

Mathematics Notes

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Abbreviations

RL	Reinforcement Learning
prob.	probability
params.	parameters
func.	function
pdf.	Probability Density Function
SVD	Singular Value Decomposition
K-L	Kullback–Leibler
IG	Information Gain
i.f.f.	if and only if
LP	Linear Programming
QP	Quadratic Programming
TSP	Travelling Salesman Problem

1 Matrix

1.1 Singular Value Decomposition

Singular Value Decomposition ([SVD](#))

MLcoban.com

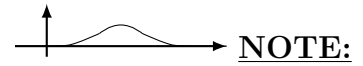
2 Probabilities

2.1 General

2.1.1 Basic Definitions

- If x is discrete: $\sum_x p(x) = 1$ with $\forall 0 \leq p(x) \leq 1$
- If x is continuous: $\int p(x) dx = 1 \Rightarrow \exists$ a **Probability Density Function (pdf.)**

$p(x)$ can take any positive value, as long as $\int p(x) dx = 1$
: theoretically $p(x) = 0, \forall x$



- Common types

Joint probability: $p(x_i, y_i) = p(X = x_i, Y = y_i)$

Marginal probability: $p(x_i) = p(X = x_i)$

Conditional probability: $p(y_i|x_i) = p(Y = y_i|X = x_i)$

- Sum rule: \sum joint probability (prob.) = marginal prob.
 \Rightarrow Marginalization

– discrete variable: $p(x) = \sum_y p(x, y)$

– continuous variable: $p(x) = \int p(x, y) dy$

- Product rule: Product of marginal prob. and conditional prob. = joint prob.

2.1.2 Expectation

For variable x : $\mathbb{E}[x] = \sum_x x.p(x) \quad \left(= \int x.p(x)dx \right)$

For function $f(\cdot)$: $\mathbb{E}[f(x)] = \sum_x f(x).p(x) \quad \left(= \int f(x).p(x)dx \right)$

2.1.3 Independence and Variability

- Independence. E.g.: x, y are independent, then

$$\begin{cases} p(x|y) = p(x) \\ p(y|x) = p(y) \end{cases} \Leftrightarrow p(x, y) = p(x).p(y)$$

- Variability

2 Probabilities

- variance: how much variability there is in $f(x)$ around its mean value $\mathbb{E}[f(x)]$

$$\text{var}[f] = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

- covariance: for two random variables x, y

$$\text{cov}[x, y] = \mathbb{E}_{x, y}[xy] - \mathbb{E}[x] \cdot \mathbb{E}[y]$$

- covariance matrix: if x, y are vectors

$$\begin{aligned}\text{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x}, \mathbf{y}}[\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\} \{\mathbf{y}^T - \mathbb{E}[\mathbf{y}^T]\}] \\ &= \mathbb{E}_{\mathbf{x}, \mathbf{y}}[\mathbf{x}\mathbf{y}^T] - \mathbb{E}[\mathbf{x}] \cdot \mathbb{E}[\mathbf{y}^T]\end{aligned}$$

2.1.4 Bayes Rule

$$\begin{aligned}p(x_i|y_i) \cdot p(y_i) &= p(y_i|x_i) \cdot p(x_i) = p(x_i, y_i) \\ \Rightarrow p(y_i|x_i) &= \frac{p(x_i|y_i) \cdot p(y_i)}{p(x_i)} = \frac{p(x_i|y_i) \cdot p(y_i)}{\sum_y p(x_i|y_i) \cdot p(y_i)}\end{aligned}$$

\Rightarrow the Bayes equation:

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{normalization factor}}$$

2.2 Types of Probability Distributions

Reference source: machinelearningcoban.com.

2.2.1 Bernoulli Distribution

Bernoulli Distribution is a distribution to describe binary discrete variables. It's the case that the variable can only take value in 2 classes $x \in \{0, 1\}$. E.g., the probability of throwing a coin. The Bernoulli distribution is defined with parameter $\lambda \in [0, 1]$:

$$p(x) = \text{Bern}_x[\lambda] = \begin{cases} p(x=1) = \lambda \\ p(x=0) = 1 - \lambda \end{cases} \quad (2.1)$$

