Introduction to Optimization

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Multi-agent optimization
Mathematical economics
Alexandrov geometry in optimization
Optimal transport

Topic Overview

This introduction shall covers the following topics:

- Introduction to Optimization Modeling
- Unconstrained Optimization
  - Principles of Unconstrained Optimization
  - Gradient Descent Algorithm and its Variants
  - Numerical Examples
- Constrained Optimization
  - Principles of Constrained Optimization
  - Constrained Optimization Solvers
- Heuristic Approach

Constrained Optimization

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A point x that satisfies the constraint (i.e. $x \in C$) is said to be *feasible*.

Structured Constrained Optimization Problem

Very often, the constraint set C is described by inequalities and equalities:

$$C = \left\{ x \in \mathbb{R}^n \;\middle|\; \begin{array}{ll} g_i(x) \le 0, & \forall i = 1, 2, \cdots, r \\ h_j(x) = 0, & \forall j = 1, 2, \cdots, l \end{array} \right\}$$

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In this case, $Min(f, C)$ and $LMin(f, C)$ will be represented by $Min(f, g, h)$ $LMin(f, g, h)$, respectively, with

$$Min(f, g, h) \quad \left\{ \begin{array}{lll} \min & f(x) & \\ \text{s.t.} & g_i(x) \le 0 & \forall i = 1, 2, \cdots, r \\ & h_j(x) = 0 & \forall j = 1, 2, \cdots, l. \end{array} \right.$$

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If there is no equality constraints, then we just write $Min(f, g)$.

Karush-Kuhn-Tucker (KKT) Conditions

To solve a structured constrained optimization problem, one resorts to the KKT conditions:

$$\begin{cases} \nabla f(x) + \sum_{i=1}^{r} \lambda_i \nabla g_i(x) + \sum_{j=1}^{l} \mu_j \nabla h_j(x) = 0, \\ \lambda_i g_i(x) = 0 \qquad \text{for all } i = 1, \cdots, r, \end{cases}$$

for some scalars $\lambda_1, \cdots, \lambda_r \geq 0$ and $\mu_1, \cdots, \mu_l \in \mathbb{R}$.

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The second conditions are called the *complementarity conditions*, which states that if an inequality constraint $g_i(x) < 0$ holds strictly (i.e. it is inactive), then $\lambda_i = 0$. This 'deactivate' the participation of its gradient $\nabla g_i(x)$ in the first condition.

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We write $\bar{x} \in KKT(f, g, h)$ if the KKT conditions holds at $\bar{x}$ for some scalars $\lambda_1, \cdots, \lambda_r \geq 0$ and $\mu_1, \cdots, \mu_l \in \mathbb{R}$.

Principles of Structured Constrained Optimization Problems

Necessity: Under some ‘technical’ assumptions,

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$$d^\top \nabla_x^2 L(\bar{x}, \bar{\lambda}, \bar{\mu}) d > 0, \quad \forall d : \begin{cases} \nabla g_i^\top(\bar{x}) d \leq 0 & \text{if } g_i(\bar{x}) = 0, \\ \nabla g_i^\top(\bar{x}) d = 0 & \text{if } g_i(\bar{x}) = 0 \text{ and } \bar{\lambda}_i > 0, \\ \nabla h_j(\bar{x})^\top d = 0 & \text{for all } j = 1, \cdots, l, \end{cases}$$

then $\bar{x} \in LMin(f, g, h)$.

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then $\bar{x} \in LMin(f, g, h)$.

In the above expression, $L(x, \lambda, \mu) = f(x) + \sum_i \lambda_i \nabla g_i(x) + \sum_j \mu_j \nabla h_j(x)$.

