

Decision Making Modelling

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A Summary of Decision Making Modelling
Learning Note

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Abstract

This thesis presents a comprehensive investigation into [research topic]. The primary contribution of this work is the development of [main contribution]. Through extensive experimentation and analysis, we demonstrate that the proposed approach achieves [key results].

The research addresses several critical challenges in [field], including [specific challenges]. Our methodology combines [technique A] with [technique B] to achieve superior performance compared to existing methods. Experimental results on [number] benchmark datasets show improvements of [percentage] in accuracy and [percentage] in efficiency.

This work has significant implications for [application areas] and provides a foundation for future research in [related fields]. The findings contribute to both theoretical understanding and practical applications of [research domain].

Keywords: keyword1, keyword2, keyword3, keyword4, keyword5

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Dedication

I dedicate this thesis to my parents, for their unwavering support and love.

Contents

Abstract	i
Acknowledgements	ii
Dedication	iii
1 Reinforcement Learning(RL)	2
1.1 Markov Decision Process	2
1.1.1 Basic Formulation and terminology	2
1.1.2 Algorithm to solve a Markov Decision Process	10
1.1.3 Value Learning	10
1.1.4 Policy Learning	11
1.2 Deep Reinforcement Learning	13
1.2.1 Deep Q-Network (DQN)	14
1.2.2 Deep Policy Gradients	19
1.2.3 Multi-agent Actor Critic(MAC)	23
1.3 Partially Observable Markov Decision Process	25
1.3.1 Basic Formulation and terminology	25
1.4 How solve a Partially Observable Markov Decision Process	32
1.5 Common Implementations	33
1.6 Recent Advances	33
1.6.1 Machine Learning Techniques	33
1.7 Research Gaps	33
2 Active Inference(AIF)	37
2.1 Active Inference	37
2.1.1 Data Collection	41
2.2 Algorithm Design	42
2.3 Experimental Setup	42

3 Structural Integration Management	43
3.1 simple example	43
3.1.1 Problem Formulation: 1D Beam with deteriorating stiffness	43
3.2 Proposed Framework	48
A Appendices	50
A.1 Probability Basis	50
A.1.1 Random Variables	50
A.1.2 Random Process	51

List of Figures

1.1	Sequential Probabilistic Graphical Model of Markovian Decision Process	2
1.2	Deep Q-Network approximate the Q function for every available action using state as input $Q(s_t, a_t)$	14
1.3	Dueling Network architecture	18
1.4	NN approximates $\pi(a_t s_t)$	19
1.5	Actor Critic Neural Network architecture	20
1.6	Deep Centralized Multi-agent Actor Critic Neural Network architecture	23
1.7	Deep Decentralized Multi-agent Actor Critic Neural Network architecture	24
1.8	Probabilistic Graphical Model of Partially Observable Markovian Decision Process defined in State Space	25
1.9	Probabilistic Graphical Model of Partially Observable Markovian Decision Process defined in Belief Space	28
1.10	Deep Q-Network approximate the Q function for every available action using belief as input $Q(b_t, a_t)$	35
1.11	Dueling Network architecture	36
2.1	Original POMDP Model	37
2.2	Graphical Representation of the Generative Process(based on the true states s^*) in the world and the corresponding (internal) generative model (based on probabilistic beliefs random variables s) that best explain the outcomes o . The outcomes are shared between the generative process and model. [sajid2021active]	40
3.1	Flowchart diagram	44
3.2	Geometrical Property of Steel Truss Bridge Structure	45
3.3	Gradual deterioration realization plot modeled by a simple rate function	46
3.4	sudden deterioration realization plot modelled by a CPP process	47
3.5	Flowchart POMDP diagram	49

A.1	Extreme Value distribution for Maximum	52
A.2	Bernoulli Process and its associated Probability Distribution	53
A.3	Poisson Process and its associated Probability Distribution	54
A.4	Compound Process Process and its associated Probability Distribution	56
A.5	Gamma Process and its associated Probability Distribution	57

List of Tables

1.1	Example of a table estimation for the optimal state-action value function $Q(S, A)$	10
1.2	Example of a table estimation for $Q^\pi(S, A)$	12
1.3	Comparison of traditional methods	33
2.1	The physical meaning of variational free energy \mathcal{F}	39
3.1	Configuration of Steel Truss Bridge Structure	43
3.2	Prior distribution of deterioration model parameters	46
3.3	Cost Definition in the beam monitoring process	48

Contents

Chapter 1

Reninforcement Learning(RL)

1.1 Markov Decision Process

1.1.1 Basic Formulation and terminology

A **Markov Decision Process (MDP)** has the following four key components: states space \mathbb{S} , action space \mathbb{A} , transition model \mathbf{T} , reward model \mathbf{r} . In some literature the discount factor γ may be treated as the fifth components of a MDP. The reward is commonly chosen to be one scalar for simplicity, so a MDP can be written as a 5-tuple $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$.

The relative definitions are summaried in the following subsections. A basic MDP means the state space and actions spaces are finite, time steps are discrete. Classical Dynamic Programming algorithms can be used to solve this case.

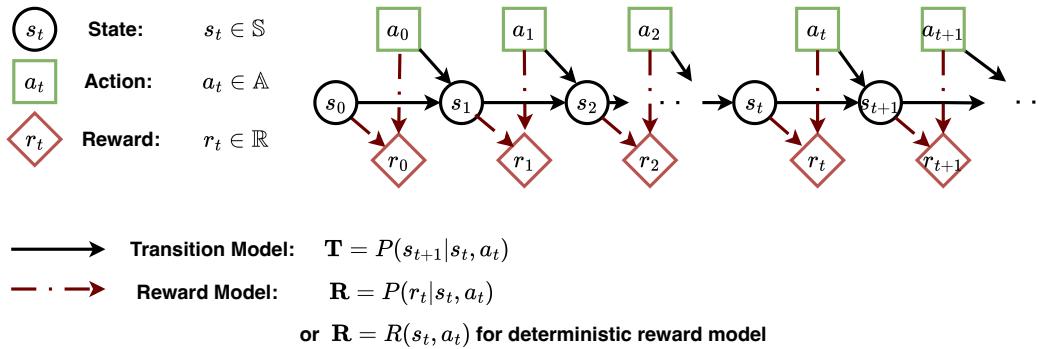


Figure 1.1: Sequential Probabilistic Graphical Model of Markovian Decision Process

State space \mathbb{S}

a finite set of states \mathbb{S} . It is very important to choose the state variables to represent the key information of the environment. In real life there are multiple state variables representing different properties of the environment. We may use the $d_{\mathbb{S}}$ to represent the number of features we choose as state variables. e.g. The healthy state of a person contain mental health and physical health two aspects, $d_{\mathbb{S}} = 2$. For each kind of state variable, its value could be discrete or continuous.

- Discrete State Variable, has the number of N possible values, e.g. the mental health level could be {"Happy", "Depressive", "sad", "angry"}, then $N = 4$
- Continuous State Variable

Action space \mathbb{A}

a finite set of actions \mathbb{A} ; $a_{i \geq t} \in \mathbb{A}$

Policy $\pi(a|s)$

A policy $\pi(a|s)$: the state-dependent sequence of actions

- Deterministic policy $\pi(a|s) : \mathbb{S} \rightarrow \mathbb{A}$
- or Stochastic policy $\pi(a|s) : \mathbb{S} \times \mathbb{A} \rightarrow \mathbb{R} \in [0, 1]$

In the reinforcement learning, we need to let the agent and the environment interact with each other, and record all observed states, actions, rewards trajectories to learn a best policy from these experiences. Here we need to distinguish two kinds of policies: Behavior policy μ : the policy we use to collect experience; Target policy π : the finally trained policy

- If the Behavior policy μ and the target policy π are the same, which means $a_{i \geq t} \sim \pi$, then it is called the On-policy.
- If the Behavior policy μ and the target policy π are different, which means $a_{i > t} \sim \pi$, $a_t \sim \mu$, then it is called the Off-policy. The advantage of Off-policy is that we could use the behavior policy to collect experience, save (s_t, a_t, r_t, s_{t+1}) to an array and use such array (aka. replay buffer) repeatedly to update the target policy. This training method is called the experience replay.

The commonly-chosen behavior policy is ϵ -greedy policy:

$$a_t = \begin{cases} \arg \max_a Q^*(s_t, a; \theta) & \text{with the prob. } 1 - \epsilon, \\ \text{randomly choose one action from } \mathbb{A} & \text{with the prob. } \epsilon. \end{cases} \quad (1.1)$$

The random behavior policy could explore more unknown states and it is good to enlarge the ϵ at the beginning (e.g. $\epsilon = 0.5$) and reduce it during the training process (e.g. $\epsilon = 0.01$)

State Transition Model T

- It could be a deterministic transition function: e.g. $s_{t+1} = f(s_t, a_t)$;
- or a transition probability: $P(s_{t+1}|s_t, a_t, \dots, s_1, a_1)$ ($P(s_{t+1}|s_t, a_t)$ under the Markov Assumption), naturally we have

$$\sum_{s_{t+1} \in \mathcal{S}} P(s_{t+1}|s_t, a_t) = 1$$

Reward model R (negative cost function)

If we consider deterministic reward model, $\mathbf{R} = P(r_{t+1}|a_t, s_t)$ can be written as $\mathbf{R} = R(a_t, b_t)$ A reward model(negative cost function) could be formulated as:

- A general reward function $R(s_t, a_t, s_{t+1})$
- Or an immediate reward function $R(s_t, a_t)$

The cumulative weighted total return $U^\pi(s_t, a_t, \dots, s_T, a_T)$

The cumulative weighted total return is a function of all the states and actions from time t when taking a policy π :

$$U_t^\pi = U^\pi(s_t, a_t, \dots, s_T, a_T) = k_t R(s_t, a_t, s_{t+1}) + \dots + k_T R(s_T, a_T, s_{T+1}) = \sum_{i=t}^T k_i R(s_i, a_i, s_{i+1}) = \sum_{i=t}^T k_i R(s_i, a_i, s_{i+1}) \quad (1.2)$$

where the discount factor $\gamma \in [0, 1]$: weighting the relative importance of the current reward against the future reward. In extreme cases when $\gamma = 0$, means only the current reward matters.

The Expected cumulative weighted total return J^π

The Expected cumulative weighted total return is a measure of the policy π :

$$J^\pi = \mathbb{E}_{S_{i \geq t} \sim T, A_{i \geq t} \sim \pi} [U^\pi(s_t, a_t, S_{t+1}, A_{t+1}, \dots, S_T, A_T)] \quad (1.3)$$

where $T = P(s_t|s_{t-1}, a_{t-1})$ is the transition probability distribution of state s_t and π is the probability of action (aka. the stochastic policy).

The State-Action Value function $Q^\pi(s_t, a_t)$

The State-Action value function $Q^\pi(s_t, a_t)$ describes the value of the policy π given a State-Action Pair $Q^\pi(s_t, a_t)$. It is a measure of the State-Action pair at time step t and the policy π from time step $t + 1$. That is why we need to reduce all the randomness from all the future state and future action.

The value of taking an action a_t at the state s_t and using the strategy π for the rest of time span until T is calculated by the expectation of all the state and actions from time t to T .

$$Q^\pi(s_t, a_t) = \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi(s_t, a_t, S_{t+1}, A_{t+1}, \dots, S_T, A_T) | s_t, a_t] \quad (1.4)$$

where $T = P(s_t | s_{t-1}, a_{t-1})$ is the transition probability distribution of state s_t and π is the probability of action (aka. the stochastic policy).

The State Value Function $V^\pi(s_t)$

The State Value Function $V^\pi(s_t)$ is a measure of the value of current state s_t and that is why we need to further eliminate the randomness of action at time A_t .

The value of a state s_t when taking a policy from this time step t until the rest of the time span can be expressed by the expected total return, mathematically written as:

$$V^\pi(s_t) = \mathbb{E}_{A_t \sim \mu} [Q^\pi(s_t, A_t)] \quad (1.5a)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi, A_t \sim \mu} [U^\pi(s_t, A_t, \dots, S_T, A_T) | s_t, a_t] \quad (1.5b)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi(s_t, a_t, \dots, S_T, A_T)] \quad (1.5c)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} \left[\sum_{i=t}^T \gamma^{i-t} R(s_i, a_i, s_{i+1}) \middle| s_t \right], \quad (1.5d)$$

where μ shows the probability distribution of a_t at time t specifically, which is not necessarily equal to the policy π chosen to taken actions from time $t + 1$ on.

The Optimal State Action Value Function $Q^*(s_t, a_t)$

The Optimal State Action Value function $Q^*(s_t, a_t)$ is a measure of values of the current state-action pair s_t . Based on the State Action Value function $Q^\pi(s_t, a_t)$ we need to further eliminate the randomness of the policy π :

$$Q^*(s_t, a_t) = \max_\pi \mathbb{E}_{S_{i>t} \sim T} \left[\sum_{i=t}^T \gamma^{i-t} R(s_i, a_i, s_{i+1}) \middle| s_t, a_t \right] \quad (1.6)$$

The Optimal State Value Function $V^*(s_t)$

The Optimal State Value function $V^*(s_t)$ is a measure of values of the current state s_t only. Based on the State Value function $V^\pi(s_t)$ we need to further eliminate the randomness of the policy π :

$$V^*(s_t) = \max_{\pi} \mathbb{E}_{S_{i>t} \sim T} \left[\sum_{i=t}^T \gamma^{i-t} R(s_i, a_i, s_{i+1}) \middle| s_t \right] \quad (1.7)$$

Bellman Equation for State-Action Value Function $Q^\pi(s_t, a_t)$

Now we will derive the Bellman equation for the state-action value function

$$Q^\pi(s_t, a_t) = \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi(s_t, a_t, \dots, S_T, A_T) | s_t, a_t] \quad (1.8a)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} \left[\sum_{i=t}^T \gamma^{i-t} R(s_i, a_i, s_{i+1}) \middle| s_t, a_t \right] \quad (1.8b)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} \left[R(s_t, a_t, S_{t+1}) + \gamma \sum_{i=t+1}^T \gamma^{i-(t+1)} R(s_i, a_i, s_{i+1}) \middle| s_t, a_t \right] \quad (1.8c)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [R(s_t, a_t, S_{t+1}) + \gamma U^\pi(s_{t+1}, a_{t+1}, \dots, S_T, A_T) | s_t, a_t] \quad (1.8d)$$

$$= \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [R(s_t, a_t, S_{t+1})] + \gamma \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi(S_{t+1}, A_{t+1}, \dots, S_T, A_T) | s_t, a_t] \quad (1.8e)$$

With the assumption of discrete states and discrete actions, the first expectation can be written as:

$$\mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [R(s_t, a_t, S_{t+1}) | s_t, a_t] = \sum_{s_{t+1} \in \mathcal{S}} R(s_t, a_t, s_{t+1}) P(s_{t+1} | s_t, a_t) \quad (1.9)$$

The second expectation

$$\mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi_{t+1} | s_t, a_t] = \sum_{s_{t+1} \in \mathcal{S}} P(s_{t+1} | s_t, a_t) \sum_{a_{t+1} \in \mathcal{A}} \pi(a_{t+1} | s_{t+1}) \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [U^\pi_{t+1} | s_{t+1}, a_{t+1}] \quad (1.10a)$$

$$= \sum_{s_{t+1} \in \mathcal{S}} P(s_{t+1} | s_t, a_t) \sum_{a_{t+1} \in \mathcal{A}} \pi(a_{t+1} | s_{t+1}) \mathbb{E}_{S_{i>t+1} \sim \rho, A_{i>t+1} \sim \pi} [U^\pi_{t+1} | s_{t+1}, a_{t+1}] \quad (1.10b)$$

Combining the two equations we have

$$Q^\pi(s_t, a_t) = \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) \left[R(s_t, a_t, s_{t+1}) + \gamma \sum_{a_{t+1} \in \mathbb{A}} \pi(a_{t+1}|s_{t+1}) \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi} [U^\pi_{t+1}|s_{t+1}, a_{t+1}] \right] \quad (1.11a)$$

$$= \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) \left[R(s_t, a_t, s_{t+1}) + \gamma \sum_{a_{t+1} \in \mathbb{A}} \pi(a_{t+1}|s_{t+1}) Q^\pi(s_{t+1}, a_{t+1}) \right] \quad (1.11b)$$

If we can simplify the reward function as $R(s_t, a_t, s_{t+1}) = R(s_t, a_t)$, then the above recursive equation can be written as

$$Q^\pi(s_t, a_t) = R(s_t, a_t) + \gamma \sum_{s_{t+1} \in \mathbb{S}} \sum_{a_{t+1} \in \mathbb{A}} P(s_{t+1}|s_t, a_t) \pi(a_{t+1}|s_{t+1}) Q^\pi(s_{t+1}, a_{t+1}) \quad (1.12)$$

Written in expectation form as

$$Q^\pi(s_t, a_t) = R(s_t, a_t) + \gamma \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi} [Q^\pi(S_{t+1}, A_{t+1})] \quad (1.13)$$

Bellman Equation for State Value Function $V^\pi(s_t)$

Now we will derive the Bellman equation for the state value function

$$V^\pi(s_t) = \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} [U^\pi(s_t, A_t, \dots, S_T, A_T)|s_t] \quad (1.14a)$$

$$= \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} \left[\sum_{i=t}^T \gamma^{i-t} R(s_i, a_i, s_{i+1}) | s_t \right] \quad (1.14b)$$

$$= \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} \left[R(s_t, A_t, S_{t+1}) + \gamma \sum_{i=t+1}^T \gamma^{i-(t+1)} R(s_i, a_i, s_{i+1}) | s_t \right] \quad (1.14c)$$

$$= \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} [R(s_t, A_t, S_{t+1}) + \gamma U^\pi(s_{t+1}, a_{t+1}, \dots, s_T, a_T) | s_t] \quad (1.14d)$$

$$= \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} [R(s_t, A_t, S_{t+1}) | s_t] + \gamma \mathbb{E}_{S_{t+1} \sim T, A_{t+1} \sim \pi, A_t \sim \mu} [U^\pi(s_{t+1}, a_{t+1}, \dots, s_T, a_T) | s_t] \quad (1.14e)$$

Now we can look at the two expectations separately. Assume that the state and actions are discrete, then the first expectation can be written as:

$$\mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi, A_t \sim \mu} [R(s_t, A_t, S_{t+1})|s_t] = \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi} [R(s_t, a_t, S_{t+1})|s_t, a_t] \quad (1.15a)$$

$$= \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \sum_{s_{t+1} \in \mathbb{S}} R(s_t, a_t, s_{t+1}) p(s_{t+1}|s_t, a_t) \quad (1.15b)$$

The second expectation $\gamma \mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi, A_t \sim \mu} [U^\pi(S_{t+1}, A_{t+1}, \dots, S_T, A_T)|s_t]$:

$$\mathbb{E}_{S_{i>t} \sim T, A_{i>t} \sim \pi, A_t \sim \mu} [U_{t+1}^\pi|s_t] = \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) \mathbb{E}_{S_{i>t+1} \sim \rho, A_{i>t+1} \sim \pi, A_{t+1} \sim \pi} [U_{t+1}^\pi|s_{t+1}] \quad (1.16a)$$

$$= \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) V^\pi(s_{t+1}) \quad (1.16b)$$

Combining these two expectations, we have

$$V^\pi(s_t) = \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) (R(s_t, a_t, s_{t+1}) + \gamma V^\pi(s_{t+1})) \quad (1.17)$$

With the simplification of $R(s_t, a_t, s_{t+1}) = R(s_t, a_t)$, then the above recursive equation can be written as

$$V^\pi(s_t) = \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) (R(s_t, a_t) + \gamma V^\pi(s_{t+1})) \quad (1.18a)$$

$$= \sum_{a_t \in \mathbb{A}} \mu(a_t|s_t) \left(R(s_t, a_t) + \gamma \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) V^\pi(s_{t+1}) \right) \quad (1.18b)$$

$$= \mathbb{E}_{A_{i=t} \sim \mu} [R(s_t, A_t)] + \gamma \mathbb{E}_{A_t \sim \mu, S_{t+1} \sim T} [V^\pi(s_{t+1})] \quad (1.18c)$$

Optimal Bellman Equation for State Action Value Function $Q^*(s_t, a_t)$

Bellman Equation for Optimal State Value Function $V^*(s_t)$ is also known as Optimal Bellman Equation.