In short form, the above equation can be combined into one:

$$p(x) = \lambda^x (1 - \lambda)^{(1-x)} \Rightarrow \begin{cases} p(0) = \lambda^0 (1 - \lambda)^1 = 1 - \lambda \\ p(1) = \lambda^1 (1 - \lambda)^0 = \lambda \end{cases} \quad (2.2)$$

2.2.2 Categorical Distribution

Categorical Distribution is the generalization of *Bernoulli Distribution* for K classes of the discrete variable $x \in \{1, 2, \dots, K\}$. Accordingly, there will be K parameters to describe this pdf: $\lambda = [\lambda_1, \lambda_2, \dots, \lambda_K]$, with $\lambda_k \geq 0$ and $\sum \lambda_k = 1$. Each λ_k represents the probability to take the output k : $p(x = k) = \lambda_k$. In short: $p(x) = \text{Cat}_x[\lambda]$.

Another common way to represent the output is the one-hot vector, $\mathbf{x} \in \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_K\}$ with \mathbf{e}_k is the k -unit vector, which has all 0-element, except the k -element equal to 1. E.g., given 3 classes: $\mathbf{e}_1 = [1, 0, 0]^T$, $\mathbf{e}_2 = [0, 1, 0]^T$, $\mathbf{e}_3 = [0, 0, 1]^T$. We will then have:

$$p(\mathbf{x} = \mathbf{e}_k) = \prod_{j=1}^K \lambda_j^{x_j} = \lambda_k \quad (2.3)$$

because for $\mathbf{x} = \mathbf{e}_k$, only $x_k = 1$, while $x_j = 0, \forall j \neq k$.

2.2.3 Univariate Normal Distribution

Univariate Normal Distribution is also known as the Gaussian distribution. For single dimension data (in 1D): $x \in (-\infty, \infty)$, the mean $\mu \in \mathbb{R}$, and the variance σ^2 with $\sigma \in \mathbb{R}$.

$$p(x) = \text{Norm}_x[\mu, \sigma^2] = \mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right) \quad (2.4)$$

NOTE:

- **Marginals** **prob.** of **Gaussian** are again **Gaussian**.
- When estimating the parameters (**params.**) of a Gaussian, beware the underestimation problem.

$$\begin{aligned} \mathbb{E}[\mu_{ML}] &= \mu \\ \mathbb{E}[\sigma_{ML}^2] &= \left(\frac{N-1}{N}\right) \sigma^2 \\ \Rightarrow \tilde{\sigma}^2 &= \left(\frac{N}{N-1}\right) \sigma_{ML}^2 = \frac{1}{N-1} \sum_{n=1}^N (x_n - \hat{\mu})^2 \end{aligned}$$

2.2.4 Multivariate Normal Distribution

Multivariate Normal Distribution is the extension of *Univariate Normal Distribution* to multi-dimensional data: $\mathbf{x}, \boldsymbol{\mu} \in \mathbb{R}^D, \sigma^2 \Rightarrow \Sigma \in \mathbb{S}_{++}^D$ (\mathbb{S}_{++}^D is the set of positive definite symmetric matrix)

$$p(\mathbf{x}) = \text{Norm}_x[\boldsymbol{\mu}, \Sigma] = \mathcal{N}(\boldsymbol{\mu}, \Sigma) = \frac{1}{2\pi^{D/2} |\Sigma|^{\frac{1}{2}}} \cdot \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})\right) \quad (2.5)$$