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$$\bar{x} \in KKT(f, g, h) \implies \bar{x} \in LMin(f, g, h).$$

Principles of Structured Constrained Optimization Problems

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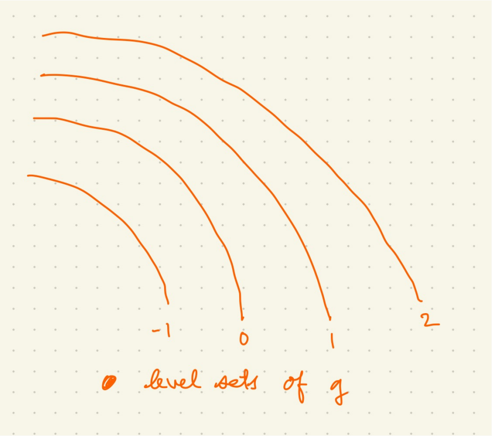
$$\bar{x} \in KKT(f, g, h) \implies \bar{x} \in Min(f, g, h).$$

Principles of Structured Constrained Optimization Problems

To find a point $\bar{x} \in LMin(f, g, h)$:
Filter: Find all KKT points $\bar{x}$ with multipliers $\bar{\lambda}$ and $\bar{\mu}$.
Confirm: Check the positivity of $\nabla_x^2 L(\bar{x}, \bar{\lambda}, \bar{\mu})$ at each KKT points.

KKT conditions explained



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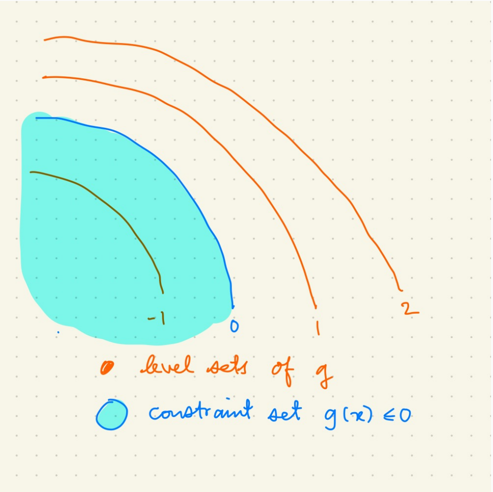

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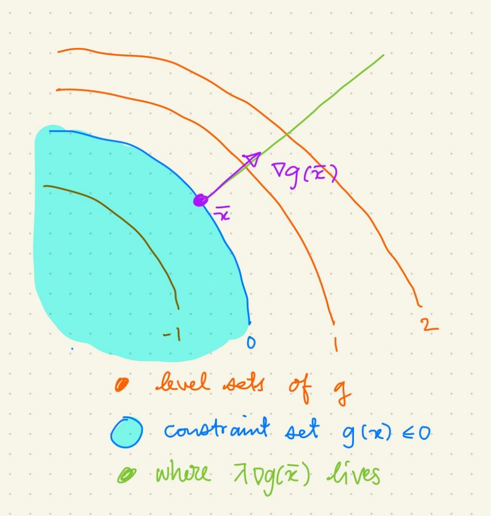

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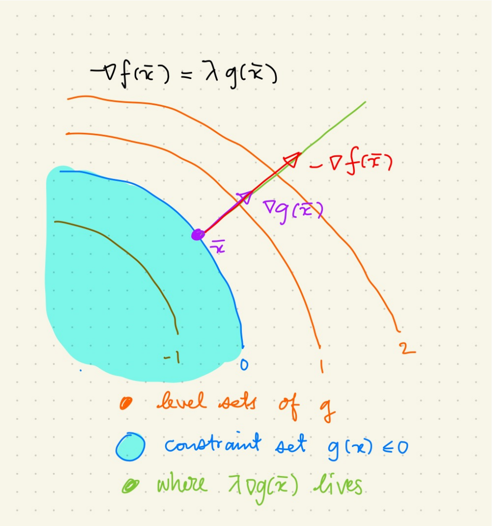

