# 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

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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:

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

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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

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

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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

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

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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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# Principles of Structured Constrained Optimization Problems

Necessity (linear constraints): If all $g_i$'s and $h_j$'s are affine, then

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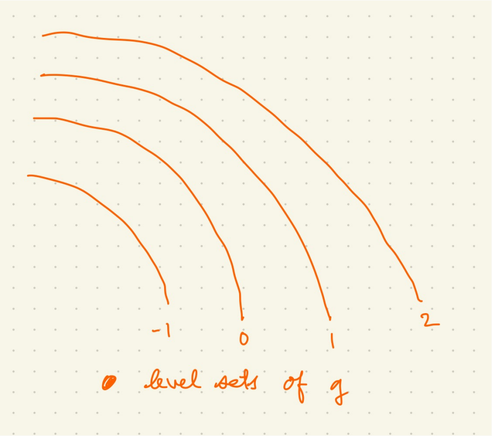
$$\bar{x} \in KKT(f, g, h) \implies \bar{x} \in Min(f, g, h).$$

# 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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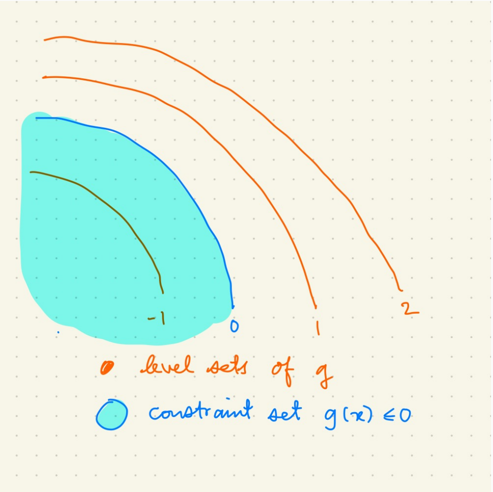

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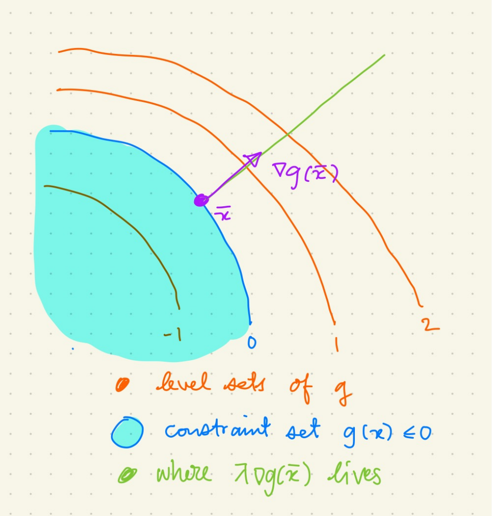

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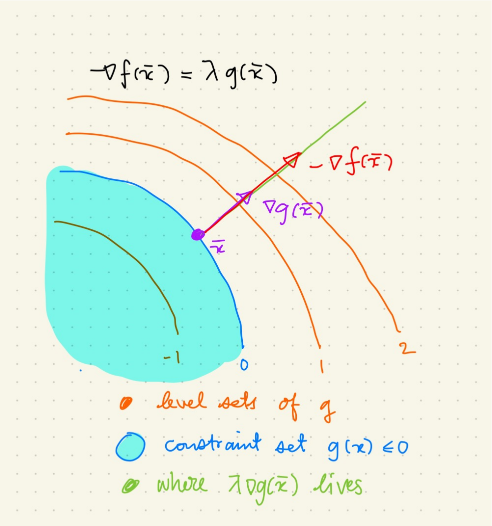