Under standard conditions for discounted MDPs, out of all possible policies there exists at least one deterministic policy that is optimal, maximizing the value of state $V^\pi(s_t)$. For a deterministic policy, with a given transition probability

$P(s_{t+1}|s_t, a_t)$, the optimal state-action value function is denoted as $Q^*(s_t, a_t)$ and the optimal state value function is denoted as $V^*(s_t)$. The optimal Bellman equation of the state-action value function is:

$$Q^*(s_t, a_t) = \mathbb{E}_{S_{t+1} \sim T} [R(s_t, a_t, S_{t+1}) + \gamma V^*(s_{t+1})] \quad (1.19a)$$

$$= \mathbb{E}_{S_{t+1} \sim T} \left[R(s_t, a_t, S_{t+1}) + \gamma \max_{a_{t+1} \in \mathcal{A}} Q^*(s_{t+1}, a_{t+1}) \right] \quad (1.19b)$$

$$= \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) \left[R(s_t, a_t, s_{t+1}) + \gamma \max_{a_{t+1} \in \mathcal{A}} Q^*(s_{t+1}, a_{t+1}) \right] \quad (1.19c)$$

with the simplification of $R(s_t, a_t, s_{t+1}) = R(s_t, a_t)$, we can write the above optimal Bellman equation as

$$Q^*(s_t, a_t) = R(s_t, a_t) + \gamma \mathbb{E}_{S_{t+1} \sim T} \left[\max_{a_{t+1} \in \mathcal{A}} Q^*(s_{t+1}, a_{t+1}) \right] \quad (1.20a)$$

$$= R(s_t, a_t) + \gamma \sum_{s_{t+1} \in \mathbb{S}} \left[\max_{a_{t+1} \in \mathcal{A}} P(s_{t+1}|s_t, a_t) Q^*(s_{t+1}, a_{t+1}) \right] \quad (1.20b)$$

$$= R(s_t, a_t) + \gamma \sum_{s_{t+1} \in \mathbb{S}} \left[\max_{a_{t+1} \in \mathcal{A}} P(s_{t+1}|s_t, a_t) Q^*(s_{t+1}, a_{t+1}) \right] \quad (1.20c)$$

Optimal Bellman Equation for State Value Function $V^*(s_t)$

Bellman Equation for Optimal State Value Function $V^*(s_t)$ is also known as Optimal Bellman Equation.

Under standard conditions for discounted MDPs, out of all possible policies there exists at least one deterministic policy that is optimal, maximizing the value of state $V^\pi(s_t)$. For a deterministic policy, with a given transition probability $P(s_{t+1}|s_t, a_t)$, the optimal state-action value function is denoted as $Q^*(s_t, a_t)$ and the optimal state value function is denoted as $V^*(s_t)$.

The optimal Bellman equation of the state value function is

$$V^*(s_t) = \max_{a_t \in \mathcal{A}} Q^*(s_t, a_t) \quad (1.21a)$$

$$= \max_{a_t \in \mathcal{A}} \mathbb{E}_{S_{t+1} \sim \rho} (R(s_t, a_t, S_{t+1}) + \gamma V^*(s_{t+1})) \quad (1.21b)$$

$$= \max_{a_t \in \mathcal{A}} \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) (R(s_t, a_t, s_{t+1}) + \gamma V^*(s_{t+1})) \quad (1.21c)$$

with the simplification of $R(s_t, a_t, s_{t+1}) = R(s_t, a_t)$, we can write the above optimal Bellman equation as

$$V^*(s_t) = \max_{a_t \in \mathbb{A}} \{R(s_t, a_t) + \gamma \mathbb{E}_{s_{t+1} \sim T} [V^*(s_{t+1})]\} \quad (1.22a)$$

$$= \max_{a_t \in \mathbb{A}} \left\{ R(s_t, a_t) + \gamma \sum_{s_{t+1} \in \mathbb{S}} P(s_{t+1}|s_t, a_t) V^*(s_{t+1}) \right\} \quad (1.22b)$$

1.1.2 Algorithm to solve a Markov Decision Process

1.1.3 Value Learning

Value Learning is a reinforcement learning methods where we want to estimate the value function ($Q(s, a)$, $V(s)$, $Q^\pi(s, a)$, $V^\pi(s)$) as accurate as possible.

The old way of estimation is to build a table to approximate the value function. This is only applicable for discrete state space and discrete action space. For example in Table 1.1:

Table 1.1: Example of a table estimation for the optimal state-action value function $Q(S, A)$

$Q(S, A)$	A_1	A_2	A_3	A_4
S_1	380	-95	20	173
S_2	-7	64	-195	210
S_3	152	72	413	-80

The more widely used estimation is to build a neural network $Q(s, a; \theta^Q)$, $V(s; \theta^V)$, $Q^\pi(s, a; \theta^{Q^\pi})$, $V^\pi(s; \theta^{V^\pi})$ to estimate the corresponding value $Q(s, a)$, $V(s)$, $Q^\pi(s, a)$, $V^\pi(s)$.

- Deep Q-Network (DQN): To learn optimal value function $Q(s, a)$ or $V(s)$. It requires 5-tuple $\{s_t, a_t, r_t, s_{t+1}\}$ generated from any policy stored in experience replay. It belongs to the off-policy learning.
- State Action Reward State Action (SARSA): To learn policy-based value function $Q^\pi(s, a)$ or $V^\pi(s)$. As suggested by the name, SARSA requires a five-tuple $\{s_t, a_t, r_t, s_{t+1}, a_{t+1}\}$. It belongs to the on-policy algorithm. The policy-based value learning is usually combined with policy learning, which is usually called Actor-Critic Algorithm

To train any one of the Neural Network estimated Value function, we will make use of the Bellman equation, take $Q(s, a)$ as an example, the Bellman equation of

the optimal state action value function is given in Eq. 1.19

$$Q(s_t, a_t) = \mathbb{E}_{s_{i>t} \sim \rho} [U_t^\pi | s_t, a_t] = \mathbb{E}_{s_{i>t} \sim \rho} [R_t + \gamma V(S_{t+1})] = \mathbb{E}_{s_{i>t} \sim \rho} \left[r_t + \gamma \max_{a_{t+1} \in \mathcal{A}} Q(S_{t+1}, a_{t+1}) \right] \quad (1.23)$$

where $U_t^\pi = \sum_{i=t}^T \gamma^i R_i$ and $R_t = R(s_t, a_t, s_{t+1})$.

Neural Network approximation is $\hat{q}_t = Q(s_t, a_t; \theta^Q)$. The loss function is defined as $L(\theta^Q) \stackrel{\text{def}}{=} \mathbb{E}[\hat{q}_t - \hat{y}_t]^2$ e.g. $L(\theta^Q) \stackrel{\text{def}}{=} \frac{1}{2}[\hat{q}_t - \hat{y}_t]^2$. We hope to minimize the loss function and based on the gradient descent:

$$\nabla_{\theta^Q} L(\theta^\pi) = (\hat{q}_t - \hat{y}_t) \cdot \nabla_{\theta^Q} \hat{q}_t \quad (1.24)$$

To minimize the loss function, we need to update the parameter like this

$$\theta^Q \leftarrow \theta^Q - \alpha(\hat{q}_t - \hat{y}_t) \nabla_{\theta^Q} \hat{q}_t = \theta^Q - \alpha \delta_t \nabla_{\theta^Q} \hat{q}_t \quad (1.25)$$

There are usually two ways of training the parameters of the neural network:

- Monte Carlo estimation: The target is the real observation of one episode (the return of one episode) starting from s_t and taking action a_t :

$$\hat{y}_t = u_t = \sum_{i=t}^T \gamma^i r_i \quad (1.26)$$

- Temporal Difference estimation: The m-step TD target is combined of the first m observations and the expected return of the remaining steps:

$$\hat{y}_t = \sum_{i=t}^m \gamma^i r_i + \gamma^m \max_{a_{t+m} \in \mathcal{A}} q(s_{t+m}, a_{t+m}; \theta^Q) \quad (1.27)$$

1.1.4 Policy Learning

Policy learning is to find the best policy $\pi(a|s)$ directly. Policy learning is usually combined with also the value learning of this policy $q^\pi(s, a; \theta^{Q^\pi})$ or $v(s; \theta^{V^\pi})$. Take $Q^\pi(s, a)$ as an example, the Bellman equation of the state action value function is given in equation Eq. 1.8

$$Q^\pi(s_t, a_t) = \mathbb{E}_{s_{i>t} \sim \rho, A_{i>t} \sim \pi} [U_t^\pi | s_t, a_t] = \mathbb{E}_{s_{i>t} \sim \rho, A_{i>t} \sim \pi} [R_t + \gamma Q^\pi(S_{t+1}, A_{t+1})] \quad (1.28)$$

For discrete states and discrete action space, we could also use a table for estimation shown in Table 1.2:

Or using neural Network approximation is $\hat{Q}_t = Q(s_t, a_t; \theta^{Q^\pi})$.

Similarly we can build the loss function and update the parameters as following

$$\theta^{Q^\pi} \leftarrow \theta^{Q^\pi} - \alpha(\hat{Q}_t - \hat{y}_t) \nabla_{\theta^{Q^\pi}} \hat{Q}_t = \theta^{Q^\pi} - \alpha \delta_t \nabla_{\theta^{Q^\pi}} \hat{Q}_t \quad (1.29)$$

There are usually two ways of training the parameters of the neural network:

Table 1.2: Example of a table estimation for $Q^\pi(S, A)$

$Q^\pi(S, A)$	A_1	A_2	A_3	A_4
S_1	380	-95	20	173
S_2	-7	64	-195	210
S_3	152	72	413	-80

- Monte Carlo estimation: The target is the real observation of one episode (the return of one episode) starting from s_t and taking action a_t :

$$\hat{y}_t = u_t = \sum_{i=t}^T \gamma^i r_i \quad (1.30)$$

- Temporal Difference estimation: The m-step TD target is combined of the first m observations and the expected return of the remaining steps:

$$\hat{y}_t = \sum_{i=t}^m \gamma^i r_i + \gamma^m q(s_{t+m}, a_{t+m}; \theta^{Q^\pi}) \quad (1.31)$$

There will be a neural network estimation of the policy function $\pi(a, s; \theta^\pi)$. The objective function is the so-called J function:

$$J(\theta^\pi) \stackrel{\text{def}}{=} \mathbb{E}_{S_t \sim \rho}[V^\pi(S_t)] = \mathbb{E}_{S_t \sim \rho}[\mathbb{E}_{A_t \sim \pi}[Q^\pi(S_t, A_t)]] \quad (1.32)$$

$$g \stackrel{\text{def}}{=} \nabla_{\theta^\pi} J(\theta^\pi) \approx \mathbb{E}_{S_t \sim \rho, A_t \sim \pi}[Q^\pi(S_t, A_t) \cdot \nabla_{\theta^\pi} \ln \pi(A_t | S_t; \theta^\pi)] \quad (1.33)$$

Here we hope to maximize the J function, so we will use the gradient ascent to update the parameter by Eq. 1.34

$$\theta^\pi \leftarrow \theta^\pi + \beta \nabla_{\theta^\pi} J(\theta^\pi) \quad (1.34)$$

We need some more approximation and advanced techniques to represent the gradient $\nabla_{\theta^\pi} J(\theta^\pi)$: Usually we will add baseline $b = V^\pi(S)$ for better training result

$$g_b \stackrel{\text{def}}{=} \nabla_{\theta^\pi} J(\theta^\pi) \approx \mathbb{E}_{S_t \sim \rho, A_t \sim \pi}[(Q^\pi(S_t, A_t) - V^\pi(S_t)) \cdot \nabla_{\theta^\pi} \ln \pi(A_t | S_t; \theta^\pi)] \quad (1.35)$$

The advantage function is defined as

$$A^\pi(s_t, a_t) \stackrel{\text{def}}{=} Q^\pi(s_t, a_t) - V^\pi(s_t) \quad (1.36)$$

We could see that in the gradients calculation for policy learning, we need to also know the value of this policy Q^π or V^π . There are many possible ways to handle this:

- REINFORCE: without base line

$$\tilde{g}_{\text{REINFORCE}}(s_t, a_t; \theta^\pi) = q(s_t, a_t; \theta^{Q^\pi}) \cdot \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) \quad (1.37)$$

Considering baseline, we will use the real observed return to approximate $Q^\pi(S_t, A_t)$, and use another neural network $v(s_t; \theta^{V^\pi})$ to approximate $V^\pi(S_t)$

$$\tilde{g}_{\text{REINFORCE}_b}(s_t, a_t; \theta^\pi) = [u_t - v(s_t; \theta^{V^\pi})] \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) \quad (1.38)$$

- Actor Critic (AC):

$$\tilde{g}_{\text{AC}}(s_t, a_t; \theta^\pi) = q(s_t, a_t; \theta^{Q^\pi}) \cdot \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) \quad (1.39)$$

When Actor-Critic considers the baseline, it becomes Advantage-Actor-Critic (A2C): First due to the Bellman equation of the state action value function Eq. 1.8

$$Q^\pi(s_t, a_t) = \mathbb{E}_{S_{t+1} \sim p(\cdot | s_t, a_t)} [R_t + \gamma V^\pi(S_{t+1})] \quad (1.40)$$

the expression in equation Eq. 1.35 $\mathbb{E}_{S_t \sim p, A_t \sim \pi, S_{t+1} \sim p(\cdot | s_t, a_t)} [(Q^\pi(S_t, A_t) - V^\pi(S_t)) \cdot \nabla_{\theta^\pi} \ln \pi(A_t | S_t; \theta^\pi)]$ could be transferred to

$$\nabla_{\theta^\pi} J(\theta^\pi) \approx \mathbb{E}_{S_t \sim p, A_t \sim \pi, S_{t+1} \sim p(\cdot | s_t, a_t)} [R_t + \gamma V^\pi(S_{t+1}) - V^\pi(S_t)] \cdot \nabla_{\theta^\pi} \ln \pi(A_t | S_t; \theta^\pi) \quad (1.41)$$

So the gradient in actor-critic algorithm is now approximated as

$$\tilde{g}_{\text{A2C}} = (r_t + \gamma v(s_{t+1}; \theta^{V^\pi}) - v(s_t; \theta^{V^\pi})) \cdot \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) \quad (1.42)$$

$$\theta^\pi \leftarrow \theta^\pi + \beta(r_t + \gamma v(s_{t+1}; \theta^{V^\pi}) - v(s_t; \theta^{V^\pi})) \cdot \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) = \theta^\pi - \beta \delta_t \cdot \nabla_{\theta^\pi} \ln \pi(a_t | s_t; \theta^\pi) \quad (1.43)$$

The one-step TD error of value learning δ_t is defined as $\delta_t \stackrel{\text{def}}{=} -(r_t + \gamma v(s_{t+1}; \theta^{V^\pi}) - v(s_t; \theta^{V^\pi}))$.

1.2 Deep Reinforcement Learning

Deep Reinforcement Learning is the Reinforcement Learning employed the deep neural networks.

Neural networks (like any other approximation structure like polynomials, splines, radial basis functions) can approximate any continuous function within a compact set. In other words, given a continuous function $f(x)$, a finite range

for the input $x \in [a, b]$ and an expected approximation accuracy ϵ , there exists a neural network that approximate $f(x)$ with an approximation error less than ϵ everywhere within $[a, b]$.

According to the universal approximation theorem, any continuous function can be arbitrarily closely approximated by a multi-layer perceptron with only one hidden layer and a finite number of neurons [info10040122, cybenko1989approximation, hornik1989multilayer, yarotsky2017error, cuomo2022scientific]. Deep neural networks is a type of artificial neural network with more than two layers.

The key idea of DRL is to utilize the deep neural networks as function approximators to provide arbitrarily accurate proxies of the original functions in large state spaces, such as:

$$F \simeq F(\cdot | \theta^F), \quad (1.44)$$

where F is one of the previously defined functions Q^π, V^π, Q, V, π and $\theta^F \in \Theta$ are real-valued vectors of parameters. Thereby, the whole problem of determining values at each point of a high-dimensional space $A \times S$ to the lower-dimensional space Θ , $|\Theta| \ll |S \times A|$.

1.2.1 Deep Q-Network (DQN)

Deep Q-Network is based on the off-policy Q-learning scheme using the NN to approximate the optimal Q-function. The general DQN concept is shown in Figure 1.2. State s_t is introduced as input to a deep neural network, with an appropriate number of hidden layers and nonlinear unit activations, which output an approximation of the action-value function $Q(s_t, a_t | \theta^Q) \in \mathbb{R}^{|\mathcal{A}|}$. If the state is

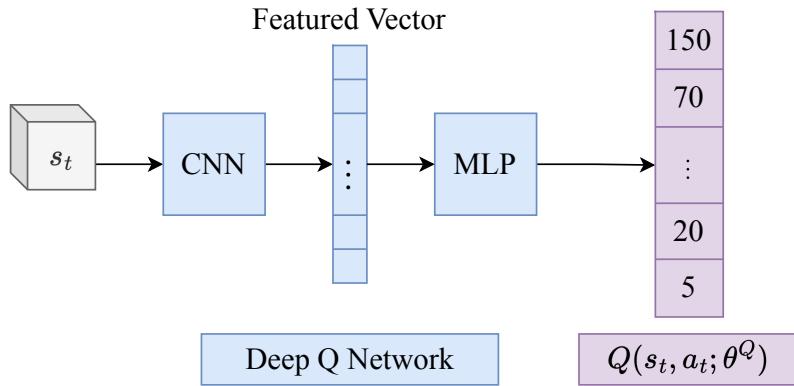


Figure 1.2: Deep Q-Network approximate the Q function for every available action using state as input $Q(s_t, a_t)$

matrix or multi-dimensional tensor, we will use Convolutional Neural Network ; if the state is a vector, then we can use Multi-layer Perceptron (MLP) directly.

The objective function that is minimized during training to determine θ^Q is given by the loss function

$$L_Q(\theta^Q) = \mathbb{E} [(Q(s_t, a_t | \theta^Q) - y_t)^2], \quad (1.45)$$

where μ is the behaviour policy of off-policy learning with $\mu \neq \pi$, ρ is the limiting distribution of states for policy μ , and $y_t \stackrel{\text{def}}{=} R(s_t, a_t) + \gamma \max_{a_{t+1} \in \mathbb{A}} Q(s_{t+1}, a_{t+1})$.

