 integer (900 binary)

Coefficient statistics:

Matrix range [1e+00, 1e+00]

Objective range [1e+00, 1e+00]

Bounds range [1e+00, 1e+00]

RHS range [1e+00, 1e+01]

(continued....)

Found heuristic solution: objective 81.0000000

Presolve removed 1662 rows and 554 columns

Presolve time: 0.00s

Presolved: 721 rows, 346 columns, 2274 nonzeros

Variable types: 0 continuous, 346 integer (346 binary)

Root relaxation: objective 0.000000e+00, 161 iterations, 0.00 se

Nodes	Current Node	Obj.	Bounds	Work	Expl	Unexpl	Obj	Depth
IntInf	Incumbent	BestBd	Gap	It/Node	Time			

0	0	0.0	0	58	81.00	0.00	100%	-	0s
H	0	0			34.00	0.00	100%	-	0s
0	0	0.0	0	85	34.00	0.00	100%	-	0s
0	0	1.5	0	127	34.00	1.50	95.6%	-	0s
0	0	1.5	0	124	34.00	1.50	95.6%	-	0s
0	2	1.5	0	121	34.00	1.50	95.6%	-	0s
*	271	239		17	32.00	9.04	71.7%	103	0s
H	494	297			29.00	10.35	64.3%	93.5	0s

(continued....)

H	630	351		28.00	11.21	59.9%	94.5	0s
*	633	335	18	27.00	11.21	58.5%	94.3	0s
H	691	316		25.00	12.30	50.8%	95.0	0s
H	974	354		24.00	13.91	42.0%	95.5	1s

Explored 4392 nodes (369175 simplex iterations) in 3.98 seconds

Optimal solution found (tolerance 1.00e-04)

Best objective 2.400e+01, best bound 2.400e+01, gap 0.0000%

369175 simplex iterations

4392 branch-and-cut nodes

Cutting planes:

Gomory: 3

MIR: 7

Zero half: 26

RLT: 128

BQP: 60

Solving IPs: computation time

- Consider the following LP formulation

$$\begin{aligned} & \text{minimize} && c^T x \\ & \text{subject to} && A^1 x \geq b^1, \\ & && A^2 x = b^2, \\ & && x \geq 0 \end{aligned}$$

- The **non-zeroes** of this formulation is the number of nonzero entries in the matrices A^1 and A^2 .
- LPs are solved using either simplex or interior point algorithms,
- In both cases one has to solve (many, many) linear equations
- The computational burden per iteration typically grows with the number of non-zero entries of the constraint matrices A^1 and A^2
- It also grows with the number of rows of A^1 and A^2 .
- IP solution time depends on the number of B&B nodes and the LP solution time at each node.