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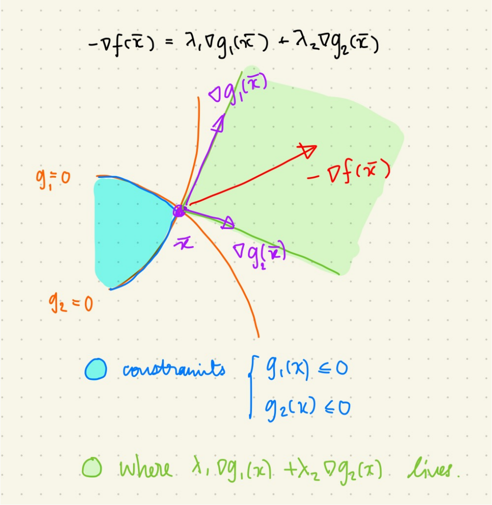

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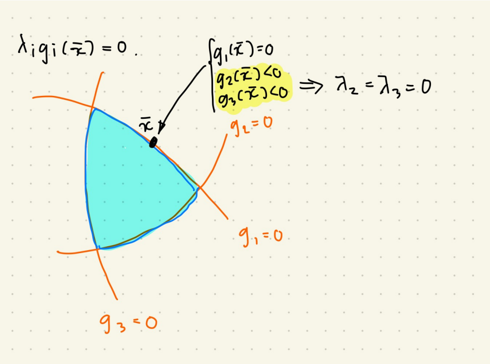

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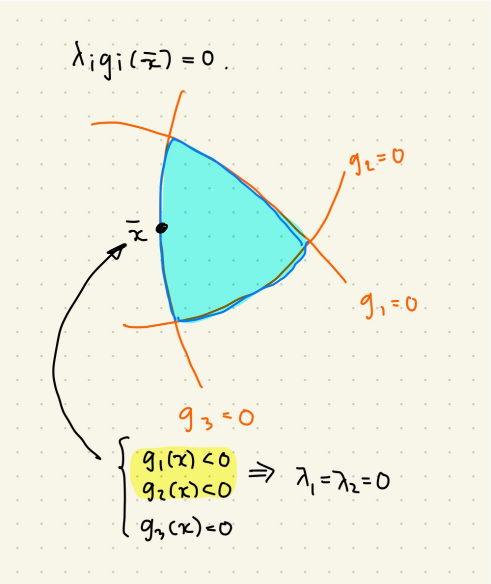

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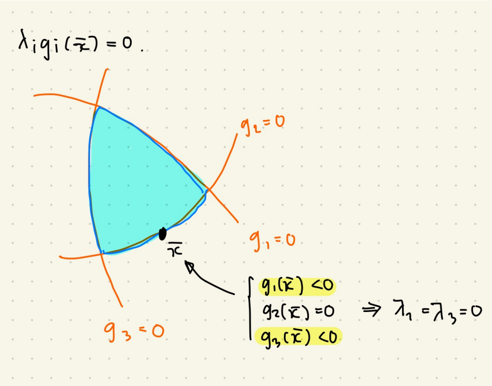

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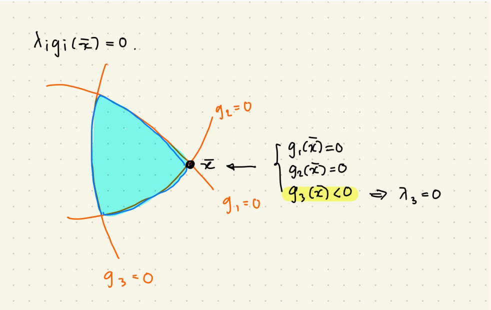

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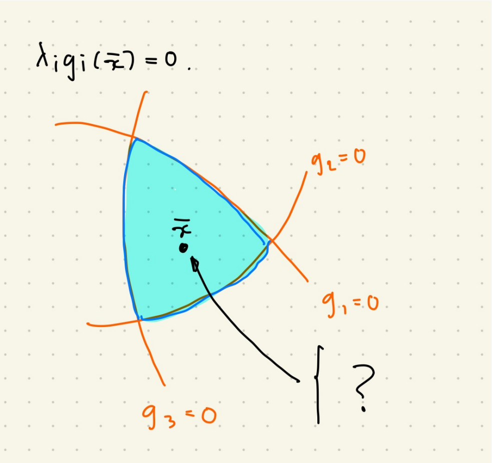