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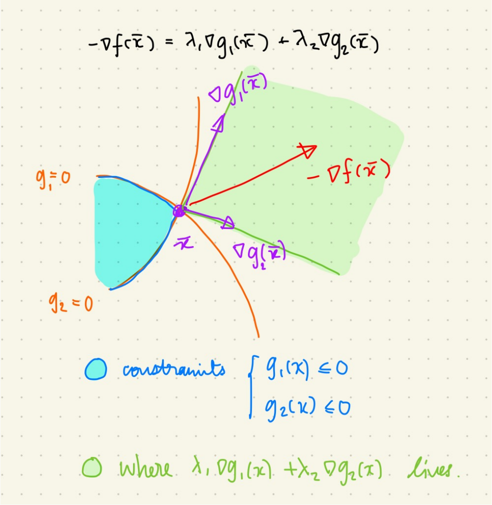

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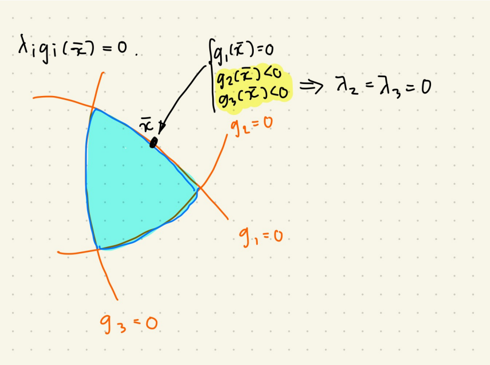

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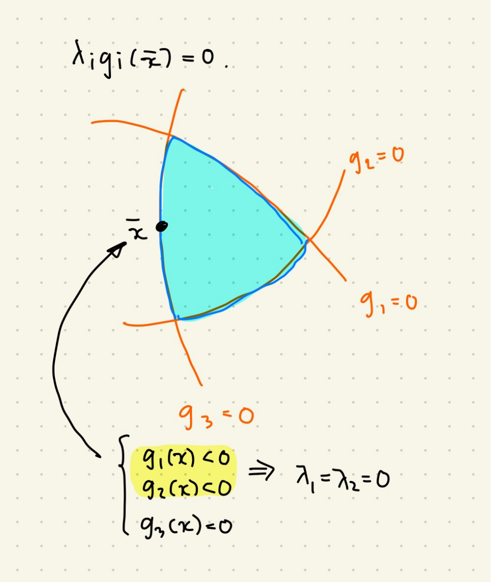

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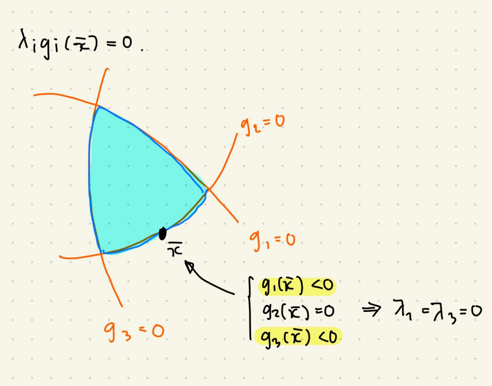

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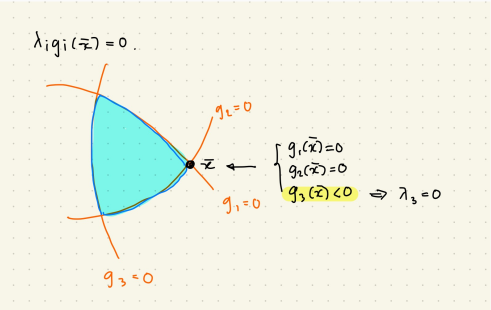

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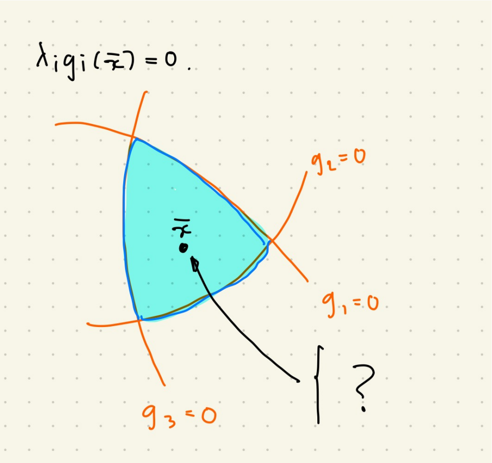