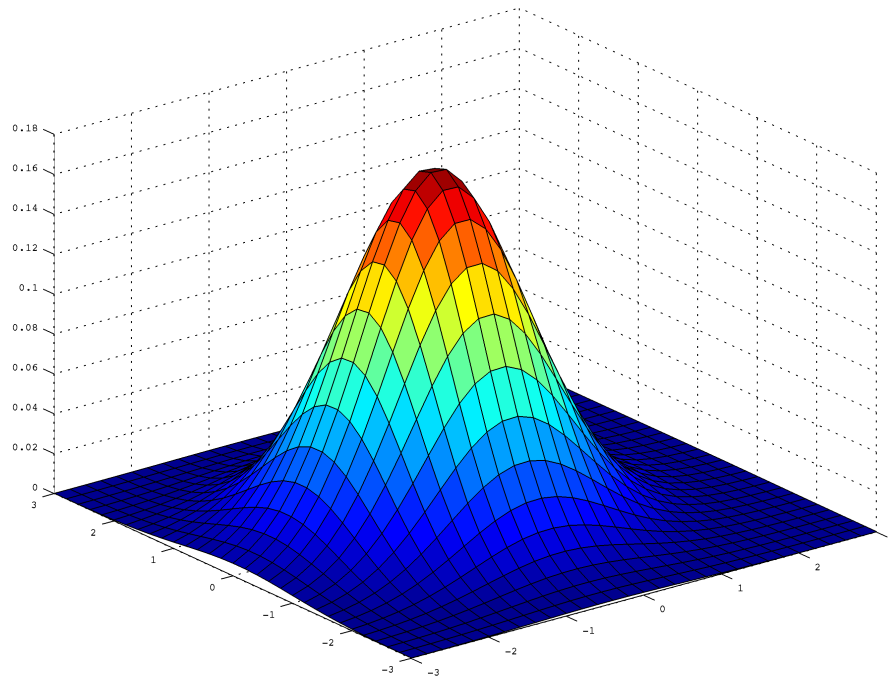


Figure 2.1: Bivariate Gaussian distribution ([src](#)).

2.2.5 Beta Distribution

This distribution describes the parameter for another distributions. E.g., Dirichlet [pdf](#). describes Categorical Distribution (Subsec. [2.2.2](#))

3 Information Theory

[TODO: intro]

3.1 Entropy

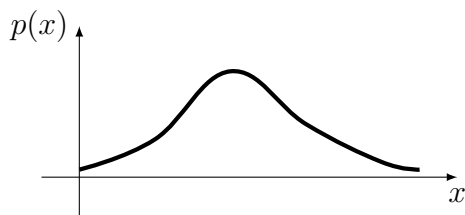
$$p(\mathbf{x}) \quad \text{-- distribution (e.g. over observation } \mathbf{x}) \quad (3.1)$$

$$\mathcal{H}(p) = -\mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[\log p(\mathbf{x})] \quad \text{-- entropy - how "broad" } p(\mathbf{x}) \text{ is} \quad (3.2)$$

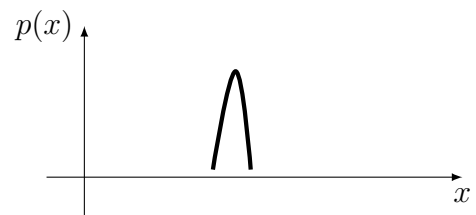
$$= -\sum_{i=1}^N p(\mathbf{x}_i) \log p(\mathbf{x}_i) \quad (3.3)$$

Intuition:

- How *random* is the variable?
The more random the variable, the higher the entropy (Fig. 3.1)
- How large is the log [prob.](#) in expectation *under* itself?
 - If you mostly see low log [prob.](#), then there are many places with similar [prob.](#), and the entropy, as negative log, would be high (Fig. 3.1a).
 - If you mostly see high log [prob.](#), then the variable focuses around only a few place, thus, the entropy, as negative log, would be low (Fig. 3.1b).



(a) Example of $p(x)$ with high entropy.



(b) Example of $p(x)$ with low entropy.

Figure 3.1: Examples of $p(x)$ with different entropy.

3.2 Cross Entropy

The cross entropy between two given [prob.](#) distributions p and q is defined as:

$$H(p, q) = \mathbb{E}_p[-\log q] \quad (3.4)$$

With \mathbf{p}, \mathbf{q} as discrete variables:

$$H(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^C p_i \log q_i \quad (3.5)$$

NOTE: $\nexists \log(0) \Rightarrow$ condition: $\mathbf{q} > 0$

3.3 Kullback - Leiber Divergence

The Kullback–Leibler (**K-L**)-divergence tells:

- How *different* are two distributions?
- How small is the expected log **prob.** of one distribution under another, **minus entropy**?