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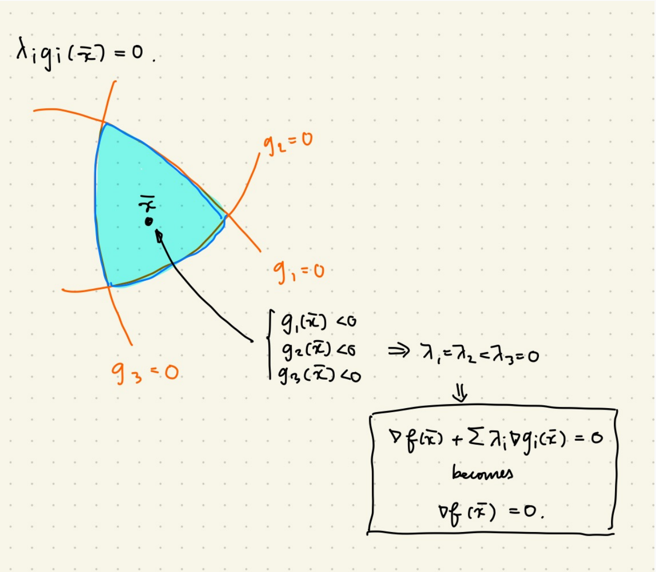

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Consider the problems

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

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

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

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

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

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

$$\left.\begin{aligned} 1 + 2\mu x_1 &= 0 \\ 1 + 2\mu x_2 &= 0 \end{aligned}\right\} \Rightarrow \left.\begin{aligned} x_1 &= -\frac{1}{2\mu} \\ x_2 &= -\frac{1}{2\mu} \end{aligned}\right\} \quad (*)$$

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

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

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 $\rho_k$ 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)

| | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 |
|---|---|---|---|---|---|
| $B_0$ | $x_5$ 0.25% | $x_6$ 0.25% | $x_7$ 0.25% | $x_8$ 0.25% | $x_9$ 0.25% |
| $B_1$ | $x_1$ 2% | | | | |
| $B_2$ | | | | | $x_2$ 4% |
| $B_3$ | | $x_3$ 6% | | | |
| $B_4$ | | $x_4$ 6% | | | |

# `linprog` **for sequential investment planning (2)**

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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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The tool `fmincon` solves a structured linearly constrained quadratic program that takes the form

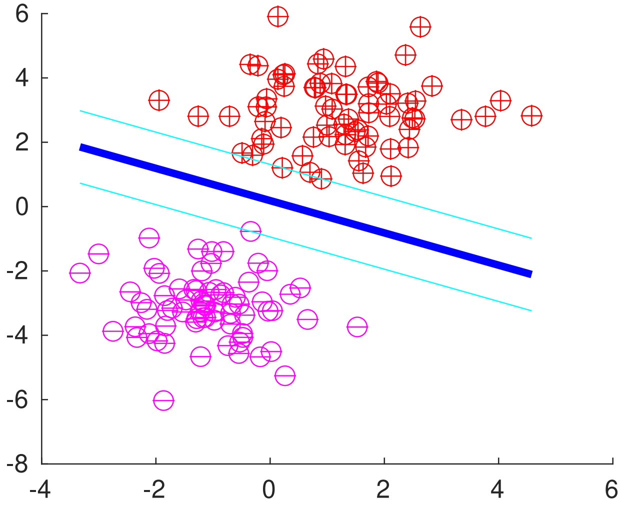
$$\begin{cases} \min & \frac{1}{2}x^\top Hx + f^\top x \\ \text{s.t.} & Ax \leq b \\ & Aeq \cdot x = beq \\ & lb \leq x \leq ub. \end{cases}$$

by the command

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

**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).`

**Ex.** Let's try `intlinprog` with a service provider problem.

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Other problem-specific constraints.

# `intlinprog` in logistics (1)

**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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# `intlinprog` in logistics (2)

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 |

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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.

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

PARTICLE SWARM OPTIMIZATION.

**Initialization:**
Generate an initial population of particles (points in the search space).
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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.