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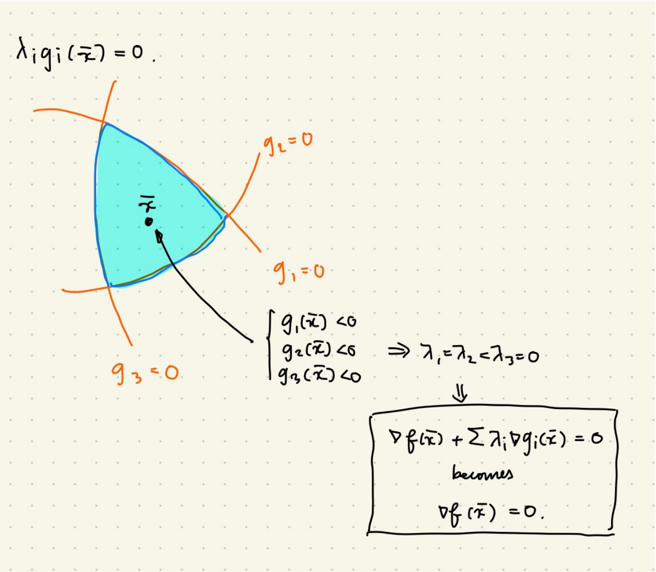

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Consider the problems

$$\begin{cases} \min & x_1 + x_2 \\ \text{s.t.} & x_1^2 + x_2^2 = 1. \end{cases} \tag{1}$$

and

$$\begin{cases} \min & x_1 + x_2 \\ \text{s.t.} & (x_1^2 + x_2^2 - 1)^2 = 0. \end{cases} \tag{2}$$

KKT conditions explained

$$\min \; x_1 + x_2 \quad \rightarrow f(x_1, x_2) \rightarrow \nabla f(x_1,x_2) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\text{s.t. } x_1^2 + x_1^2 - 1 = 0 \quad \rightarrow h_1(x_1, x_2) \rightarrow \nabla h_1(x_1,x_2) = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix}$$

$$\nabla f(x) + \mu \nabla h_1(x) = 0$$

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \mu \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} = 0$$

$$\left.\begin{array}{l} 1 + 2\mu x_1 = 0 \\ 1 + 2\mu x_2 = 0 \end{array}\right. \Rightarrow \left.\begin{array}{l} x_1 = -\frac{1}{2\mu} \\ x_2 = -\frac{1}{2\mu} \end{array}\right\} \; (*)$$

From the constraint,

$$x_1^2 + x_2^2 = 1$$

$$\frac{1}{4\mu^2} + \frac{1}{4\mu^2} = 1$$

$$\frac{1}{2\mu^2} = 1$$

$$\mu = \frac{1}{\sqrt{2}}$$

From (*), we get $x_1 = x_2 = -\frac{1}{\sqrt{2}}$.

The candidate for the local solution is $x = \begin{bmatrix} -1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$.

KKT conditions explained

$$\min \quad x_1 + x_2$$
$$\text{s.t.} \quad (x_1^2 + x_2^2 - 1)^2 = 0$$

$$\nabla f(x) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\nabla h_2(x) = \begin{bmatrix} 4x_1 (x_1^2 + x_2^2 - 1) \\ 4x_2 (x_1^2 + x_2^2 - 1) \end{bmatrix}.$$

KKT condition:

$$\begin{bmatrix} -1 \\ -1 \end{bmatrix} = \mu \begin{bmatrix} 4x_1 (x_1^2 + x_2^2 - 1) \\ 4x_2 (x_1^2 + x_2^2 - 1) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

← no solution on the constraint set.

If the constraint is satisfied, then $(x_1^2 + x_2^2 - 1) = 0$

The gradient $\nabla h_2(x) = 0$ for all $x \in C_2$.

Some MATLAB Solvers for Structured Problems

Well-known solvers

The following solvers are well known and many of them can be called in Matlab.