Example reference: [countbayesie](#)

$$H = - \sum_{i=1}^N p(x_i) \log p(x_i) \quad (3.6)$$

$$D_{KL}(p||q) = \sum_{i=1}^N p(x_i) [\log p(x_i) - \log q(x_i)] \quad (3.7)$$

$$= \sum_{i=1}^N p(x_i) \log \frac{p(x_i)}{q(x_i)} \quad (3.8)$$

$$= \mathbb{E}_{x \sim p(x)} [\log p(x) - \log q(x)] \quad (3.9)$$

\Rightarrow How many bits of info we expect to loose

\Rightarrow **A function** that we can **optimized**

cross entropy = entropy + KL Divergence

$$H(p, q) = H(p) + D_{KL}(p||q) \quad (3.10)$$

E.g.: KL divergence between two normal distributions $\mathcal{N}(\mu_1, \sigma_1)$ and $\mathcal{N}(\mu_2, \sigma_2)$:

$$D_{KL}(p, q) = \log \frac{\sigma_2}{\sigma_1} + \frac{\sigma_1^2 + (\mu_1 - \mu_2)^2}{2\sigma_2^2} - \frac{1}{2} \quad (3.11)$$

PSEUDO CODE: with $\mu_2 = 0, \sigma_2 = 1$

$$\mu, \sigma = \text{encoder}(\hat{x}) \quad (3.12)$$

$$z = \mu + \sigma * \text{random_normal}(0, 1) \quad (3.13)$$

$$y = \text{decoder}(z) \quad (3.14)$$

$$\text{recon_loss} = x.\log(y) + (1-x)\log(1-y) \quad (3.15)$$

$$\text{KL_loss} = \frac{1}{2}[\mu^2 + \sigma^2 - \log(\sigma^2 + 1e^{-8}) - 1] \quad (3.16)$$

$$\text{ELBO} = \text{recon_loss} - \text{KL_loss} \quad (3.17)$$

$$\text{loss} = -\text{ELBO} \quad (3.18)$$

3.4 Mutual Information

$$p(x) \quad - \text{distribution (e.g. over observation } \mathbf{x}) \quad (3.19)$$

$$\mathcal{H}(p(\mathbf{x})) = -\mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[\log p(\mathbf{x})] \quad - \text{entropy - how "broad" } p(\mathbf{x}) \text{ is} \quad (3.20)$$

$$\mathcal{I}(\mathbf{x}; \mathbf{y}) = D_{KL}(p(\mathbf{x}, \mathbf{y}) || p(\mathbf{x})p(\mathbf{y})) \quad - \text{mutual information} \quad (3.21)$$

$$= \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim p(\mathbf{x}, \mathbf{y})} \left[\log \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})p(\mathbf{y})} \right] \quad (3.22)$$

$$= \mathcal{H}(p(\mathbf{y})) - \mathcal{H}(p(\mathbf{y}|\mathbf{x})) \quad - \text{relates to IG} \quad (3.23)$$

The last equation implies that we can interpret mutual information $\mathcal{I}(\mathbf{x}; \mathbf{y})$ as [IG](#), how much more do we know about \mathbf{y} after receiving observation about \mathbf{x} .

E.g.:

- If \mathbf{x} and \mathbf{y} are independent of each others, then $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y})$, thus $\mathcal{I}(\mathbf{x}; \mathbf{y}) = 0$
- If \mathbf{x} and \mathbf{y} depends on each others more and more, the different between the joint [prob.](#) $p(\mathbf{x}, \mathbf{y})$ and the product of marginal [prob.](#) $p(\mathbf{x})p(\mathbf{y})$ grows, thus the $\mathcal{I}(\mathbf{x}; \mathbf{y})$ is larger.

4 Convexity

4.1 Convex Sets

- Definition 1: line connects 2 points of a convex set lies within the set
- Definition 2: \mathcal{C} is a convex set if for $\forall x_1, x_2 \in \mathcal{C}$:

$$x_\theta = \theta x_1 + (1 - \theta)x_2 \in \mathcal{C}, \quad \forall 0 \leq \theta \leq 1$$

- Hyperplane is a convex set

$$a_1 x_1 + a_2 x_2 + \dots + a_n x_n = \mathbf{a}^T \mathbf{x} = b, \quad b, a_i \in \mathbb{R}, \quad i \in \mathbb{N}$$

- Half-space is a convex set

$$a_1 x_1 + a_2 x_2 + \dots + a_n x_n = \mathbf{a}^T \mathbf{x} \leq b, \quad b, a_i \in \mathbb{R}, \quad i \in \mathbb{N}$$

- Matrix A is positive definite if:

$$\mathbf{x}^T \mathbf{A} \mathbf{x} \geq 0, \quad \forall \mathbf{x} \in \mathbb{R}^n \iff \boxed{A \succ 0}$$

because $\exists A^{-1} \Rightarrow \forall \lambda \neq 0$ (eigenvalues)

- Intersection of convex sets is a convex set
 \Rightarrow Polyhedra, which is the intersection of halfspaces and hyperplanes is convex.
- x is said to be a convex combination of x_1, x_2, \dots, x_k if

$$x = \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_k x_k \quad \text{with} \quad \theta_1 + \theta_2 + \dots + \theta_k = 1$$

- Convex hull of a set (x_1, x_2, \dots, x_k) is a set of all possible convex combination of that set.