To increase the training stability and robustness, we can also use two central features in the DQN algorithm [[mnih2013playing](#)]: the first is the experience replay (replay buffer) and the second is the use of a separate target network.

Algorithm 1: Deep Q Network(DQN) Training

Input: The decision process model MDP $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$, or POMDP $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{r}, \mathbf{O}, \gamma\}$

Output: The optimal state-action value function $Q(s, a)$

- 1 Collect the training data: Use any policy (e.g. use the ϵ -greedy policy) to interact with the environment and get many trajectories(where each trajectory consists of the following elements $s_1, a_1, r_1, \dots, s_T, a_T, r_T$):

$$a_t = \begin{cases} \operatorname{argmax}_{a_t} Q(s_t, a_t; \theta^Q), & \text{with prob. } 1 - \epsilon \\ \text{randomly select from the action space } \mathbb{A}, & \text{with prob. } \epsilon. \end{cases} \quad (1.46)$$

Store the most recent 10^4 most recent (s, a, r, s_{t+1}) tuples in the replay buffer;

- 2 Update the parameters θ^Q :
 - 3 **repeat**
 - 4 Select one four-tuple from the replay buffer based on prioritized experience replay;
 - 5 TD target $\hat{y}_t = r_t + \gamma \max_{a_{t+1} \in \mathbb{A}} Q(s_{t+1}, a_{t+1}; \theta^Q)$;
 - 6 TD error $\delta_t = \hat{q}_t = Q(s_t, a_t, \zeta; \mu^Q, \sigma^Q) - \hat{y}_t$;
 - 7 $\theta^Q \leftarrow \theta^Q - \alpha \delta_t \cdot \nabla_{\theta^Q} Q(s_t, a_t; \theta^Q)$
 - 8 **until** θ^Q converges;
-

Disadvantages of DQN

The Deep Q Network has two problems: Overestimating and bootstrapping:

- Overestimating due to maximization : Wiithout detailed proofs, it could be shown that: Assume that x_1, \dots, x_d are d random real numbers. After

adding random noise with zero expectation, we could get random variables Z_1, \dots, Z_d , it can be proved that

$$\begin{cases} \mathbb{E}[\text{mean}(Z_1, Z_2, \dots, Z_d)] = \text{mean}(x_1, \dots, x_d) \\ \mathbb{E}[\max(Z_1, Z_2, \dots, Z_d)] \geq \max(x_1, \dots, x_d) \end{cases} \quad (1.47)$$

Which means that the random noise will not affect the expectation value, but will increase the maximization value.

Look back at the Deep Q Network (DQN) $q(s, a; \theta^Q)$. Assume for all actions $a \in \mathbb{A}$ and states $s \in \mathbb{S}$, the output of DQN is the real value plus random noise with zero expectation ϵ

$$q(s, a; \theta^Q) = Q(s, a) + \epsilon \quad (1.48)$$

So obviously, $q(s, a; \theta^Q)$ is the unbiased estimation of $Q(s, a)$, and the following inequality holds:

$$\mathbb{E}_\epsilon \left[\max_{a \in \mathbb{A}} q(s, a; \theta^Q) \right] \geq \max_{a \in \mathbb{A}} Q(s, a) \quad (1.49)$$

Recall that our TD target is $\hat{y}_t = r_t + \gamma \cdot \max_{a_{t+1} \in \mathbb{A}} q(s_{t+1}, a_{t+1}; \theta^Q)$. And Temporal difference algorithm encourages the estimation $q(s_t, a_t; \theta^Q)$ to come close to the TD target. That is why the estimation $q(s, a; \theta^Q)$ would overestimate the true value $Q(s, a)$.

- Bootstrapping: bootstrapping means the problem when we evaluate ourselves based on our value. For the Temporal Difference algorithm, the overestimating at time step $t + 1$ will propagate to the time step t .

Improve the training algorithm

To overcome the above overestimating problem of Temporal Difference Training algorithm, we could use another target network or double Q learning Review that for the basic Q learning algorithm: the TD target is calculated as

$$\hat{y}_t = r_t + \gamma \max_{a_{t+1} \in \mathbb{A}} q(s_{t+1}, a_{t+1}; \theta^Q) = r_t + \gamma q \left(s_{t+1}, \underset{a_{t+1} \in \mathbb{A}}{\text{argmax}} q(s_{t+1}, a_{t+1}; \theta^Q); \theta^Q \right) \quad (1.50)$$

- Q-learning with target network could alleviate bootstrapping TD target is

$$\hat{y}_t = r_t + \gamma q \left(s_{t+1}, \underset{a_{t+1} \in \mathbb{A}}{\text{argmax}} q(s_{t+1}, a_{t+1}; \theta^{Q-}); \theta^{Q-} \right) \quad (1.51)$$

- Double Q-learning: could alleviate bootstrapping and overestimating TD target is

$$\hat{y}_t = r_t + \gamma q \left(s_{t+1}, \underset{a_{t+1} \in \mathbb{A}}{\operatorname{argmax}} q(s_{t+1}, a_{t+1}; \theta^Q); \theta^{Q-} \right) \quad (1.52)$$

Improved the Neural Network Architecture

Now we will focus on the techniques to improve the architecture design and the training algorithm is kept the same as the previous DQN:

- Dueling Network: Divide the state-action value to the state value and the advantage function shown in Figure 1.3:

$$Q(s_t, a_t) = V(s_t) + D(s_t, a_t) \quad (1.53)$$

To assure the uniqueness, the dueling network is designed as

$$Q(s_t, a_t; \theta^Q) \stackrel{\text{def}}{=} V(s_t; \theta^V) + V(s_t, a_t; \theta^D) - \max_{a_t \in \mathbb{A}} D(s_t, a_t; \theta^D) \quad (1.54)$$

or

$$Q(s_t, a_t; \theta^Q) \stackrel{\text{def}}{=} V(s_t; \theta^V) + V(s_t, a_t; \theta^D) - \text{mean}_{a_t \in \mathbb{A}} D(s_t, a_t; \theta^D) \quad (1.55)$$

And $\theta^Q = (\theta^D, \theta^V)$

- Noisy net: Replace the parameters of the Neural Network with the mean and standard deviation

$$\theta = \mu + \sigma \odot \zeta, \quad (1.56)$$

where \odot is the element-wise product, ζ is random noise following standard normal distribution $\mathcal{N}(0, 1)$; μ and σ are parameters to be learned. Thus the parameters of noisy network is doubled. The adding noise will contribute to the exploration and robustness of the result. Based on the previous algorithm of DQN 1, the modifications are the following:

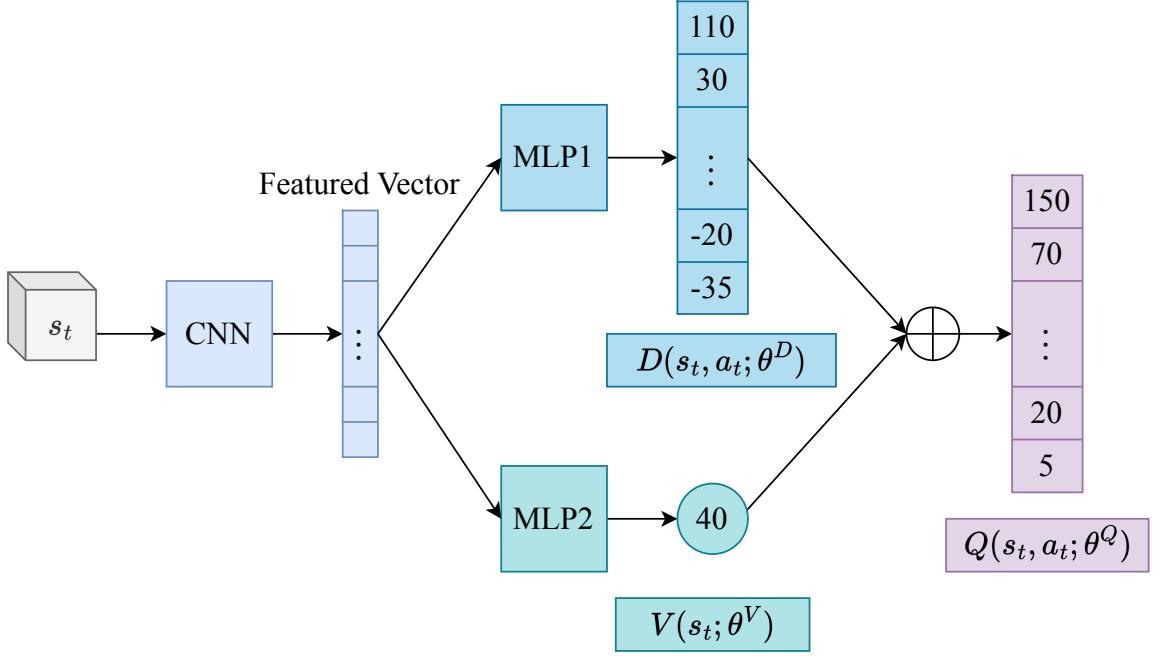


Figure 1.3: Dueling Network architecture

Algorithm 2: Deep Q Network(DQN) with Noisy Net Training

Input: The decision process model MDP $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$, or POMDP $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{r}, \mathbf{O}, \gamma\}$

Output: The optimal state-action value function $Q(s, a)$

- 1 Collect the training data: Use any policy (e.g. here we can directly use the noisy DQN) to interact with the environment and get many trajectories(where each trajectory consists of the following elements $s_1, a_1, r_1, \dots, s_T, a_T, r_T$):

$$a_t = \underset{a_t}{\operatorname{argmax}} Q(s_t, a_t, \zeta; \mu^Q, \sigma^Q) \quad (1.57)$$

Store the most recent 10^4 most recent (s, a, r, s_{t+1}) tuples in the replay buffer;

- 2 Update the parameters μ^Q, σ^Q :
 - 3 **repeat**
 - 4 Select one four-tuple from the replay buffer based on prioritized experience replay;
 - 5 TD target $\hat{y}_t = r_t + \gamma \max_{a_{t+1} \in \mathbb{A}} Q(s_{t+1}, a_{t+1}, \zeta; \mu^Q, \sigma^Q)$;
 - 6 TD error $\delta_t = Q(s_t, a_t, \zeta; \mu^Q, \sigma^Q) - \hat{y}_t$;
 - 7
$$\begin{cases} \mu^Q & \leftarrow \mu^Q - \alpha_\mu \delta_t \nabla_{\mu^Q} Q(s_t, a_t, \zeta; \mu^Q, \sigma^Q) \\ \sigma^Q & \leftarrow \sigma^Q - \alpha_\sigma \delta_t \nabla_{\sigma^Q} Q(s_t, a_t, \zeta; \mu^Q, \sigma^Q) \end{cases} \quad (1.58)$$
 - 8 **until** θ^Q converges;
-

After training, we will use the trained network to make decisions. At this stage, no noise is necessary and the noisy network becomes standard DQN

$$Q(s, a, \zeta; \mu^Q, \sigma^Q = 0) = Q(s, a; \mu^Q) \quad (1.59)$$

1.2.2 Deep Policy Gradients

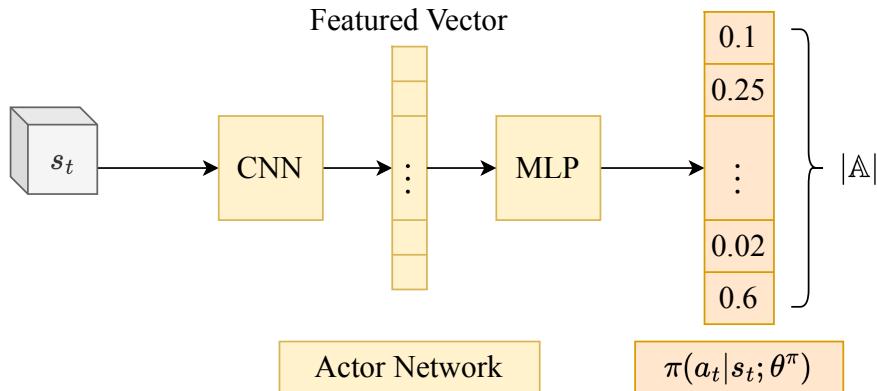


Figure 1.4: NN approximates $\pi(a_t|s_t)$

Commonly used policy gradients algorithms are REINFORCE and Actor Critic. Actor-Critic method shown in the Figure 1.5 and its advanced version like Advantage Actor-Critic (A2C). When it comes to multi-agent actor critic training algorithm, the so-called Asynchronous Advantage Actor-Critic (A3C) is used very often.

Actor-Critic Algorithm

Here is the basic training process of Actor-Critic is the following:

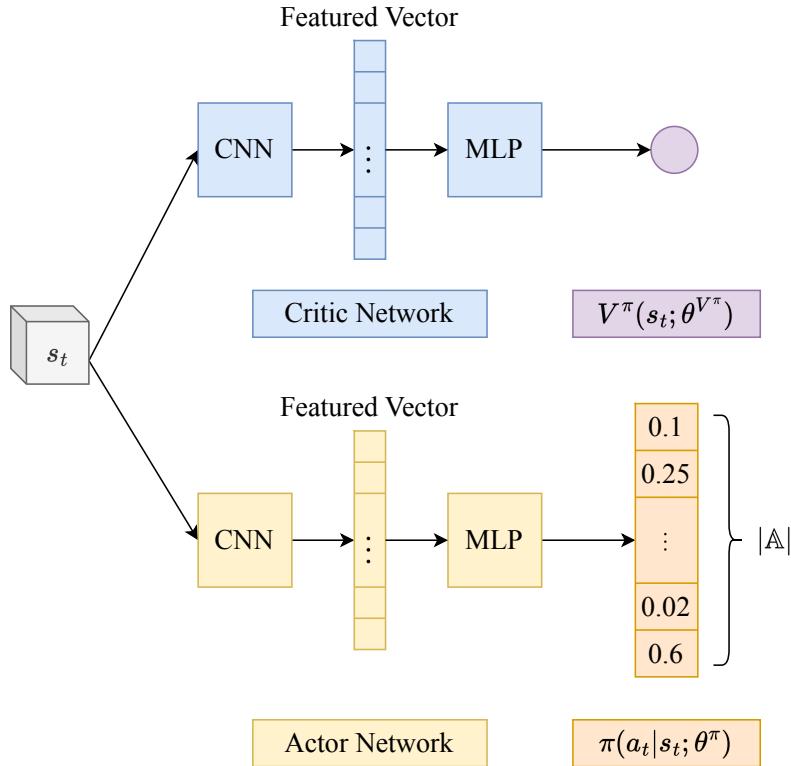


Figure 1.5: Actor Critic Neural Network architecture

Algorithm 3: Actor-Critic(AC)

Input: The decision process model MDP $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$, or POMDP $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{r}, \mathbf{O}, \gamma\}$

Output: The optimal state-action-policy value function $Q^\pi(s, a)$ and the policy function $\pi(a|s)$

- 1 Initialize the policy network and the value network randomly as $\pi(s, a; \theta^\pi)$ and $q(s, a; \theta^{Q^\pi})$; **repeat**
- 2 Take action according to policy network $a_t = \pi(\cdot|s_t; \theta^\pi)$ and perform action a_t ;
- 3 Observe the reward $r_t = r(s_t, a_t)$ and the new state s_{t+1} from the environment;
- 4 Take action according to policy network $\tilde{a}_{t+1} = \pi(\cdot|s_{t+1}; \theta^\pi)$ but not perform action \tilde{a}_{t+1} ;
- 5 Use the value network to evaluate the two time steps:

$$\begin{cases} \hat{q}_t &= q(s_t, a_t; \theta^{Q^\pi}) \\ \hat{q}_{t+1} &= q(s_{t+1}, \tilde{a}_{t+1}; \theta^{Q^\pi}) \end{cases} \quad (1.60)$$

- 6 Calculate TD target and TD error

$$\begin{cases} \hat{y}_t &= r_t + \gamma \hat{q}_{t+1} \\ \delta_t &= \hat{q}_t - \hat{y}_t \end{cases} \quad (1.61)$$

- 7 Update the parameters

To alleviate the bootstrapping problem of time difference algorithm, we can also introduce a target value network separately to calculate TD target $q(s, a; \theta^{Q^{\pi-}})$, then the Actor Critic C algorithm 3 becomes:

Algorithm 4: Actor-Critic(AC) with target network

Input: The decision process model MDP $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$, or POMDP $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{r}, \mathbf{O}, \gamma\}$

Output: The optimal state-action-policy value function $Q^\pi(s, a)$ and the policy function $\pi(a|s)$

- 1 Initialize the policy network and the value network randomly as $\pi(s, a; \theta^\pi)$ $q(s, a; \theta^{Q^\pi})$, and the target value network $q(s, a; \theta^{Q^{\pi-}})$;

2 repeat

- 3 Take action according to policy network $a_t = \pi(\cdot|s_t; \theta^\pi)$ and perform action a_t ;
- 4 Observe the reward $r_t = r(s_t, a_t)$ and the new state s_{t+1} from the environment;
- 5 Take action according to policy network $\tilde{a}_{t+1} = \pi(\cdot|s_{t+1}; \theta^\pi)$ but not perform action \tilde{a}_{t+1} ;
- 6 Use the value network to evaluate the two time steps:

$$\begin{cases} \hat{q}_t &= q(s_t, a_t; \theta^{Q^\pi}) \\ \hat{q}_{t+1} &= q(s_{t+1}, \tilde{a}_{t+1}; \theta^{Q^{\pi-}}) \end{cases} \quad (1.63)$$

- 7 Calculate TD target and TD error

$$\begin{cases} \hat{y}_t &= r_t + \gamma \hat{q}_{t+1} \\ \delta_t &= \hat{q}_t - \hat{y}_t \end{cases} \quad (1.64)$$

- 8 Update the parameters

$$\begin{cases} \theta^\pi &\leftarrow \theta^\pi - \beta \cdot \hat{q}_t \cdot \nabla_{\theta^\pi} \ln \pi(a_t|s_t; \theta^\pi) \\ \theta^{Q^\pi} &\leftarrow \theta^{Q^\pi} - \alpha \cdot \delta_t \cdot \nabla_{\theta^Q} Q(s_t, a_t; \theta^{Q^\pi}) \\ \theta^{Q^{\pi-}} &\leftarrow \tau \cdot \theta^{Q^\pi} + (1 - \tau) \theta^{Q^{\pi-}}, \end{cases} \quad (1.65)$$

where $\tau \in (0, 1)$

- 9 **until** $Q(s, a; \theta^{Q^\pi})$ and $\pi(a|s; \theta^\pi)$ converges;
-

Advantage Actor-Critic (A2C) Algorithm

Algorithm 5: Advantage Actor-Critic(A2C) with target network

Input: The decision process model MDP $\{\mathbb{S}, \mathbb{A}, \mathbf{T}, \mathbf{r}, \gamma\}$, or POMDP $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{r}, \mathbf{O}, \gamma\}$

Output: The optimal state-action-policy value function $V^\pi(s, a)$ and the policy function $\pi(a|s)$

- 1 Initialize the policy network and the value network randomly as $\pi(s, a; \boldsymbol{\theta}^\pi)$ $v(s; \boldsymbol{\theta}^{V^\pi})$, and the target value network $v(s; \boldsymbol{\theta}^{V^\pi-})$;
- 2 **repeat**
- 3 Take action according to policy network $a_t = \pi(\cdot|s_t; \boldsymbol{\theta}^\pi)$ and perform action a_t ;
- 4 Observe the reward $r_t = r(s_t, a_t)$ and the new state s_{t+1} from the environment;
- 5 Take action according to policy network $\tilde{a}_{t+1} = \pi(\cdot|s_{t+1}; \boldsymbol{\theta}^\pi)$ but not perform action \tilde{a}_{t+1} ;
- 6 Use the value network to evaluate the two time steps:

$$\begin{cases} \hat{v}_t &= v(s_t, a_t; \boldsymbol{\theta}^{V^\pi}) \\ \hat{v}_{t+1} &= v(s_{t+1}, \tilde{a}_{t+1}; \boldsymbol{\theta}^{V^\pi-}) \end{cases} \quad (1.66)$$

- 7 Calculate TD target and TD error

$$\begin{cases} \hat{y}_t &= r_t + \gamma \hat{v}_{t+1} \\ \delta_t &= \hat{q}_t - \hat{y}_t \end{cases} \quad (1.67)$$

- 8 Update the parameters

$$\begin{cases} \boldsymbol{\theta}^{V^\pi} &\leftarrow \boldsymbol{\theta}^{V^\pi} - \alpha \cdot \delta_t \cdot \nabla_{\boldsymbol{\theta}^{V^\pi}} v(s_t; \boldsymbol{\theta}^{V^\pi}) \\ \boldsymbol{\theta}^\pi &\leftarrow \boldsymbol{\theta}^\pi - \beta \cdot \delta_t \cdot \nabla_{\boldsymbol{\theta}^\pi} \ln \pi(a_t|s_t; \boldsymbol{\theta}^\pi) \\ \boldsymbol{\theta}^{V^\pi-} &\leftarrow \tau \cdot \boldsymbol{\theta}^{V^\pi} + (1 - \tau) \boldsymbol{\theta}^{V^\pi-}, \end{cases} \quad (1.68)$$

where $\tau \in (0, 1)$

- 9 **until** $Q(s, a; \boldsymbol{\theta}^Q)$ and $\pi(a|s; \boldsymbol{\theta}^\pi)$ converges;
-

Asynchronous Advantage Actor Critic (A3C) Algorithm

A3C is the parallel computing based on A2C. Parallel gradient descent

1.2.3 Multi-agent Actor Critic(MAC)

When there are multiple agents in the environment e.g. there are m components in the system and n control units, the system state is determined by components state $s_t = \{s_t^j\}_{j=1}^m$. And the final action is also a combination of all control units $a_t = \{a_t^i\}_{i=1}^n$.