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Keep in mind that there is no algorithm that can be used to find a true (local) optimum for general nonlinear programs.

Hence, eventhough the above solvers succeeded, the the reported result can be incorrect.

The tool `fmincon` solves a structured constrained optimization problem that takes the form

$$\begin{cases} \min & f(x) \\ \text{s.t.} & c_i(x) \leq 0 \quad \forall i = 1, 2, \cdots, r \\ & ceq_j(x) = 0 \quad \forall j = 1, 2, \cdots, l \\ & Ax \leq b \\ & Aeq \cdot x = beq \\ & lb \leq x \leq ub. \end{cases}$$

by the command

```
fmincon(f,x0,A,b,Aeq,beq,lb,ub,nonlcon)
```

where `nonlcon` outputs the nonlinear constraints *c* and *ceq* in a vector form.

Ex. Let's try `fmincon` with the soft drink manufacturing problem.

The tool `fmincon` solves a structured linear program that takes the form

$$\begin{cases} \min & f^\top x \\ \text{s.t.} & Ax \le b \\ & Aeq \cdot x = beq \\ & lb \le x \le ub. \end{cases}$$

by the command

```
linprog(f,A,b,Aeq,beq,lb,ub).
```

Ex. Let's try `linprog` with the portfolio optimization problem.

`linprog` for sequential investment planning (1)

General purpose. Suppose that you have an initial amount of money C_0 to invest over a time period of T years in N zero-coupon bonds. Each bond k pays an interest rate ρ_k that compounds each year, and pays the principal plus compounded interest at the end of a maturity period m_k. The objective is to maximize the total amount of money after T years.

linprog for sequential investment planning (2)

Ex. Invest \$1,000 in $N = 4$ types of bonds $B_1, \cdots, B_4$ over the period of $T = 5$ years.

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B_1: Can be purchased in Year 1. Maturity period of 4 years.
Interest rate of 2%.

B_2: Can be purchased in Year 5. Maturity period of 1 year.
Interest rate of 4%.

B_3: Can be purchased in Year 2. Maturity period of 4 years.
Interest rate of 6%.

B_4: Can be purchased in Year 2. Maturity period of 3 years.
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We also create B_0 for the choice not to invest in any bonds. The interest rate for B_0 is bank interest rate $\rho_0 = 0.25\%$, which is assumed to be fixed over the period.

`linprog` for sequential investment planning (2)

<table>
<tr><th></th><th>Year 1</th><th>Year 2</th><th>Year 3</th><th>Year 4</th><th>Year 5</th></tr>
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0.25%</td><td>x_6
0.25%</td><td>x_7
0.25%</td><td>x_8
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2%</td><td></td></tr>
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4%</td></tr>
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Let x_k denotes the amount of investment according to the above table and $r_k = (1 + \rho_k/100)^{m_k}$ denotes the net return of B_k.

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Profit after Year 5 = $r_2 x_2 + r_3 x_3 + r_9 x_9$.

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`linprog` for sequential investment planning (2)

	Year 1	Year 2	Year 3	Year 4	Year 5
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The tool `fmincon` solves a structured linearly constrained quadratic program that takes the form

$$\begin{cases} \min & \frac{1}{2}x^\top Hx + f^\top x \\ \text{s.t.} & Ax \le b \\ & Aeq \cdot x = beq \\ & lb \le x \le ub. \end{cases}$$

by the command

```
quadprog(H,f,A,b,Aeq,beq,lb,ub).
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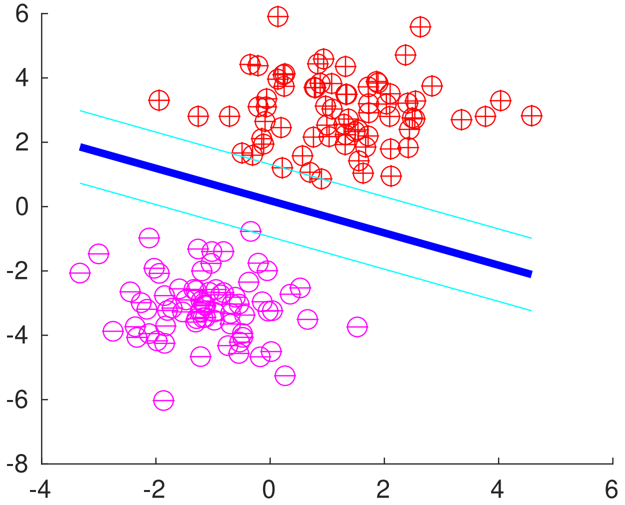
Ex. Let's try to use `quadprog` to find an optimal separating plane in the SVM model.

`quadprog` for SVMs



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by the command