Convex hull of a set is the smallest convex set that contains that set.

- Two convex sets \mathcal{C} and \mathcal{D} are disjoint then exist a, b such:

$$\begin{cases} \mathbf{a}^T \mathbf{x} \leq b & \forall \mathbf{x} \in \mathcal{C} \\ \mathbf{a}^T \mathbf{x} \geq b & \forall \mathbf{x} \in \mathcal{D} \end{cases}$$

Set of all \mathbf{x} that $\mathbf{a}^T \mathbf{x} - b = 0$ is a hyperplane that separate \mathcal{C} and \mathcal{D}

\Rightarrow separating hyperplane

4.2 Convex function

Definition: $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is a convex function if the domain $\text{dom}(f)$ is a convex set and:

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y), \quad \forall x, y \in \text{dom}(f), \quad 0 \leq \theta \leq 1$$

- A function f is **strictly convex** if:

$$f(\theta x + (1 - \theta)y) < \theta f(x) + (1 - \theta)f(y)$$

If there is a minimum point that it is the only minimum point and a global minimum

- **Affine function**: $f(\mathbf{x}) = \mathbf{a}^T \mathbf{x} + b$ is both convex and concave

If the variable is a matrix \mathbf{X} : $f(\mathbf{X}) = \text{trace}(\mathbf{A}^T \mathbf{X}) + b$

- **Quadratic form**: $f(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$ is
 - convex if $A \succeq 0$
 - concave if $-A \succeq 0$
- A function satisfies 3 norm conditions \Rightarrow convex
- α -subset level of $f : \mathbb{R}^n \rightarrow \mathbb{R}$: $\mathcal{C}_\alpha = \{\mathbf{x} \in \text{dom} f \mid f(\mathbf{x}) \leq \alpha\}$

Checking if f is convex:

- First order condition if and only if (i.f.f.): $\begin{cases} \text{differentiable with convex domain} \\ f(x) \geq f(x_0) + \nabla f(x_0)^T (x - x_0), \quad \forall x, x_0 \in \text{dom} f \end{cases}$
- Second order condition: the Hessian $\nabla^2 f(x) \succeq 0$

5 Optimization

Problem:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} f_0(\mathbf{x}) \quad \text{subject to} \quad \begin{cases} f_i(\mathbf{x}) \leq 0, i = 1, 2, \dots, m & \text{(inequality constraints)} \\ h_j(\mathbf{x}) = 0, j = 1, 2, \dots, p & \text{(equality constraints)} \end{cases} \quad (5.1)$$

$$\text{feasible set } \mathcal{D} = \bigcap_{i=0}^m \text{dom} f_i \cap \bigcap_{j=0}^p \text{dom} h_j \Rightarrow \text{set of all } \mathbf{x} \text{ satisfying all constraints} \quad (5.2)$$

5.1 Convex Optimization Problem

Problem:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} f_0(\mathbf{x}) \quad (5.3)$$

$$\text{subject to} \quad \begin{cases} f_i(\mathbf{x}) \leq 0, i = 1, 2, \dots, m & \text{(inequality constraints)} \\ \mathbf{a}_j^T \mathbf{x} - b_j = 0, j = 1, 2, \dots, p & \text{(equality constraints)} \\ f_0 \text{ is convex func.} \\ f_i \text{ is convex func.} \\ h_j \text{ is affine func.} \end{cases} \quad (5.4)$$

$$\Rightarrow \begin{cases} f_i(x) \leq 0 \Rightarrow 0\text{-sublevel set of } f_i \\ h_j(x) = 0, \quad \forall x \Rightarrow \text{hyperplane} \end{cases} \quad (5.5)$$

\Rightarrow we optimize a convex function in a convex set domain.