Depends on the relationship of all components, there are typically four assumptions: fully cooperative mode, fully competitive mode, mixed cooperative & competitive and self-interested.

Fully cooperative mode

In fully cooperative assumption, the reward , return, value are the same for all agents. All agent uses one same value network

Deep Centralized Multi-agent Actor Critic (DCMAC)

Deep Centralized Multi-agent Actor Critic Architecture [andriotis2019managing] is shown in Figure 1.6:

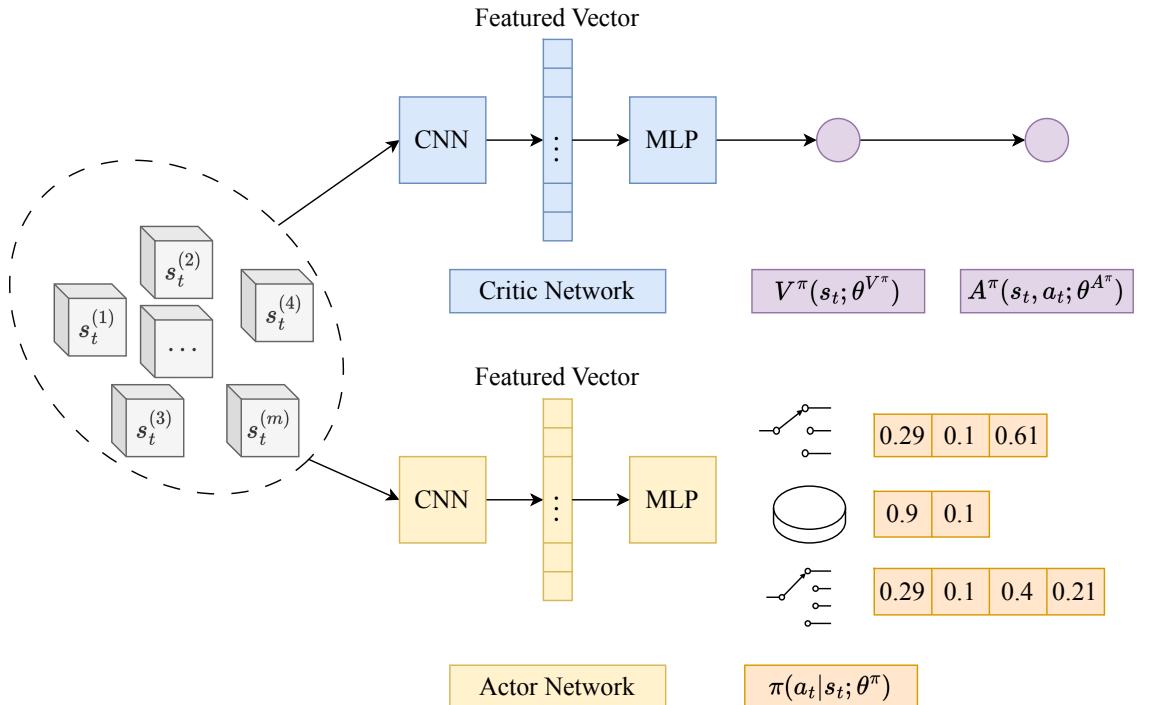


Figure 1.6: Deep Centralized Multi-agent Actor Critic Neural Network architecture

Deep Decentralized Multi-agent Actor Critic (DDMAC)

Deep Decentralized Multi-agent Actor Critic Architecture [andriotis2021deep] is shown in Figure 1.7:

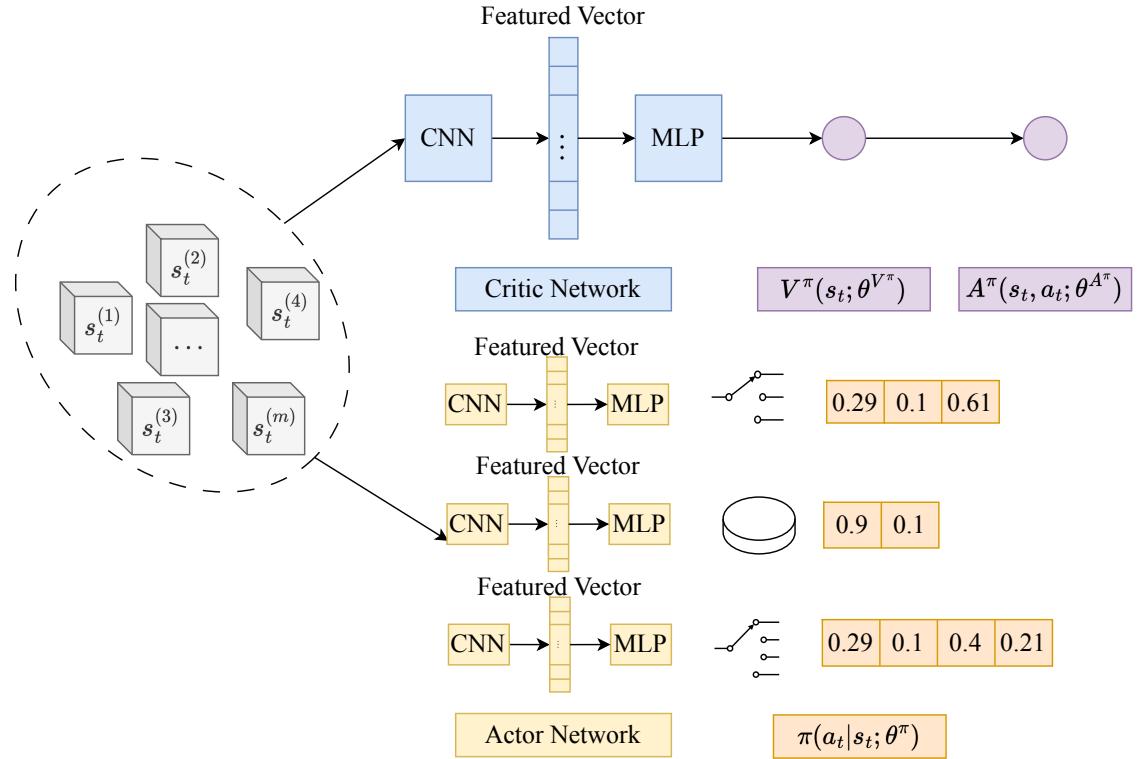


Figure 1.7: Deep Decentralized Multi-agent Actor Critic Neural Network architecture

Hierarchical Resource Allocation and Continuous-control Reinforcement Learning

Hierarchical Resource Allocation and continuous-control reinforcement learning [andriotis2023struct]

1.3 Partially Observable Markov Decision Process

1.3.1 Basic Formulation and terminology

Based on the Markov Decision Process (MDP), the Partially Observable MDP can not fully observe the state, but instead, obtain some observation of the state. Thus we need to add observation space \mathbb{O} and observation model $P(o_t|s_t, a_{t-1})$ in the original MDP. It can be written a 7-tuple $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{R}, \mathbf{O}, \gamma\}$. The sequential Probabilistic Graphical Model of POMDP is shown in Figure 1.8. The shaded round node denoting the state variable is not directly observable, but a hidden variable.

A Markov Decision Process shows the markovian property, where the next state s_{t+1} can be predicted just based on the current state s_t and action a_t , regardless of the whole past history $s_{0:t}, a_{0:t}$ ¹. In other words, s_t, a_t already contains all the information needed to predict the next state s_{t+1} .

But for Partially observable MDP, just the current observation o_t and the current action a_t could not provide all of the necessary information needed to make decisions. e.g. the Tiger problem, we could not confidently choose the side when hearing the sound once behind another door. The whole history $o_{0:t}$ are necessary for making decisions.

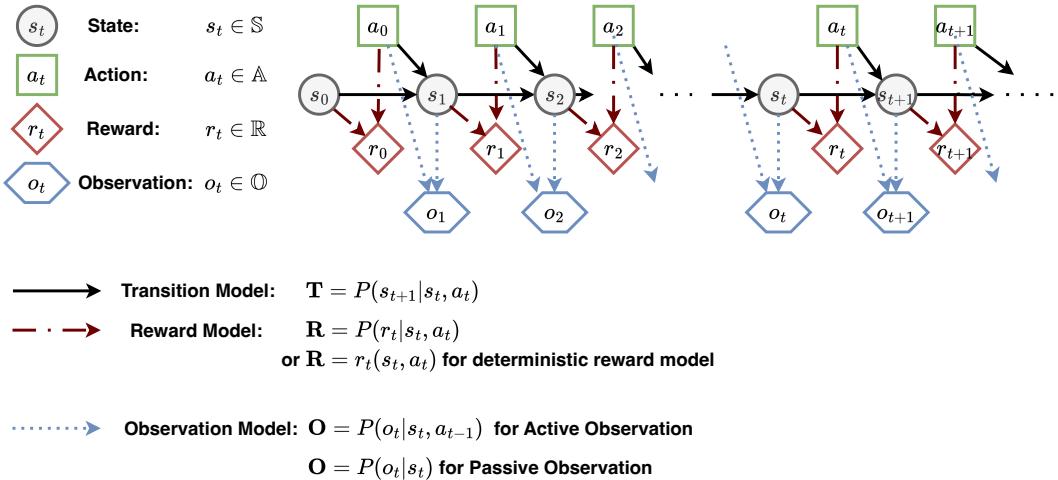


Figure 1.8: Probabilistic Graphical Model of Partially Observable Markovian Decision Process defined in State Space

¹ $s_{0:t}$ is a short notation of s_0, s_1, \dots, s_t and $a_{0:t}$ a short notation of a_0, a_1, \dots, a_t

Belief Space \mathbb{B}

To implement those methods for solving MDP in solving POMDP, we can introduce the belief of the state variable, which is the probability distribution over the whole state space. to transfer the POMDP as a belief-MDP.

$$\mathbf{b}_t(s) \stackrel{\text{def}}{=} P(S_t = s | o_{1:t}, a_{0:t-1}) \quad (1.69)$$

$\mathbf{b}_t \in \mathbb{B}$ is the our believed-distrubution of all possible state variables based on all history observations and actions until time t . The dimension of the belief state space is dependent on the original state space \mathbb{S} .

- For discrete state space, the belief \mathbf{b} is the Probability Mass Function (PMF). If the discrete state has N possible values, then the belief state \mathbf{b}_t is a point in the $(N - 1)$ -simplex Δ^{N-1} . The definition of a simplex is

$$\Delta^{N-1} = \left\{ (p_1, p_2, \dots, p_N) \in \mathbb{R}^N \middle| p_i > 0 \forall i \text{ and } \sum_{i=1}^N p_i = 1 \right\} \quad (1.70)$$

- if $N = 2$, where the original state space is a 2D space, the belief state \mathbf{b}_t is a point on a line between $(1, 0)$ and $(0, 1)$, e.g. $\mathbf{b}_t = (0.4, 0.6)$;
- if $N = 3$, where the original state space is a 3D space, the belief state \mathbf{b}_t is a point on a triangle between $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$, e.g. $\mathbf{b}_t = (0.3, 0.2, 0.5)$
- For continuous state space, the belief \mathbf{b} is the Probability Density Function (PDF). If there are more than one chosen state variables are continuous, the belief of those states are also the joint PDF. In real life application, Under some assumptions, if we could parameterize the PDF, then the number of parameters determine the dimension of the belief space.

- If we assume the Multi-gaussian Distribution for these d_S continuous state variables, for every continuous state variables, we have the mean and standard deviation to describe them. Considering also the correlation between those variables. The total number of parameters is calculated as:

$$d_B = d_S + \frac{d_S(d_S + 1)}{2} \quad (1.71)$$

- If we assuem the Gaussian Mixture Distribution for these d_S continuous state variables, the number of parameters is calculated as

$$d_B = K(d_S + \frac{d_S(d_S + 1)}{2} + 1) - 1 \quad (1.72)$$

\mathbf{b}_t contains the probability of the whole state space.

Belief Update Rule

When we connecting with the Bayesian updating, the belief \mathbf{b}_t is actually the posterior distribution.

The belief \mathbf{b}_t is our current guess of the state distributions based on the information we have until time t , it is not stationary, and it will update dynamically when we perform new actions a_t and the new observation o_{t+1} . If we have performed action a_t and obtained the new observation o_{t+1} , how to update our belief \mathbf{b}_{t+1} ?

$$b_{t+1}(s_{t+1}) \stackrel{\text{def}}{=} P(S_{t+1} = s_{t+1} | o_{t+1}, a_t, b_t) = \frac{P(O_{t+1} = o_{t+1} | s_{t+1}, a_t, b_t)P(S_{t+1} = s_{t+1} | a_t, b_t)}{P(O_{t+1} = o_{t+1} | a_t, b_t)} \quad (1.73)$$

where

- $P(O_{t+1} = o_{t+1} | s_{t+1}, a_t, b_t) = P(O_{t+1} = o_{t+1} | s_{t+1}, a_t)$, which is the observation model defined in POMDP
- $P(S_{t+1} = s_{t+1} | a_t, b_t) = \int_{s_t \in \mathbb{S}} P(S_{t+1} = s_{t+1} | s_t, a_t) b_t(s_t) ds_t$
- $P(O_{t+1} = o_{t+1} | a_t, b_t) = \int_{s_{t+1} \in \mathbb{S}} P(O_{t+1} = o_{t+1} | s_{t+1}, a_t) \int_{s_t \in \mathbb{S}} P(S_{t+1} = s_{t+1} | s_t, a_t) b_t(s_t) ds_t ds_{t+1}$

Then the simplified Belief Update equation becomes

$$b_{t+1}(s_{t+1}) \stackrel{\text{def}}{=} P(s_{t+1} | o_{t+1}, a_t, b_t) = \frac{P(o_{t+1} | s_{t+1}, a_t)P(s_{t+1} | a_t, b_t)}{P(o_{t+1} | a_t, b_t)} \quad (1.74)$$

As in the real case, multi-dimensional integral are difficult to calculate. We will use the sequential Monte Carlo Simulation to update the belief (the posterior distribution) at each time step.

Use the particle filtering method to approximate the quantity of interest like value function, State action value function etc.

Belief-MDP

After introducing the belief, the POMDP becomes the Belief-MDP shown in Figure 1.9, since the next belief state \mathbf{b}_{t+1} is only dependent on the current belief state \mathbf{b}_t and current action a_t . The belief state transition model can be derived from the above belief update formula:

$$P(\mathbf{b}_{t+1} | \mathbf{b}_t, a_t) = \int_{o_{t+1} \in \mathcal{O}} P(\mathbf{b}_{t+1} | \mathbf{b}_t, a_t, o_{t+1}) P(o_{t+1} | \mathbf{b}_t, a_t) do_{t+1} \quad (1.75)$$

$$P(b_{t+1}|b_t, a_t) = \sum_{o_{t+1} \in \mathcal{O}} P(b_{t+1}|b_t, a_t, o_{t+1}) P(o_{t+1}|b_t, a_t) \quad (1.76)$$

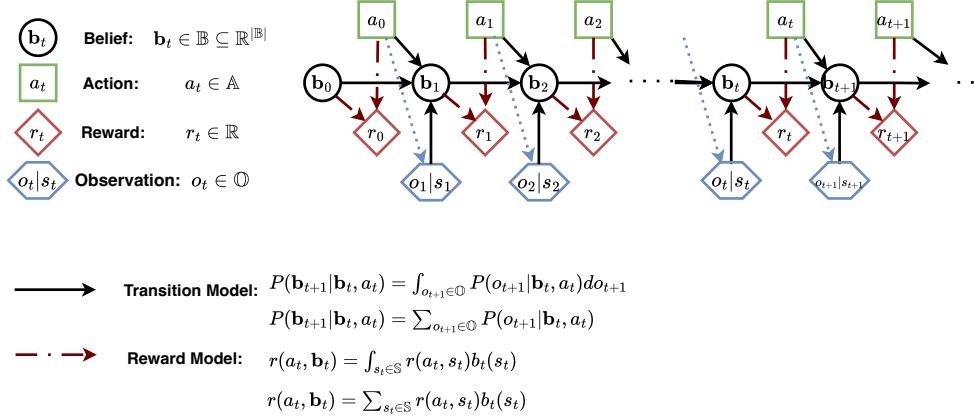


Figure 1.9: Probabilistic Graphical Model of Partially Observable Markovian Decision Process defined in Belief Space

Observation Model of Belief-MDP $P(o_{t+1}|b_t, a_t)$

- For continuous State space

$$P(o_{t+1}|b_t, a_t) = \int_{s_{t+1} \in \mathbb{S}} P(o_{t+1}|s_{t+1}, a_t) \int_{s_t \in \mathbb{S}} P(s_{t+1}|s_t, a_t) b_t(s_t) ds_t ds_{t+1} \quad (1.77)$$

- For discrete State space

$$P(o_{t+1}|b_t, a_t) = \sum_{s_{t+1} \in \mathbb{S}} P(o_{t+1}|s_{t+1}, a_t) \sum_{s_t \in \mathbb{S}} P(s_{t+1}|s_t, a_t) b_t(s_t) \quad (1.78)$$

State Transition Model of Belief-MDP T_{belief}

- For continuous Observation space

$$P(b_{t+1}|b_t, a_t) = \int_{o_{t+1} \in \mathcal{O}} P(b_{t+1}|b_t, a_t, o_{t+1}) P(o_{t+1}|b_t, a_t) do_{t+1} = \int_{o_{t+1} \in \mathcal{O}} P(o_{t+1}|b_t, a_t) do_{t+1} \quad (1.79)$$

- For discrete Observation space

$$P(b_{t+1}|b_t, a_t) = \sum_{o_{t+1} \in \mathcal{O}} P(b_{t+1}|b_t, a_t, o_{t+1}) P(o_{t+1}|b_t, a_t) = \sum_{o_{t+1} \in \mathcal{O}} P(o_{t+1}|b_t, a_t) \quad (1.80)$$

Reward Model of Belief-MDP $\mathbf{R}_{\text{belief}}$

If we consider deterministic reward model, $\mathbf{R}_{\text{belief}} = P(r_{t+1}|a_t, b_t)$ can be written as $\mathbf{R}_{\text{belief}} = r_{\text{belief}}(a_t, b_t)$

- For continuous Observation space

$$r_{\text{belief}}(a_t, b_t) = \int_{s_t \in \mathbb{S}} r(a_t, s_t) b_t(s_t) \quad (1.81)$$

- For discrete Observation space

$$r_{\text{belief}}(a_t, b_t) = \sum_{s_t \in \mathbb{S}} r(a_t, s_t) b_t(s_t) \quad (1.82)$$

The cumulative weighted total return $U^\pi(b_t, a_t, \dots, b_T, a_T)$

The cumulative weighted total reward is now a function of all the belief states and actions from time t when taking a policy π :

$$U_t^\pi = U^\pi(b_t, a_t, \dots, b_T, a_T) = \sum_{i=t}^T \gamma^{i-t} r_{\text{belief}}(a_i, b_i) \quad (1.83)$$

where the discount factor $\gamma \in [0, 1]$: weighting the relative importance of the current reward against the future reward. In extreme cases when $\gamma = 0$, means only the current reward matters.