```
intlinprog(f,I,A,b,Aeq,beq,lb,ub).
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Ex. Let's try `intlinprog` with a service provider problem.

`linprog`/`intlinprog` for service provider problems

General statement.

A service company that has N hubs requires to serve its M clients.

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Other problem-specific constraints.

Ex. A transportation company has 5 hubs, namely Samut Prakan (city), Pathum Thani, Chachoengsao, Nakhon Nayok, and Rayong (city), that stock empty containers. This company needs to provide these containers to the 6 ports in Samut Prakan (Bang Pu), Samut Prakan (Suvarnabhumi), Prachin Buri, Sa Kaeo, Chonburi, and Rayong (Pluak Daeng).

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The container stocks (x_i) and port demands (r_j) are as follows:

	Empty containers
Samut Prakan (city)	10
Pathum Thani	8
Chachoengsao	8
Nakhon Nayok	7
Rayong (city)	9

	Container demand
Samut Prakan (Bang Pu)	8
Samut Prakan (Suvarnabhumi)	7
Prachin Buri	7
Sa Kaeo	6
Chonburi	6
Rayong (Pluak Daeng)	7

`intlinprog` in logistics (3)

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The transportation cost bore by each lorry is directly proportional to the distance with the cost/km. = THB300. The (rounded) distances d_{ij} from hub i to port j are given in the following table.

		$j = 1$	$j = 2$	$j = 3$	$j = 4$	$j = 5$	$j = 6$
		BP	SVP	PB	SK	CB	PD
$i = 1$	SP	15	20	148	175	108	120
$i = 2$	PT	78	60	143	194	162	173
$i = 3$	CCS	100	92	69	95	72	83
$i = 4$	NN	132	107	59	110	153	161
$i = 5$	RY	153	154	186	213	54	47

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Non-negativity constraint: $x_{ij}, y_{ij} \geq 0$.

Metaheuristics

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We have to be careful with the term *global* in this context, as it rather means a local solution that is better than some other local solutions than the true global optimum that one would imagined of.

Heuristics vs Metaheuristics

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Metaheuristics, on the other hand, are designed to work with any problems without using any problem-specific knowledge. Well-known algorithms of this category are

- Particle Swarm Optimization (PSO)*
- Genetic Algorithm (GA)*
- Ant Colony Optimization
- Bee Colony Optimization
- Tabu Search
- etc.

Classical vs Metaheuristic Algorithms

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Applications that usually require metaheuristics are (hyper)parameter estimations.

PSO

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Initialization:
Generate an initial population of particles (points in the search space).
While: Not satisfied;
Evaluation: Evaluate the objective value at each candidate.
Local update: Each particle memorizes its own best-known position (local best). The new position is then compared with the previous local best.
Global update: All local bests are compared and the best one is memorized as the global best.
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Initialization:
Generate an initial population of candidate solutions. Each candidate is coded as a finite sequence of *genes*, called a *chromosome*.
While: Not satisfied;
Evaluation: Compute the fitness value of each candidates using a choice of fitness function.
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Conclusion and remarks

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- To hand-calculate the constrained optimum, we solve it through the KKT conditions.
- Most of the classical gradient-based iterative methods are based on the KKT conditions.
- GA works best with discrete search spaces.
- PSO works best with continuous search spaces.
- Metaheuristics do not require gradient information.
- No best-for-all algorithm exists.

Thank you.