5.2 Linear Programming

(Vietnamese: Quy hoạch tuyến tính)

Problem:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \mathbf{c}^T \mathbf{x} + d \quad \text{subject to} \quad \begin{cases} \mathbf{G}\mathbf{x} \leq \mathbf{h} \\ \mathbf{A}\mathbf{x} = \mathbf{b} \end{cases} \quad (5.6)$$

A standard form of Linear Programming (LP):

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \mathbf{c}^T \mathbf{x} \quad \text{subject to} \quad \begin{cases} \mathbf{Ax} = \mathbf{b} \\ \mathbf{x} \leq \mathbf{0} \end{cases} \quad (5.7)$$

Python: `cvxopt.solvers.lp`

5.3 Quadratic Programming

Problem:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \frac{1}{2} \mathbf{x}^T \mathbf{P} \mathbf{x} + \mathbf{q}^T \mathbf{x} + r \quad \text{subject to} \quad \begin{cases} \mathbf{G} \mathbf{x} \leq \mathbf{h} \\ \mathbf{Ax} = \mathbf{b} \\ P \succeq 0 \quad (P \text{ is semi-definite}) \end{cases} \quad (5.8)$$

NOTE: When $P = 0$, Quadratic Programming (QP) is LP

Python: `cvxopt.solvers.qp`

5.4 Geometric Programming

- Function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ with $\text{dom} f = \mathbb{R}_{++}^n$ (all element > 0) is a monomial function if:

$$f(x) = c x_1^{a_1} x_2^{a_2} \dots x_n^{a_n}, \quad c > 0, \quad a_i \in \mathbb{R} \quad (5.9)$$

- Function f is a posynomial function if:

$$f(x) = \sum_{k=1}^K c_k x_1^{a_{1k}} x_2^{a_{2k}} \dots x_n^{a_{nk}}, \quad c_k > 0 \quad (5.10)$$

Problem:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} f_0(\mathbf{x}) \quad \text{subject to} \quad \begin{cases} f_i(\mathbf{x}) \leq 1, & i = 1, 2 \dots m \\ h_j(\mathbf{x}) = 1, & j = 1, 2 \dots p \\ f_0, f_i \text{ are posynomial func.} \\ h_j \text{ are monomial func.} \end{cases} \quad (5.11)$$

\Rightarrow geometric programming ($x > 0$ is hidden)

$$\text{Set:} \quad \begin{cases} x_i = e^{y_i} \\ y_i = \log(x_i) \end{cases} \quad \Rightarrow f_0(\mathbf{x}) = \exp(\mathbf{a}^T \mathbf{y} + b)$$

Python: `cvxopt.solvers.gp`

6 Search Algorithms

Search problem is one common type of problem which has numerous presences in our lives. The well-known Travelling Salesman Problem (**TSP**) and its variants are search problems, in which the salesman have to find the shortest route that visit every cities. Many Reinforcement Learning (**RL**) problems can also be viewed as search problems, in which the machine find the most optimal plan to reach the goal.

A search problem consists of: an agent in a state space, a successor function, a start state and a goal state. The **agent** is the one taking the **action**, e.g., in **TSP**, the agent is the salesman, and the action is to travel; in **RL**, the agent is the robot or the machine, and the action could be to move to a different position. The **search state** represents the current situation that the agent is in, which would not necessary equivalent to the world state, which includes every possible details about the environment. E.g., in **TSP**, the state is the current city, every time the action traveling is taken, the agent moves from one city to another (one state to another). The **successor function** describes the transition from one state to another. This function usually comes with the transition action and costs.

A **solution of search problem** is a sequence of actions (a plan) which transform the start state to a goal state. **Search algorithms** find search solutions, which can be optimal, but in many practical cases, close to optimal within time limitation.

This chapter structures as follows:

- The first section describes how a search problem is formulated mathematically as a graph.
- The second section presents some well-known search algorithms.

6.1 Graph

A graph is the mathematical representation of a search problem. A graph consists of nodes and edges.

6.1.1 Undirected Graph

6.1.2 Directed Graph

6.1.3 Adjacency Matrix

6.1.4 Incidence Matrix

6.1.5 Trees and Forest

6.2 Search Algorithms

6.2.1 Properties

6.2.2 Depth-first search

6.2.3 Breadth-first search

6.2.4 Prim's Algorithm

6.2.5 Kruskal's Algorithm

6.2.6 Dijkstra's Algorithm

6.2.7 Bellman and Ford's Algorithm

6.2.8 A* Algorithm

[TODO:]