The State-Action Value Function $Q^\pi(b_t, a_t)$

The State-Action value function $Q^\pi(b_t, a_t)$ describes the value of the policy π given a State-Action Pair $Q^\pi(b_t, a_t)$. It is a measure of the State-Action pair at time step t and the policy π from time step $t + 1$. That is why we need to reduce all the randomness from all the future state and future action.

The value of taking an action a_t at the state b_t and using the strategy π for the rest of time span until T is calculated by the expectation of all the state and actions from time t to T .

$$Q^\pi(b_t, a_t) = \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}, A_{i>t} \sim \pi} [U^\pi(b_t, a_t, B_{t+1}, A_{t+1}, \dots, B_T, A_T) | b_t, a_t] \quad (1.84)$$

where $T_{\text{belief}} = P(b_t | b_{t-1}, a_{t-1})$ is the transition probability distribution of state b_t and π is the probability of action (aka. the stochastic policy).

The State Value Function $V^\pi(\mathbf{b}_t)$

The State Value Function $V^\pi(\mathbf{b}_t)$ is a measure of the value of current state \mathbf{b}_t and that is why we need to further eliminate the randomness of action at time A_t .

The value of a state \mathbf{b}_t when taking a policy from this time step t until the rest of the time span can be expressed by the expected total return, mathematically written as:

$$V^\pi(\mathbf{b}_t) = \mathbb{E}_{A_t \sim \mu} [Q^\pi(\mathbf{b}_t, A_t)] \quad (1.85a)$$

$$= \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}, A_{i>t} \sim \pi, A_t \sim \mu} [U^\pi(\mathbf{b}_t, A_t, \dots, \mathbf{b}_T, A_T) | \mathbf{b}_t, a_t] \quad (1.85b)$$

$$= \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}, A_{i>t} \sim \pi} [U^\pi(\mathbf{b}_t, a_t, \dots, \mathbf{b}_T, A_T)] \quad (1.85c)$$

$$= \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}, A_{i>t} \sim \pi} \left[\sum_{i=t}^T \gamma^{i-t} r_{\text{belief}}(a_i, b_i) \middle| \mathbf{b}_t \right], \quad (1.85d)$$

where μ shows the probability distribution of a_t at time t specifically, which is not necessarily equal to the policy π chosen to taken actions from time $t+1$ on.

The Optimal State Action Value Function $Q^*(\mathbf{b}_t, a_t)$

The Optimal State Action Value function $Q^*(\mathbf{b}_t, a_t)$ is a measure of values of the current state-action pair \mathbf{b}_t . Based on the State Action Value function $Q^\pi(\mathbf{b}_t, a_t)$ we need to further eliminate the randomness of the policy π :

$$Q^*(\mathbf{b}_t, a_t) = \max_{\pi} \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}} \left[\sum_{i=t}^T \gamma^{i-t} r_{\text{belief}}(a_i, b_i) \middle| \mathbf{b}_t, a_t \right] \quad (1.86)$$

The Optimal State Value Function $V^*(\mathbf{b}_t)$

The Optimal State Value function $V^*(\mathbf{b}_t)$ is a measure of values of the current state \mathbf{b}_t only. Based on the State Value function $V^\pi(\mathbf{b}_t)$ we need to further eliminate the randomness of the policy π :

$$V^*(\mathbf{b}_t) = \max_{\pi} \mathbb{E}_{B_{i>t} \sim T_{\text{belief}}} \left[\sum_{i=t}^T \gamma^{i-t} r_{\text{belief}}(a_i, b_i) \middle| \mathbf{b}_t \right] \quad (1.87)$$

The Optimal State Action Value Function $V^*(\mathbf{b}_t)$

Bellman Equation for Optimal State Value Function $V^*(\mathbf{b}_t)$ is also known as Optimal Bellman Equation.

Under standard conditions for discounted MDPs, out of all possible policies there exists at least one deterministic policy that is optimal, maximizing the value

of state $V^\pi(\mathbf{b}_t)$. For a deterministic policy, with a given transition probability $P(\mathbf{b}_{t+1}|\mathbf{b}_t, \mathbf{a}_t)$, the optimal state-action value function is denoted as $Q^*(\mathbf{b}_t, \mathbf{a}_t)$ and the optimal state value function is denoted as $V^*(\mathbf{b}_t)$.

The optimal Bellman equation of the state value function is

$$V^*(\mathbf{b}_t) = \max_{\mathbf{a}_t \in \mathbb{A}} Q^*(\mathbf{b}_t, \mathbf{a}_t) \quad (1.88a)$$

$$= \max_{\mathbf{a}_t \in \mathbb{A}} \mathbb{E}_{\mathbf{B}_{t+1} \sim T_{\text{belief}}} (r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t, \mathbf{B}_{t+1}) + \gamma V^*(\mathbf{b}_{t+1})) \quad (1.88b)$$

$$= \max_{\mathbf{a}_t \in \mathbb{A}} \int_{\mathbf{b}_{t+1} \in \mathbb{B}} P(\mathbf{b}_{t+1}|\mathbf{b}_t, \mathbf{a}_t) (r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t, \mathbf{B}_{t+1}) + \gamma V^*(\mathbf{b}_{t+1})) d\mathbf{b}_{t+1} \quad (1.88c)$$

with the simplification of $r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t, \mathbf{b}_{t+1}) = r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t)$, we can write the above optimal Bellman equation as

$$V^*(\mathbf{b}_t) = \max_{\mathbf{a}_t \in \mathbb{A}} \{r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t) + \gamma \mathbb{E}_{\mathbf{B}_{t+1} \sim T_{\text{belief}}} [V^*(\mathbf{b}_{t+1})]\} \quad (1.89a)$$

$$= \max_{\mathbf{a}_t \in \mathbb{A}} \left\{ r_{\text{belief}}(\mathbf{b}_t, \mathbf{a}_t) + \gamma \int_{\mathbf{b}_{t+1} \in \mathbb{B}} P(\mathbf{b}_{t+1}|\mathbf{b}_t, \mathbf{a}_t) V^*(\mathbf{b}_{t+1}) d\mathbf{b}_{t+1} \right\} \quad (1.89b)$$

$$= \max_{\mathbf{a}_t \in \mathbb{A}} \left\{ \sum_{s_t \in \mathbb{S}} r(a_t, s_t) b_t(s_t) + \gamma \sum_{o_{t+1} \in \mathbb{O}} P(o_{t+1}|\mathbf{b}_t, \mathbf{a}_t) V^*(\mathbf{b}_{t+1}) \right\} \quad (1.89c)$$

The optimal state-value function is defined over the continuous space of the belief simplex \mathbb{B} , which essentially consists of an infinite number of beliefs. However, it has been proven that the optimal value function is piece-wise linear and convex, and can thus be described by a finite number of affine hyperplanes. This important result reduces the decision problem to determining a finite set of vectors, also known as the $\hat{\alpha}$ -vectors:

$$V^*(\mathbf{b}) = \max_{\hat{\alpha} \in \Gamma} \sum_{s \in \mathbb{S}} b(s) \hat{\alpha}(s), \quad (1.90)$$

where Γ is the set comprising all α -vectors. After substituting the Eq. 1.90 for $V^*(\mathbf{b}_{t+1})$ into Eq. 1.89, we could get:

$$V^*(\mathbf{b}_t) = \max_{\mathbf{a}_t \in \mathbb{A}} \left[\sum_{s_t \in \mathbb{S}} b_t(s_t) r(a_t, s_t) + \gamma \sum_{o_{t+1} \in \mathbb{O}} P(o_{t+1}|\mathbf{b}_t, \mathbf{a}_t) \max_{\hat{\alpha} \in \Gamma} \sum_{s_{t+1} \in \mathbb{S}} b_{t+1}(s_{t+1}) \hat{\alpha}(s_{t+1}) \right] \quad (1.91)$$

Considering the belief update formular in Eq. 1.73 $b_{t+1}(s_{t+1}) \stackrel{\text{def}}{=} P(s_{t+1}|o_{t+1}, a_t, b_t) = \frac{P(o_{t+1}|s_{t+1}, a_t)P(s_{t+1}|a_t, b_t)}{P(o_{t+1}|a_t, b_t)}$

$$V^*(b_t) = \max_{a_t \in A} \left[\sum_{s_t \in S} b_t(s_t) r(a_t, s_t) + \gamma \sum_{o_{t+1} \in O} P(o_{t+1}|b_t, a_t) \max_{\hat{a} \in \Gamma} \sum_{s_{t+1} \in S} \frac{P(o_{t+1}|s_{t+1}, a_t)P(s_{t+1}|a_t, b_t)}{P(o_{t+1}|a_t, b_t)} \right] \quad (1.92)$$

After rearanging the terms, we could get

$$V^*(b_t) = \max_{a_t \in A} \left[\sum_{s_t \in S} b_t(s_t) r(a_t, s_t) + \gamma \sum_{o_{t+1} \in O} \max_{\hat{a} \in \Gamma} \sum_{s_{t+1} \in S} P(o_{t+1}|s_{t+1}, a_t)P(s_{t+1}|a_t, b_t)\hat{\alpha}(s_{t+1}) \right] \quad (1.93)$$

Since $P(s_{t+1}|a_t, b_t) = \sum_{s_t \in S} P(s_{t+1}|s_t, a_t)b_t(s_t)ds_t$ we could get

$$V^*(b_t) = \max_{a_t \in A} \left[\sum_{s_t \in S} b_t(s_t) r(a_t, s_t) + \gamma \sum_{o_{t+1} \in O} \max_{\hat{a} \in \Gamma} \sum_{s_{t+1} \in S} P(o_{t+1}|s_{t+1}, a_t) \sum_{s_t \in S} P(s_{t+1}|s_t, a_t)b_t(s_t)\hat{\alpha}(s_{t+1}) \right] \quad (1.94)$$

After arranging the sum order we could get

$$V^*(b_t) = \max_{a_t \in A} \left[\sum_{s_t \in S} b_t(s_t) r(a_t, s_t) + \gamma \sum_{o_{t+1} \in O} \max_{\hat{a} \in \Gamma} \sum_{s_t \in S} b_t(s_t) \sum_{s_{t+1} \in S} P(o_{t+1}|s_{t+1}, a_t)P(s_{t+1}|s_t, a_t)\hat{\alpha}(s_{t+1}) \right] \quad (1.95)$$

1.4 How solve a Partially Observable Markov Decision Process

Although have mentioned above, we will here emphasize the way to solve the Partially Observable Markov Decision Process based on the previous section about the Reinforcement Learning to solve the Markov Decision Process 1.2.

Partially Observable Markov Decision Process can be treated as the Belelif-MDP. Where the belief is actually the posterior distribution of the state Eq. 1.69.

All of the algorithm and neural network when solving MDP problem used to have the states as input. But here we will first use sequential Monte Carlo Simulation (particle filtering) to get the updated belief (which is actually a number of particles with its corresponding weights) as the input. Which means that, the figures 1.2 become now 1.10

Figure 1.3 becomes now figure 1.11

The theoretical foundations of this research are rooted in several key areas. [johnson2018foundations] provided a comprehensive overview of the fundamental principles.

1.5 Common Implementations

Traditional methods have primarily focused on...

Method	Accuracy	Complexity	Scalability
Method A	0.85	$O(n)$	High
Method B	0.92	$O(n^2)$	Medium
Method C	0.78	$O(n \log n)$	High

Table 1.3: Comparison of traditional methods

1.6 Recent Advances

Recent developments in the field have introduced novel approaches...

1.6.1 Machine Learning Techniques

Deep learning methods have shown remarkable performance in various applications [brown2021deeplearning]. The key architectures include:

- **Convolutional Neural Networks (CNNs):** Particularly effective for image processing...
- **Recurrent Neural Networks (RNNs):** Suitable for sequential data analysis...
- **Transformer Networks:** Revolutionized natural language processing...

1.7 Research Gaps

Despite the significant progress, several research gaps remain:

1. Limited studies addressing the scalability issues...

2. Inadequate consideration of real-world constraints...
3. Lack of comprehensive benchmarking across diverse datasets...

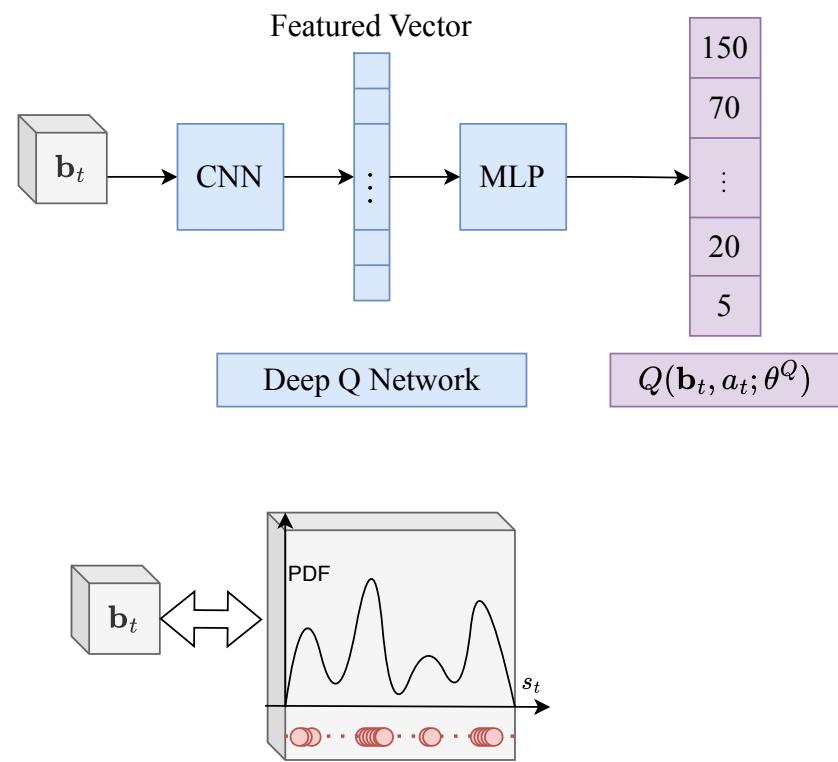


Figure 1.10: Deep Q-Network approximate the Q function for every available action using belief as input $Q(\mathbf{b}_t, a_t)$

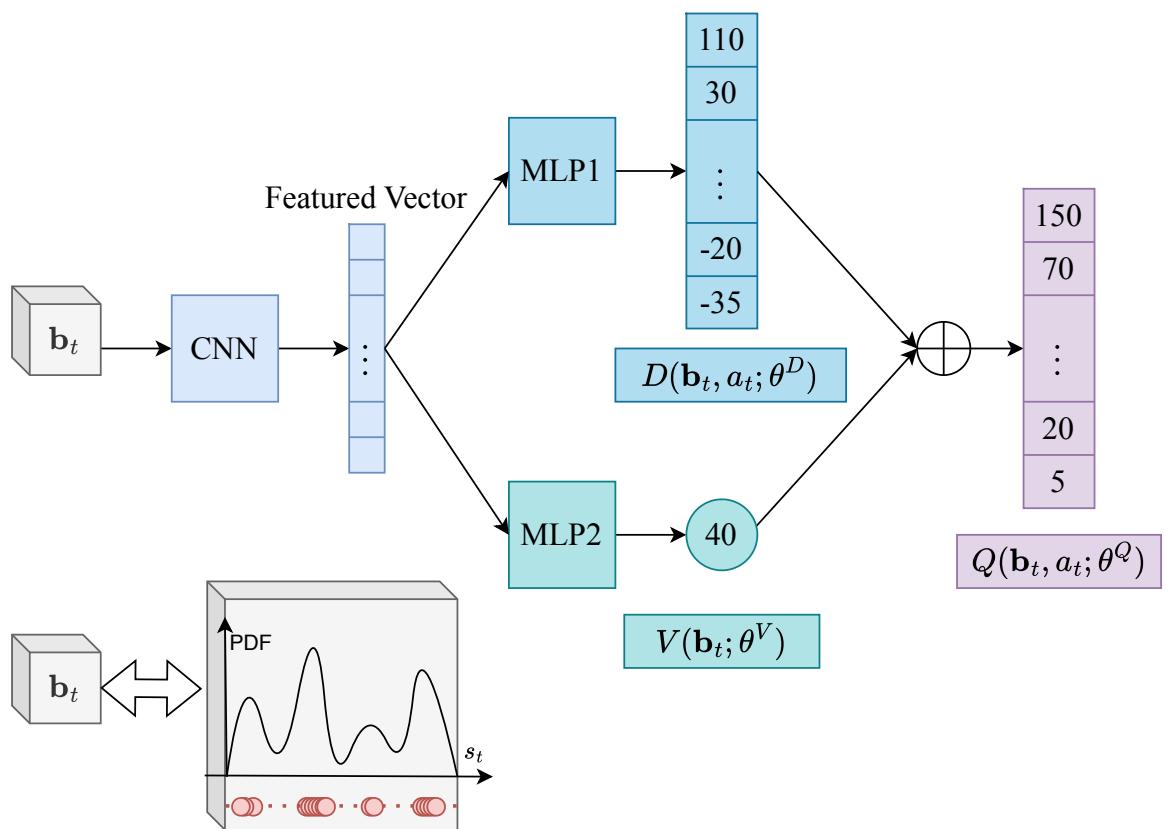


Figure 1.11: Dueling Network architecture

Chapter 2

Active Inference(AIF)

2.1 Active Inference

Recall the definition of POMDP, we will define a 7-tuple for the whole decision making process: $\{\mathbb{S}, \mathbb{A}, \mathbb{O}, \mathbf{T}, \mathbf{R}, \mathbf{O}, \gamma\}$, where at time step t , the state $s_t \in \mathbb{S}$ are hidden in the real world, its transition mechanism is illustrated by the transition model $T(s_{t+1}|s_t, a_t)$, action will be taken according to a policy $\pi(a_t|s_t)$, the observation comes from the observation model $o_t = O(o_t|s_t)$. To optimize the policy, we define a reward model $r_t = R(s_t, a_t)$ and the weighted accumulated total return $\mathbb{E}[\mathcal{U}_t^\pi] = \mathbb{E}[\sum_{i=t}^{\infty} \gamma^{i-t} r_i]$.

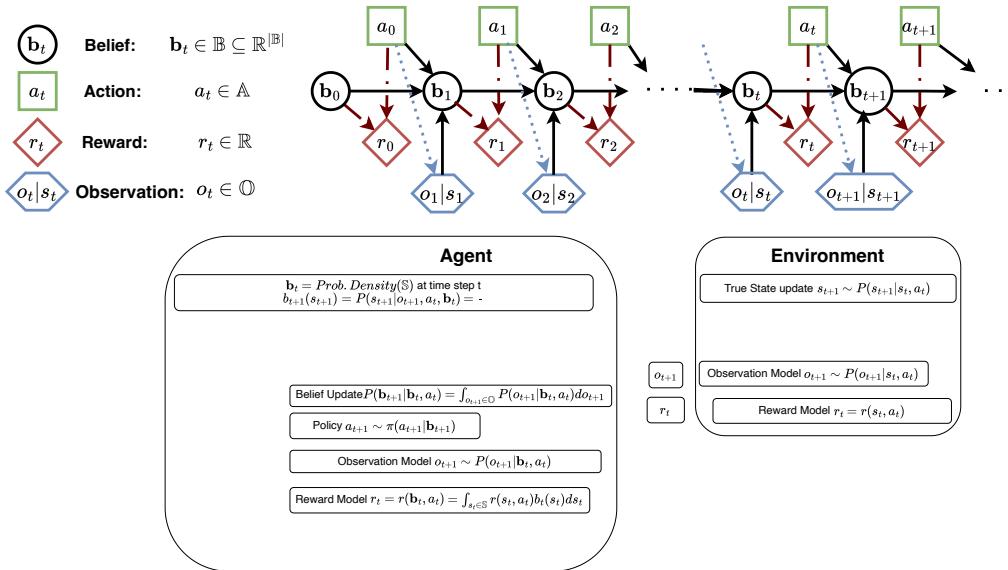


Figure 2.1: Original POMDP Model

There are only one model for the real world

After understanding the basics of Partially Observable Markov Decision Process (POMDP), we can have an basic understanding of Active Inference shown in the Figure 2.2, we should clarify that there are two models defined, i.e. the real world model described by the generative process $P^*(s^*, o)$ and the generative model $P(s, o) = P(s|o)P(o) = P(o|s)P(s)$.

The true process is always unknown, the agent has a generative model about how the outside world works. The only true connection between the interior and external world is the outcome (or observation).

The internal generative model would be updated every time observe some outcome. The prior belief is defined as the probability density of the state $P(s)$, the posterior is defined as

$$P(s|o) = \frac{P(s, o)}{P(o)} = \frac{P(o|s)P(s)}{P(o)} \quad (2.1)$$

Due to the difficulty of calculating the evidence $P(o) = \int_{S \in \mathcal{S}} P(o|S)P(S)$, we may use $Q(s)$ to approximate the posterior distribution $P(s|o)$. The information loss caused when using $Q(s)$ to approximate $P(s|o)$ is given by the relative Kullback-Divergence:

$$D_{KL}[Q(s)||P(s|o)] = \mathbb{E}_{Q(s)} [\ln(Q(s)) - \ln(P(s|o))] \quad (2.2)$$

When substitute the Eq. 2.1 to the Eq. 2.2 we could get:

$$D_{KL}[Q(s)||P(s|o)] = \mathbb{E}_{Q(s)} [\ln Q(s) - \ln P(s|o)] \quad (2.3a)$$

$$= \mathbb{E}_{Q(s)} \left[\ln Q(s) - \ln \left(\frac{P(s, o)}{P(o)} \right) \right] \quad (2.3b)$$

$$= \mathbb{E}_{Q(s)} [\ln Q(s) - \ln (P(s, o))] + \mathbb{E}_{Q(s)} [\ln P(o)] \quad (2.3c)$$

The active inference framework is based on the premise that perception and learning can be understood as minimizing a quantity known as **variational free energy** (VFE), and that action selection, planning and decision-making can be understood as minimizing the **expected free energy** (EFE).

- **Perception:** posterior state inference after each new observation
- **Learning:** slowly updating the priors and likelihood distributions in the model over many observations (which facilitates more accurate state inference in the long run).
- **Action selection, planning and deccision-making:** to select policy that will bring about future observations that minimize VFE.

Table 2.1: The physical meaning of **variational free energy** \mathcal{F}

Variational	$= D_{KL}[Q(s) P(s o)]$	$+ -\mathbb{E}_{Q(s)}[\ln P(o)]$	Eq. 2.4b
Free	= Divergence	+ Surprisal	
Energy	$= D_{KL}[Q(s) P(s)]$	- $\mathbb{E}_{Q(s)}[\ln P(o s)]$	Eq. 2.4c
\mathcal{F}	= Complexity	- Accuracy (Goodness of fit)	

Variational Free Energy (VFE) \mathcal{F}

The first term in Eq. 2.3c is defined as the **variational free energy** $\mathcal{F} \stackrel{\text{def}}{=} \mathbb{E}_{Q(s)}[\ln(Q(s)) - \ln(P(s, o))] = D_{KL}[Q(s)||P(s, o)]$. Then we can write that

$$\mathcal{F} = D_{KL}[Q(s)||P(s, o)] \quad (2.4a)$$

$$= D_{KL}[Q(s)||P(s|o)] - \mathbb{E}_{Q(s)}[\ln P(o)] \quad (2.4b)$$

$$= D_{KL}[Q(s)||P(s)] - \mathbb{E}_{Q(s)}[\ln P(o|s)] \quad (2.4c)$$

The physical meaning of the **variational free energy** (VFE) is shown in Table 2.1:

From the Eq. 2.4b, the term Divergence is the information loss when using the approximated density to approximate the posterior, which is no less than zero. Minimizing the **variational free energy** is equivalent to minimize the **surprisal** (defined as the negative log evidence) and also equivalent to maximize the evidence.

From the Eq. 2.4c, the Complexity is a measure of the difference between the approximation model and the prior density. And the accuracy is a measure of the likelihood, to show how well the model fit the observation. Minimizing VFE means only increase the accuracy of the model, also reducing the change effort when observing new observation.

In summary, by minimizing the **variational free energy**, we can perform the task of both perception and learning to find (approximately) optimal posterior beliefs after each new observation.

Expected Free Energy (EFE) \mathcal{G}

The task of action selection and planning is to select policies that will bring about future observations that minimize VFE. However, the future outcomes have not yet been observed. Actions must therefore be selected such that they minimize expected free energy (EFE).

Similarly to the previous introduced posterior approximation $P(s|o) \approx Q(s)$, the approximation of observations are written as $Q(o)$, the joint distribution of state and observation is $Q(s, o) = Q(o|s)Q(s)$

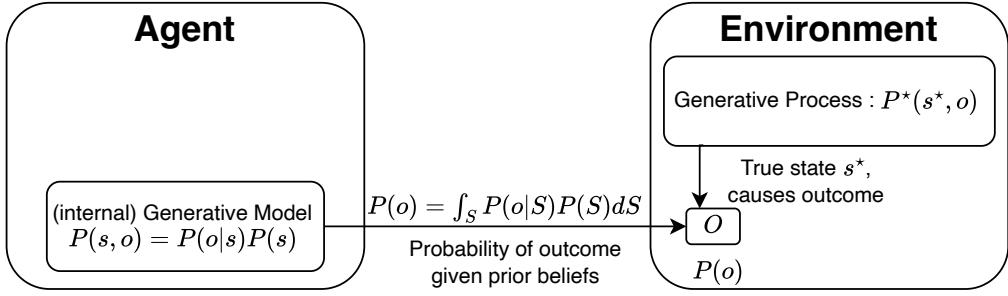


Figure 2.2: Graphical Representation of the Generative Process(based on the true states s^*) in the world and the corresponding (internal) generative model (based on probabilistic beliefs random variables s) that best explain the outcomes o . The outcomes are shared between the generative process and model. [sajid2021active]

The expected free energy can be seen as the expectation of the variational free energy over observations

$$\mathcal{G} \stackrel{\text{def}}{=} \mathbb{E}_{Q(o|s)} [\mathcal{F}] = \mathbb{E}_{Q(s,o)} [\ln Q(s) - \ln P(s,o)] \quad (2.5a)$$

$$= \mathbb{E}_{Q(o,s)} [\ln Q(s) - \ln P(s|o)] - \mathbb{E}_{Q(o,s)} [\ln P(o)] \quad (2.5b)$$

$$= \mathbb{E}_{Q(o,s)} [\ln Q(s) - \ln P(s|o)] - \mathbb{E}_{Q(o)} [\ln P(o)] \quad (2.5c)$$

$$\approx \mathbb{E}_{Q(o,s)} [\ln Q(s) - \ln Q(s|o)] - \mathbb{E}_{Q(o)} [\ln P(o)] \quad (2.5d)$$

$$\approx \mathbb{E}_{Q(o,s)} [\ln Q(s) - \ln Q(s|o)] - \mathbb{E}_{Q(o)} [\ln P(o|C)] \quad (2.5e)$$

$$= \mathbb{E}_{Q(o,s)} [\ln Q(o) - \ln Q(o|s)] - \mathbb{E}_{Q(o)} [\ln P(o|C)] \quad (2.5f)$$

$$= \mathbb{E}_{Q(o,s)} [\ln Q(o) - \ln P(o|s)] - \mathbb{E}_{Q(o)} [\ln P(o|C)] \quad (2.5g)$$

$$= D_{KL}[Q(o)||P(o|C)] + \mathbb{E}_{Q(o)} [H[P(o|s)]] \quad (2.5h)$$

where the second line Eq. 2.5b uses the product rule of probability $P(s,o) = P(s|o)P(o)$ to rearrange EFE into two terms that can be associated with information-seeking (epistemic value) and reward-seeking (pragmatic value). In active inference, we did not define the reward specifically. But instead, we have observed that the organism has an instinction to observe some thing in their expectation. If the observation aligns with their expectation, even the observation itself is a bad phenomena like a war happening or a disaster, if it was predicted by themselves, it is a signal of reward. Which means that the internal model of the world is quite effective. ??? With this explanation, we could treat the expectation of observation as the reward. And the difference between the true posterior model and the approximation could be treated as the information-seeking. Minimizing the expected free energy means minimizing the discrepancy between the approximation and the true posterior and at the same time maximizing the possibility of observing desired results.

The third line Eq. 2.5d uses a new introduced approximation of true posterior $P(s|o) \approx Q(s|o)$.

The fourth line Eq. 2.5e uses a new introduced terminology prior expectation over observations $p(o|C)$, that plays the role of preference.

The fifth line Eq. 2.5f uses the equality $\frac{Q(s)}{Q(s|o)} = \frac{Q(s)Q(o)}{Q(o|s)Q(s)} = \frac{Q(o)}{Q(o|s)}$

The sixth line Eq. 2.5g assumes that $P(o|s) = Q(o|s)$.

The final line Eq. 2.5h introduces a new terminology: Entropy of a distribution $P(x)$ is defined as $H[P(x)] \stackrel{\text{def}}{=} -\mathbb{E}_{P(x)}[\ln P(x)]$. Mutual information of x and y is defined as

$$I(x, y) \stackrel{\text{def}}{=} H[p(x)] - H[p(x|y)] = H[p(y)] - H[p(y|x)] \quad (2.6)$$

$I(x, y)$ is symmetric and scores the reduction in uncertainty (entropy) about the value of a variable x afforded by knowledge of another variable y . If these two variables are independent, mutual information is 0. To derive Eq. 2.5h, we start from Eq. 2.5g

$$\mathcal{G} = \mathbb{E}_{Q(o,s)} [\ln Q(o) - \ln P(o|s)] - \mathbb{E}_{Q(o)} [\ln P(o|C)] \quad (2.7a)$$

$$= \mathbb{E}_{Q(o,s)} \left[\ln \frac{Q(o)}{P(o|s)} \right] - \mathbb{E}_{Q(o,s)} [\ln P(o|C)] \quad (2.7b)$$

$$= \mathbb{E}_{Q(o,s)} \left[\ln \frac{Q(o)}{P(o|s)} - \ln P(o|C) \right] \quad (2.7c)$$

$$= \mathbb{E}_{Q(o,s)} \left[\ln \frac{Q(o)}{P(o|s)P(o|C)} \right] \quad (2.7d)$$

$$= \mathbb{E}_{Q(o,s)} \left[\ln \frac{Q(o)}{P(o|C)} - \ln P(o|s) \right] \quad (2.7e)$$

$$= \mathbb{E}_{Q(o,s)} \left[\ln \frac{Q(o)}{P(o|C)} \right] - \mathbb{E}_{Q(o,s)} [\ln P(o|s)] \quad (2.7f)$$

$$= \mathbb{E}_{Q(o)} \left[\ln \frac{Q(o)}{P(o|C)} \right] - \mathbb{E}_{Q(o|s)Q(s)} [\ln P(o|s)] \quad (2.7g)$$

$$= \mathbb{E}_{Q(o)} \left[\ln \frac{Q(o)}{P(o|C)} \right] - \mathbb{E}_{Q(s)} [\mathbb{E}_{Q(o|s)} [\ln P(o|s)]] \quad (2.7h)$$

$$= \mathbb{E}_{Q(o)} \left[\ln \frac{Q(o)}{P(o|C)} \right] - \mathbb{E}_{Q(s)} [\mathbb{E}_{P(o|s)} [\ln P(o|s)]] \quad (2.7i)$$

$$= D_{KL}[Q(o)||P(o|C)] - \mathbb{E}_{Q(s)} [H(P(o|s))] \quad (2.7j)$$

2.1.1 Data Collection

The research employs multiple datasets to ensure comprehensive evaluation:

- **Dataset A:** Contains 10,000 samples with 50 features...
- **Dataset B:** Comprises time-series data spanning 5 years...
- **Dataset C:** Includes multimodal data from various sources...

2.2 Algorithm Design

The proposed algorithm builds upon the foundation established by [lee2019optimization]. The pseudocode is presented in Algorithm 6.

```

Input: X, θ
Output: Best solution in P
1 Initialize population P ← ∅;
2 for i ← 1 to N do
3   | xi ← InitializeSolution();
4   | P ← P ∪ {xi};
5 end
6 while not converged do
7   | Evaluate fitness for all x ∈ P;
8   | Select parents for reproduction;
9   | Apply crossover and mutation;
10  | Update population P;
11 end
12 return best solution in P;
```

Algorithm 6: Proposed Optimization Algorithm

2.3 Experimental Setup

All experiments were conducted on a computing cluster with the following specifications:

- CPU: Intel Xeon Gold 6248R (3.0 GHz)
- GPU: NVIDIA A100 (40GB)
- Memory: 256 GB DDR4
- Storage: 2 TB NVMe SSD

Chapter 3

Structural Integration Management

3.1 simple example

Now we need to build the code block shown in the Figure 3.1 to connect all the relevant functions. In our code, we can also write the following blocks:

3.1.1 Problem Formulation: 1D Beam with deteriorating stiffness

We model a 1D fixed-fixed beam under a point load at mid-span with a pre-defined geometry, Loading condition, boundary condition, material properties are summarized in the following Table 3.1:

Table 3.1: Configuration of Steel Truss Bridge Structure

Geometry Property	length L Cross Section A	1m 1.0m ²
Machanical Property	Youngs modulus E	E(t = 0) = 210e9Pa
Material Property	Density ρ	7800kg/m ³
Loading	Mid point load F	10kN
Boundary Condition	u _L = 0, u _R = 0	

To model as a POMDP model, we will think through the following components of the model

- States space \mathbb{S} : is a continuous spaces \mathbb{R}^N containing the Youngs modulus for all elements $\mathbf{E} = [E_1, E_2, \dots, E_{n_{elements}}]$. In other words, we will assume that the only changing parameters over time is the mechanical property Youngs modulus. The mass (usually depends on density and geometry) is constant if we assume that the density and geometry do not change over time.

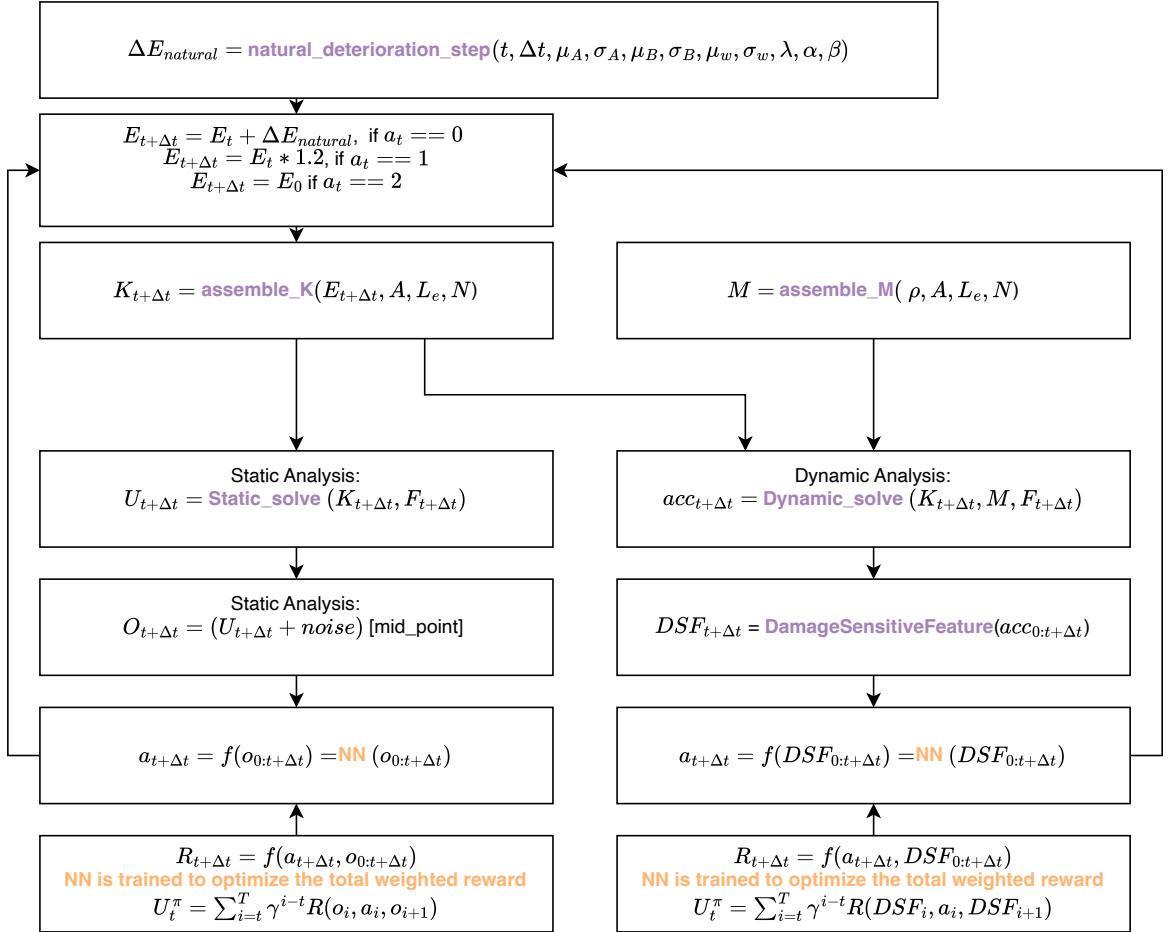


Figure 3.1: Flowchart diagram

- Action space \mathbb{A} : is a discrete space contains three elements a_0, a_1, a_2

The state-dependent sequence of actions is defined as policy π . There could be two types of policies, the deterministic policy $\pi(a|s) : \mathbb{S} \rightarrow \mathbb{A}$ (mapping from the state space to the action space) and the stochastic policy $\pi(a|s) : \mathbb{S} \times \mathbb{A} \rightarrow \mathbb{R} \in [0, 1]$ (mapping from the state space to the probability of actions). Depending on whether the action space are continuous or discrete we can have the conditional probability density function (PDF) and the conditional probability mass function (PMF).

- Observation space \mathbb{O} : is a continous observation space containing the observation of the mid-point displacement observations

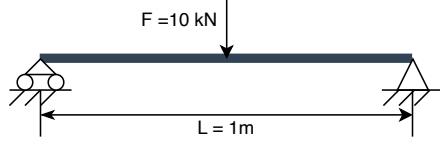


Figure 3.2: Geometrical Property of Steel Truss Bridge Structure

- Transition probability \mathbf{T} : $s_{t+\Delta t} \leftarrow \mathbf{T}(s_t, a_t)$ The natural degradation process is modelled as the basic deterioration and repairs are applied element-wise
 - a_0 : do nothing \rightarrow natural deterioration. We could define a deterioration level as $D(t) \stackrel{\text{def}}{=} E(t=0) - E(t)$ to indicate the deterioration extent from the beginning to the time t .
 - * gradual deterioration (aging process): The gradual deterioration process can be modelled as a simple rate function [**ellingwood2005risk**]:

$$D(t) \stackrel{\text{def}}{=} E(t=0) - E(t) = At^B e^{w(t)} \quad (3.1)$$

where A is the random variable modelling the deterioration rate, B is the random variable modelling the nonlinearity effect in terms of a lower law in time and $w(t)$ models the gaussian stochastic process noise. Realization plot of an aging process is shown in Figure 3.3. The changes of the deterioration can be approximated by the derivative $\frac{dD}{dt}\Delta t$ if we treat $w(t)$ as a constant number w_k

$$\Delta D(t) = E(t) - E(t + \Delta t) \approx ABt^{B-1}e^{w_k}\Delta t \quad (3.2)$$

- * sudden deterioration: The sudden deterioration can be modelled as a homogeneous compound Poisson Process(CPP) [**van2009survey**, **sanchez2016reliability**]

$$D(t) \stackrel{\text{def}}{=} E(t=0) - E(t) = \sum_{i=1}^{N(t)} D_i \sim CPP(t; \lambda, F_D(d)) \quad (3.3)$$

where the number of jumps in the time interval t $N(\Delta t) \sim \text{PoissonProcess}(\lambda)$; the amplitude of each jump $D_i \sim F_D(d)$ are independent and identically distributed random variables following a given distribution $F_D(d)$ e.g. a Gamma distribution. Realization plot of a CPP process is shown in Figure 3.4

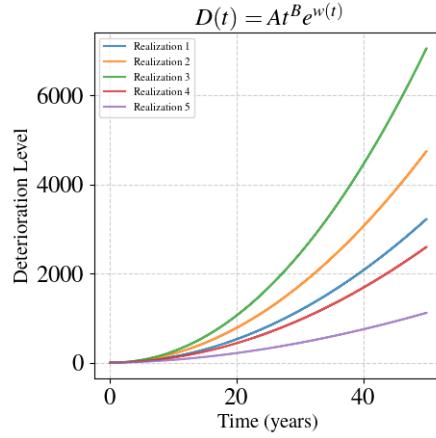


Figure 3.3: Gradual deterioration realization plot modeled by a simple rate function

The change of the deterioration during the time interval Δt is calculated as:

$$\Delta D(t) = E(t) - E(t + \Delta t) = \sum_{i=1}^{N(\Delta t)} D_i \sim CPP(\Delta t; \lambda, F_D(d)) \quad (3.4)$$

where the number of jumps in the time interval Δt $N(\Delta t) \sim \text{PoissonProcess}(\lambda)$; the amplitude of each jump $D_i \sim F_D(d)$ are independent and identically distributed random variables following a given distribution $F_D(d)$ e.g. a Gamma distribution

In summary the deterioration model parameters are defined in the Table 3.2

Table 3.2: Prior distribution of deterioration model parameters

Parameter	Distribution	Mean	cv
A	Lognormal	$1.94 \cdot 10^{-4}$	0.4
B	Normal	2.0	0.1
ω_k	Normal	-0.005	0.1
D_i	Lognormal	3.75	0.25
$N(t)$	Poisson	$0.04 \cdot t$	$0.04 \cdot t$

- a_1 : minor repair $\rightarrow E(t + \Delta t) = E(t) + (E(t = 0) - E(t)) \cdot \alpha_{\text{repair}}$
- a_2 : full replacement $\rightarrow E(t + \Delta t) = E(t = 0)$

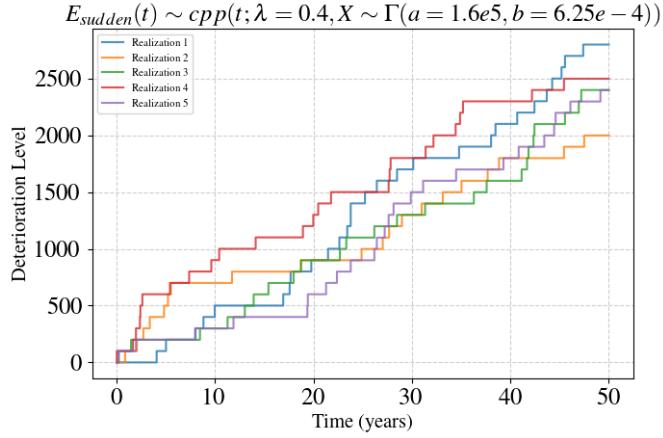


Figure 3.4: sudden deterioration realization plot modelled by a CPP process

where $\Delta t = T/N$, T is the total time span e.g. 50 years and N is the total number of decision steps.

- Observation model $\mathbf{O}(o_{t+\Delta t}|s_{t+\Delta t}, a_t)$:

- Static analysis: Observation from the static analysis is the midpoint displacement. It is continuous observation. The displacement vector is calculated via

$$u_{t+\Delta t} = \text{StaticSolver}(K(E(t + \Delta t)), F_{t+\Delta t}). \quad (3.5)$$

We could generate the synthetic observations by adding the noise

$$o_{t+\Delta t} = f(u_{t+\Delta t} + N(0, \sigma^2)). \quad (3.6)$$

- Dynamic analysis: We could generate the synthetic observation from dynamic analysis is the acceleration time series data.

$$acc_{t+\Delta t} = \text{dynamicSolver}(K(E(t + \Delta t)), F_{t+\Delta t}). \quad (3.7)$$

We could use the Vibration-based SHM method to extract the damage sensitive feature from the acceleration time series data.

$$DSF_{t+\Delta t} = \text{DamageSensitiveFeatureExtraction}(acc_{0:t+\Delta t}) \quad (3.8)$$

- Reward Model $r(s, a)$:

Accumulated Discount Reward for the whole episode T is defined as the weighted sum of reward at each time step:

$$R = R(s_0, a_0, \dots, s_T, a_T) = \sum_{i=0}^T \gamma^{i-t} R(s_i, a_i) \quad (3.9)$$

where the discount factor $\gamma \in [0, 1]$. It weights more on the current reward than the future reward. When $\gamma = 0$: only the current reward matters; when $\gamma = 1$: rewards in all steps equally matter.

The total reward is also composed of three parts: $R = R_{\text{insp}} + R_{\text{disp}} + R_{\text{repair}} + R_{\text{replace}} + R_{\text{failure}}$

Table 3.3: Cost Definition in the beam monitoring process

Cost due to displacement	$R_{\text{disp}} = -\sum_{i=1}^T k_i u_i^2$ or simpler $-\beta u_i $	$k_i = 10$ for $i = 0, \dots, T$ $\beta = 50$
Cost due to repair	$R_{\text{repair}} = -c_{\text{repair}} \cdot n_{\text{repair}}$	$c_{\text{repair}} = 500$ n_{repair} is the total repair times
Cost due to replace	$R_{\text{replace}} = -c_{\text{replace}} \cdot n_{\text{replace}}$	$c_{\text{replace}} = 2000$ n_{replace} is the total replace times
Cost due to inspection	$R_{\text{insp}} = -c_{\text{insp}} \cdot n_{\text{inspection}}$	$c_{\text{insp}} = 200$ n_{insp} is the total inspection times
Cost due to failure	$R_{\text{failure}} = -c_{\text{failure}}$	$c_{\text{failure}} = 10000$ is the equivalent in During time T , the structure failure

3.2 Proposed Framework

This section presents the proposed framework for addressing the research problem. The overall architecture is depicted in ??.

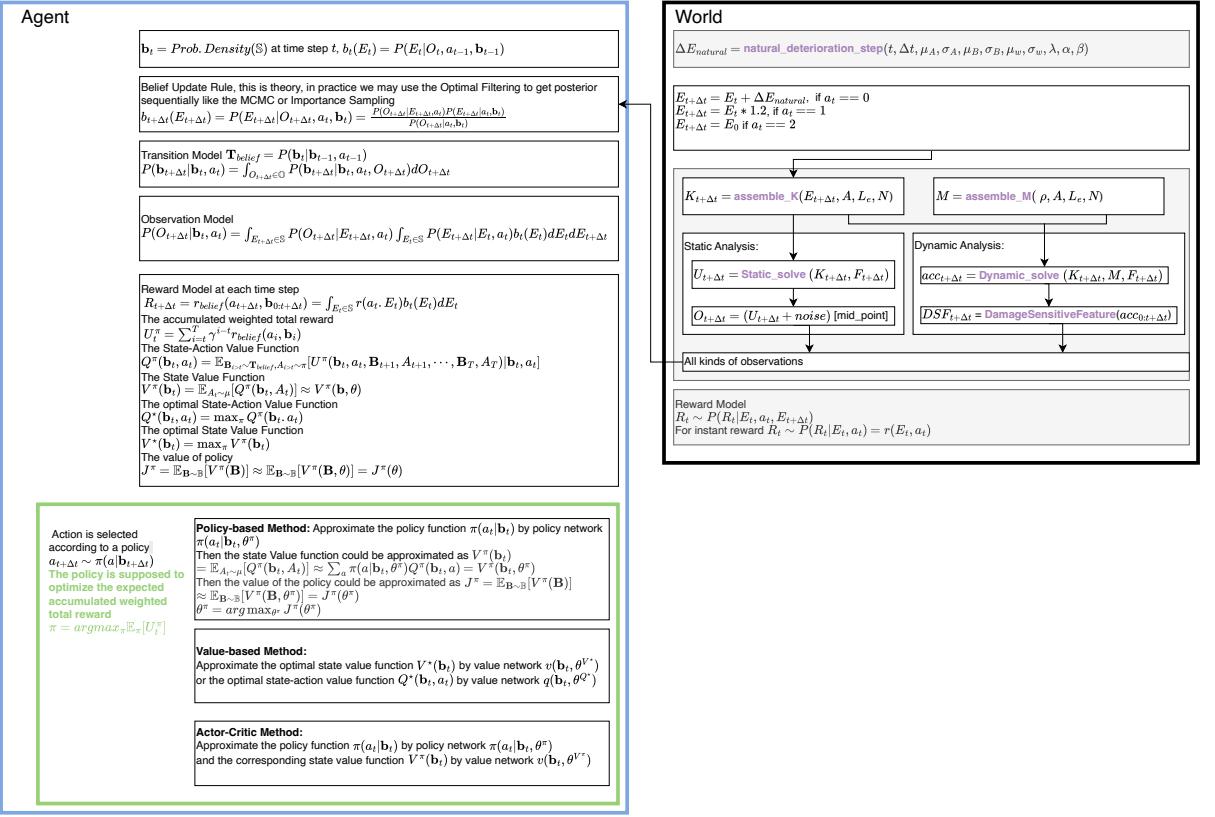


Figure 3.5: Flowchart POMDP diagram

Appendix A

Appendices

A.1 Probability Basis

A.1.1 Random Variables

Extreme Value (EV) distributions

Let $\mathbf{X} = [X_1, X_2, \dots, X_n]^T$ denote a random vector, with its smallest value denoted by X_{\min} and its largest value denoted by X_{\max} . If the distribution of \mathbf{X} is known, one can also find the distribution of X_{\min} and X_{\max} .

For the special case when X_i s are iid, one can obtain simple expressions for the distribution of X_{\min} and X_{\max} .

Let $f_X(x)$ and $F_X(x)$ denote the PDF and CDF of the X_i s, the minimum value is larger than x means than $\{X_{\min} > x\} = \{X_1 > x \cap X_2 > x \cap \dots \cap X_n > x\}$ To derive the CDF of X_{\min}

$$F_{X_{\min}}(x) = \Pr(X_{\min} \leq x) \quad (\text{A.1})$$

$$= 1 - \Pr(X_{\min} > x) \quad (\text{A.2})$$

$$= 1 - \Pr(X_1 > x \cap X_2 > x \cap \dots \cap X_n > x) \quad (\text{A.3})$$

$$= 1 - \prod_{i=1}^n \Pr(X_i > x) \quad (\text{A.4})$$

$$= 1 - [1 - F_X(x)]^n \quad (\text{A.5})$$

The PDF of X_{\min} is

$$f_{X_{\min}}(x) = \frac{dF_{X_{\min}}(x)}{dx} \quad (\text{A.6})$$

$$= n f_X(x) [1 - F_X(x)]^{n-1} \quad (\text{A.7})$$

To derive the CDF of X_{\max} , we could start from the fact that $\{X_{\max} \leq x\} = \{X_1 \leq x \cap \dots \cap X_n \leq x\}$:

$$F_{X_{\max}}(x) = \Pr(X_{\max} \leq x) \quad (\text{A.8})$$

$$= \Pr(X_1 \leq x \cap \dots \cap X_n \leq x) \quad (\text{A.9})$$

$$= \prod_{i=1}^n \Pr(X_i \leq x) \quad (\text{A.10})$$

$$= [F_X(x)]^n \quad (\text{A.11})$$

The PDF of X_{\max} is

$$f_{X_{\max}}(x) = \frac{dF_{X_{\max}}(x)}{dx} = n f_X(x) [F_X(x)]^{n-1} \quad (\text{A.12})$$

The results can be generalized to the k^{th} largest value in \mathbf{X} denoted by Y_k : the CDF of Y_k is

$$F_{Y_k}(x) = \sum_{j=k}^n C_n^j (F_X(x))^j (1 - F_X(x))^{n-j} \quad (\text{A.13})$$

The underlying X_i s are often unknown, and the above solutions are therefore not directly applicable. However, extreme value distributions that arise as asymptotic solutions of the above for $n \rightarrow \infty$ provide a useful model in these cases.

It can be shown that the solutions given above in Eqs Eq. A.1, Eq. A.6, Eq. A.8, Eq. A.12 converge to one of three distribution types, depending on the distribution of the X_i s.

The type I EV distribution for maxima is named Gumbel distribution.

A.1.2 Random Process

Bernoulli Process

A Bernoulli process is a finite or infinite sequence of independent random variables X_1, X_2, \dots , such that

- for each i , the value of X_i is either 0 or 1;
- for all values of i , the probability p is the same.

In other words, Bernoullie process is a sequence of independent identically distributed Bernoulli trials. The summary of Bernoulli process and its associated distributions are shonw in Figure A.2

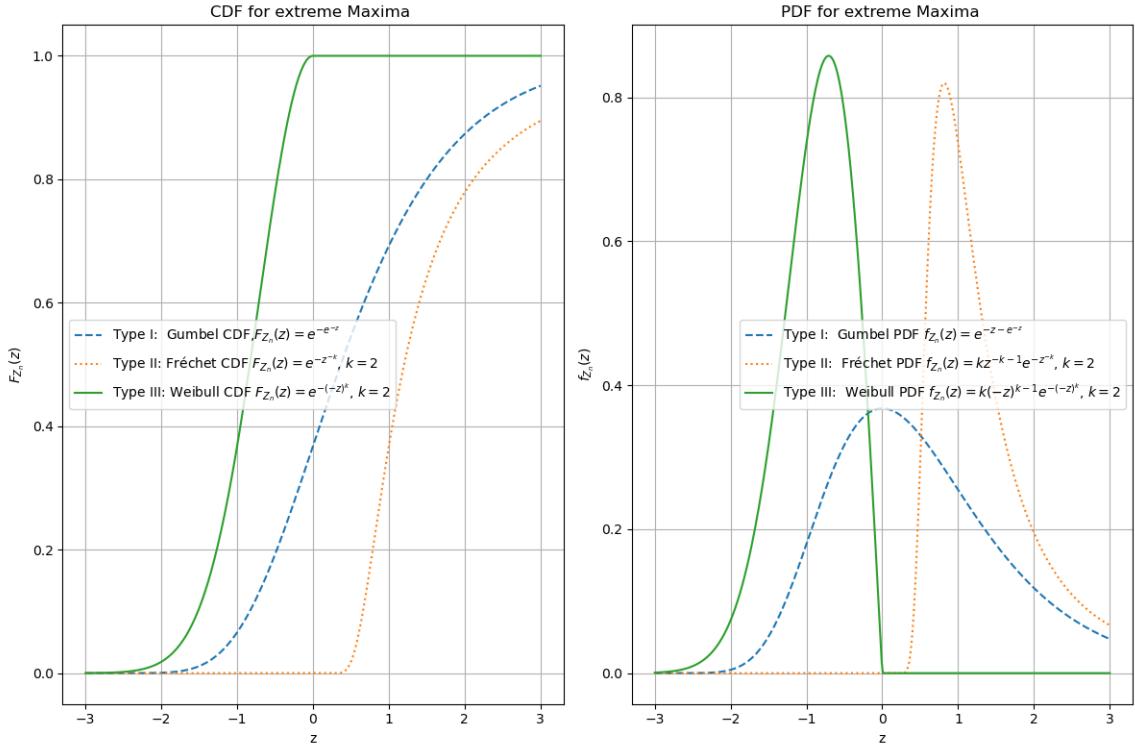


Figure A.1: Extreme Value distribution for Maximum

Poisson Process

The homogeneous Poisson process can be defined as a counting process with rate $\lambda > 0$ and follows the three properties

- Independent occurrences: In two non-overlapping intervals, the corresponding numbers of occurrences must be statistically independent of each other
- Occurrences proportional to duration: In an interval $(t, t + \Delta t)$, the probability of exactly one occurrence is asymptotically proportional to the interval length Δt as $\Delta t \rightarrow 0$
- Occurrences do not coincide: The probability of two or more occurrences within a sufficiently small interval $(t, t + \Delta t)$ must be orders of magnitude lower than the probability of one occurrence

For the homogeneous Poisson Process, the mean rate of occurrence λ is constant with time or locations, whereas for nonhomogeneous case, λ is the function of time or location.

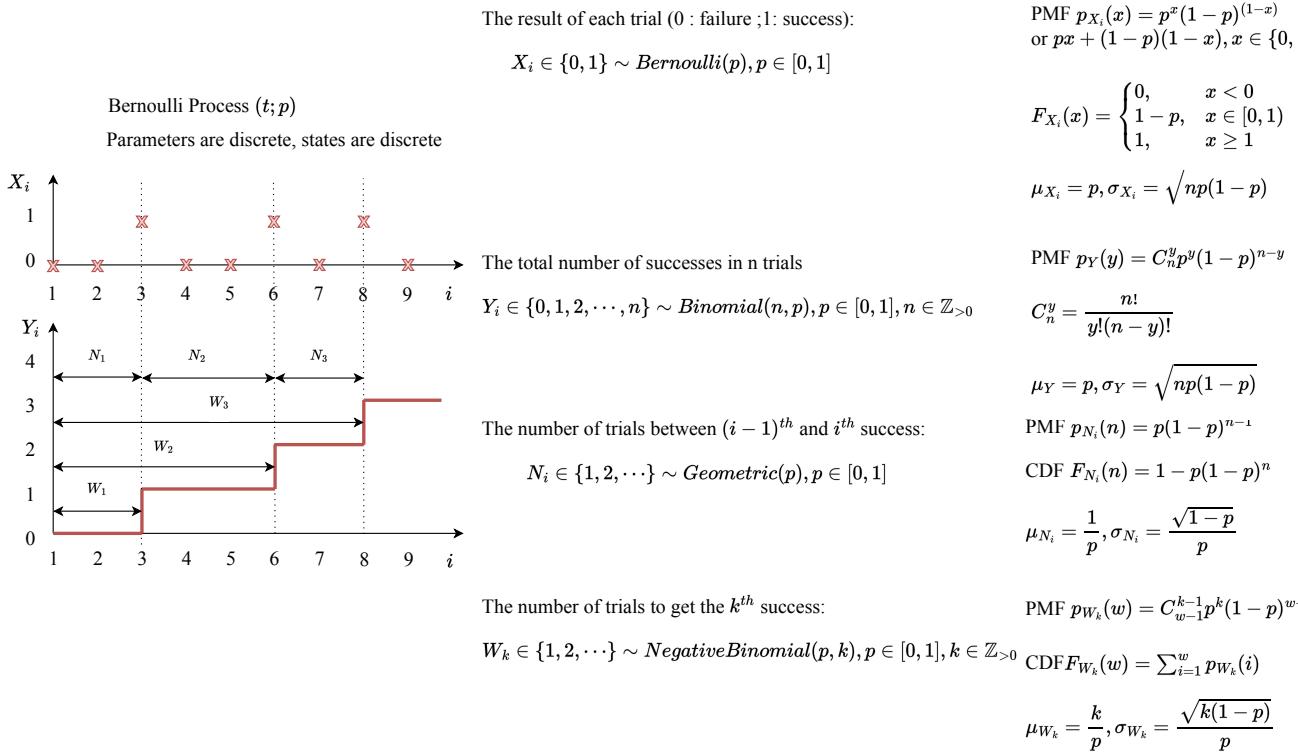


Figure A.2: Bernoulli Process and its associated Probability Distribution

Compound Poisson Process

A compound Poisson process with rate $\gamma > 0$ abd jump size distribution is a continuous-time stochastic process $\{S(t) : t \geq 0\}$ given by

$$S(t) = \sum_{i=1}^{Y(t)} X_i, \quad (\text{A.14})$$

where the sum is by convention equal to zero as long as $Y(t) = 0$. Here $\{Y(t), t \geq 0\}$ is a Poisson process with rate γ and $\{X_i; i \geq 1\}$ are independent and identically distributed random variables with distribution function f_{X_i} , which is also independent of $\{Y(t), t \geq 0\}$. The summary of Compound Poisson Process in shown in Figure A.4 Compound poisson Process builds on the Poisson process by adding randomness to the event magnitudes. The Poisson porcess models the timing of the events, while the compound Poisson Process accounts for both the timing and the accumulated effect of events.

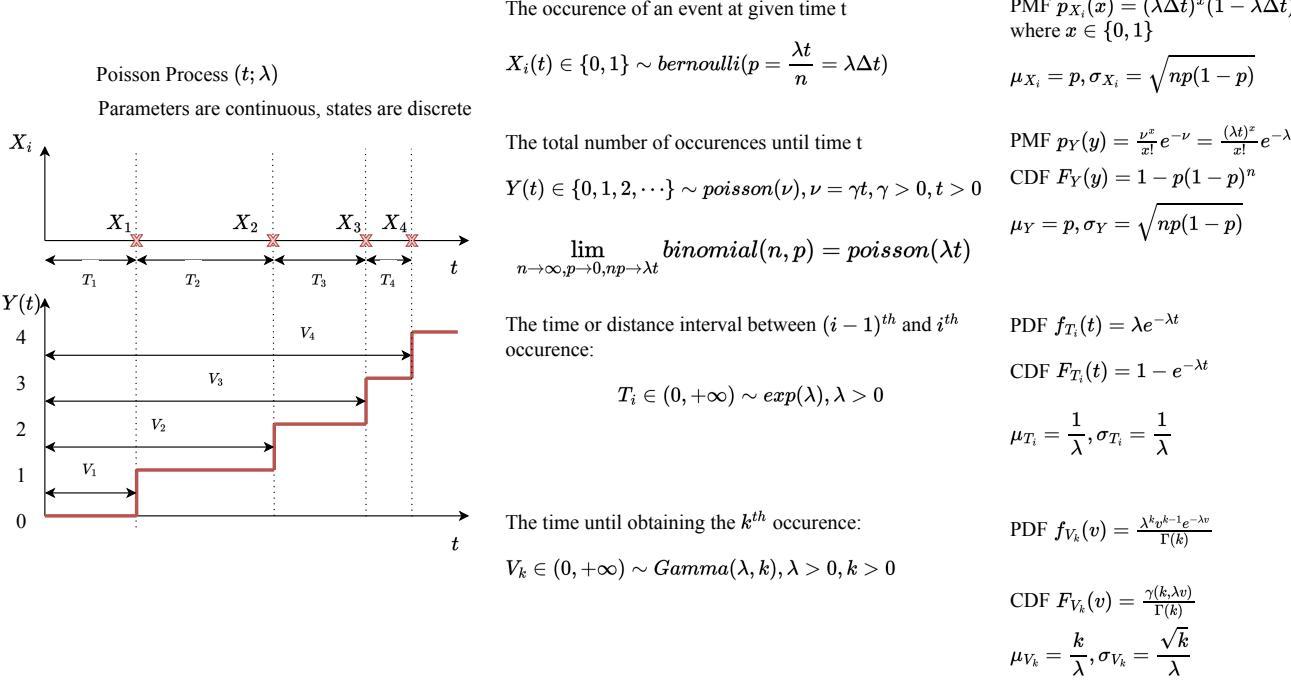


Figure A.3: Poisson Process and its associated Probability Distribution

Gamma Process

The gamma process $\Gamma(t; \gamma, \lambda)$ is a process which measures the number of occurrences of independent gamma-distributed variables over a span of time.

The gamma distribution is a two-parameter continuous probability distributions family. The exponential, Erlang and chi-squared distributions are special cases of the gamma distributions. The two parameters are the shape parameter $\gamma > 0$ and the rate parameter $\lambda > 0$ (or equivalently the scale parameter $\theta = \frac{1}{\lambda}$). Assume the random variable $X \sim \Gamma(\gamma, \lambda)$, then the probability density function is

$$f_X(x; \gamma, \lambda) = \frac{x^{\gamma-1} e^{-\lambda x} \lambda^\gamma}{\Gamma(\gamma)}, \text{ for } x > 0 \quad (\text{A.15})$$

The gamma function $\Gamma(\cdot)$ is the extension of factorial function to complex numbers. It is defined for all complex numbers z except non-positive integers.

$$\Gamma(z) = \begin{cases} (z-1)!, & z \in \mathbb{Z}_{>0} \\ \int_0^\infty t^{z-1} e^{-t} dt, & \Re(z) > 0 \end{cases} \quad (\text{A.16})$$

For the gamma process: the increment distribution is following the gamma

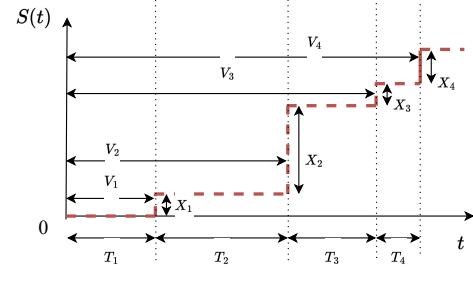
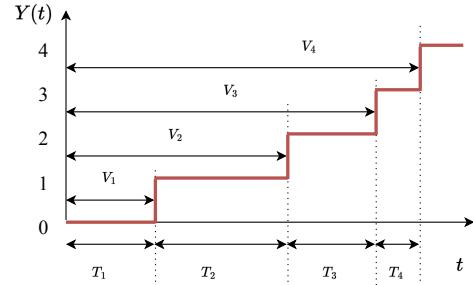
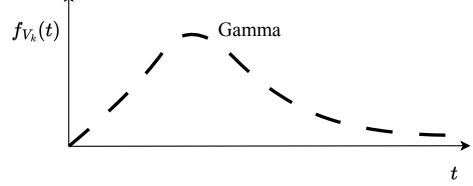
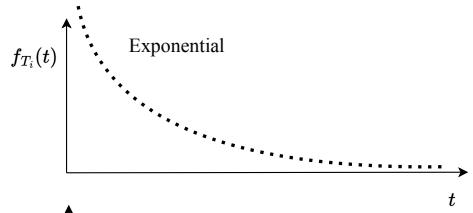
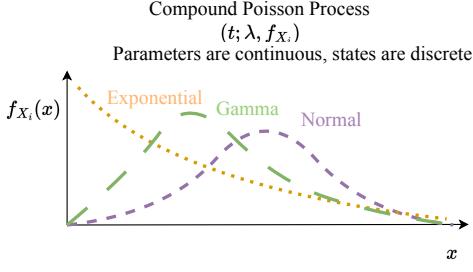
distribution.

$$S(t + \Delta t) - S(t) \sim \Gamma(\gamma \Delta t, \lambda) \quad (\text{A.17})$$

It is used to model phenomena where the cumulative total grows smoothly over time, e.g. Modelling degradation and aging in systems due to wear and tear.

In contrast the compound Poisson Process models the phenomena where discrete random events contribute to a cumulative sum, e.g. total rainfall, aggregate claims in insurance, financial losses.

The gamma process is a random process consisting of independently distributed gamma distributions where $Y(t)$ represents the number of event occurrences from time 0 to time t . The gamma distribution has shape parameter γ and rate parameter λ , often written as $\Gamma(\gamma, \lambda)$, $\gamma > 0$ and $\lambda > 0$. The gamma process is often written as $\Gamma(t; \gamma, \lambda)$ where t represents the time from 0. The process is a pure-jump increasing Levy process with intensity measure $v(x) = \gamma x^{-1} e^{(-\lambda x)}$ for all positive x . Thus jumps whose size lies in the interval $[x, x + dx]$ occur as a Poisson process with intensity $v(x)dx$. The parameter γ controls the rate of jump arrivals and the scaling parameter γ inversely controls the jump size. It is assumed the process starts from a value 0 at $t=0$, i.e. $Y(0) = 0$



The magnitude of i^{th} event
 $X_i \in (0, +\infty)$ could follow any specified distribution,
e.g. continuous dist.: normal, gamma (exponential is a
special case of gamma distribution); or discrete dist.

If X_i is gamma distribution with shape parameter a
and rate parameter b

$$X_i \in (0, +\infty) \sim \Gamma(a, b), a > 0, b > 0$$

$$\begin{aligned} \text{PDF: } f_X(x) &= \frac{x^{a-1} e^{-x/b}}{b^a \Gamma(a)} \\ \text{CDF: regularized incomplete gamma function } F_X(x) &= \frac{\gamma(a, x/b)}{\Gamma(a)} \\ \text{lower incomplete gamma function } \gamma(a, x/b) &= \int_0^{x/b} t^{a-1} e^{-t} dt \\ \Gamma(a) &= \int_0^\infty t^{a-1} e^{-t} dt \end{aligned}$$

$$\mu_X = ab, \sigma_X = \sqrt{ab}$$

The time or distance between $(i-1)^{th}$ and i^{th} success:

$$T_i \in (0, +\infty) \sim \exp(\lambda), \lambda > 0$$

$$\text{PDF } f_{T_i}(t) = \lambda e^{-\lambda t}$$

$$\text{CDF } F_{T_i}(t) = 1 - e^{-\lambda t}$$

$$\mu_{T_i} = \frac{1}{\lambda}, \sigma_{T_i} = \frac{1}{\lambda}$$

The time until obtaining the k^{th} success:Erlang dist.

$$V_k \in (0, +\infty) \sim \Gamma(k, \lambda), \lambda > 0, k = 1, 2, \dots$$

$$\text{PDF } f_{V_k}(t) = \frac{\lambda^k t^{k-1} e^{-\lambda t}}{\Gamma(k)} = \frac{\lambda^k t^{k-1} e^{-\lambda t}}{(k-1)!}$$

In numpy

$$V_k = np.random.gamma(shape=k, scale=1/lambda)$$

$$\text{CDF } F_{V_k}(t) = \frac{\gamma(k, \lambda t)}{\Gamma(k)} = \frac{\int_0^t \tau^{k-1} e^{-\tau} d\tau}{(k-1)!}$$

$$\mu_{V_k} = \frac{k}{\lambda}, \sigma_{V_k} = \frac{\sqrt{k}}{\lambda}$$

The total number of successes until time t

$$\text{PMF } p_Y(y) = \frac{\nu^y}{y!} e^{-\nu} = \frac{(\lambda t)^y}{y!} e^{-\lambda t}$$

$$Y(t) \in \{0, 1, 2, \dots\} \sim \text{poisson}(\nu), \nu = \lambda t, \lambda > 0, t > 0$$

$$\text{CDF } F_Y(y) = 1 - p(1-p)^y$$

$$\lim_{y \rightarrow \infty, p \rightarrow 0, y p \rightarrow \lambda t} \text{binomial}(y, p) = \text{poisson}(\lambda t)$$

The accumulated total amount until time t

$$S(t) = \sum_{i=1}^{Y(t)} X_i \in (0, +\infty) \sim CPP(t; \nu, F_X(x)), \nu = \lambda t, \lambda > 0, t > 0$$

$$\mathbb{E}[S(t)] = \mathbb{E}[\mathbb{E}[S(t)|Y(t)]] = \mathbb{E}[Y(t)\mathbb{E}[X(t)]] = \lambda t \mathbb{E}[X_i]$$

$$\mathbb{D}[S(t)] = \mathbb{E}[\mathbb{D}[S(t)|Y(t)]] + \mathbb{D}[\mathbb{E}[S(t)|Y(t)]] = \mathbb{E}[\sigma_X^2 Y(t)] + \mathbb{D}[\mu_X Y(t)] = \sigma_X^2 \mu_Y + \mu_X^2 \sigma_Y^2 = \lambda t \sigma_X^2$$

$$S|_{Y(t)=y} = \sum_{i=1}^y X_i \sim \Gamma(ya, b) \quad f_{S|_{Y=t}}(x) = (f_X * \dots * f_X)(x) = \frac{b^{ya} x^{ya-1} e^{-bx}}{\Gamma(ya)}$$

$$f_S(x) = \sum_{y=0}^{\infty} p_Y(y) f_{S|_{Y=y}}(x) = e^{-\lambda t} + \sum_{y=1}^{\infty} \frac{(\lambda t)^y}{y!} e^{-\lambda t} \frac{b^{ya} x^{ya-1} e^{-bx}}{\Gamma(ya)} = e^{-\lambda t} + \sum_{y=1}^{\infty} \frac{(\lambda t)^y b^{ya} x^{ya-1}}{y! \Gamma(ya)} e^{-\lambda t}$$

$$W(x, z) = \sum_{y=1}^{\infty} \frac{x^y}{y! \Gamma(zy)} \quad f_S(x) = e^{-\lambda t} + \frac{e^{-\lambda t-bx}}{x} \sum_{y=1}^{\infty} \frac{(\lambda t(bx)^a)^y}{y! \Gamma(ya)} = e^{-\lambda t} + \frac{e^{-\lambda t-bx}}{x} W(\lambda t(bx)^a)$$

$$F_S(s) = \int_0^s f_S(x) dx = e^{-\lambda t} + \int_0^s \frac{e^{-\lambda t-bx}}{x} \sum_{y=1}^{\infty} \frac{(\lambda t(bx)^a)^y}{y! \Gamma(ya)} dx$$

Figure A.4: Compound Process Process and its associated Probability Distribution

Gamma Process $\Gamma(t; \gamma, \lambda)$

Parameters are continuous, states are continuous. $S(t)$ is continuous (no jump)

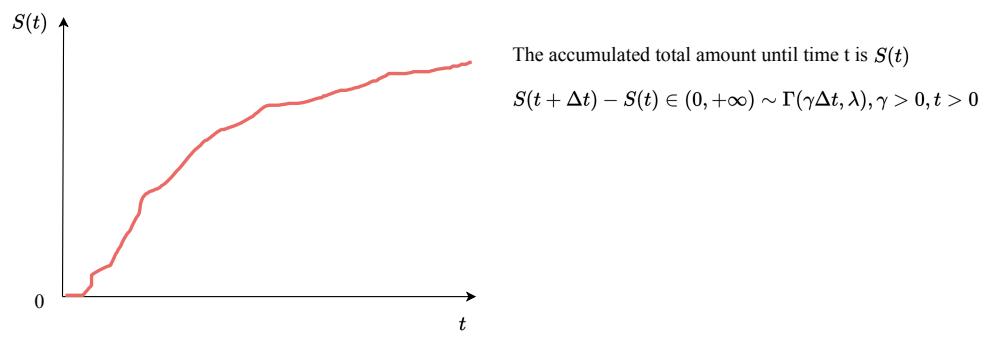


Figure A.5: Gamma Process and its associated Probability Distribution