

1 Parameter identification for DTMCs

1.1 Preliminaries

We consider a DTMC with two states, $S = \{s_A, s_B\}$, and a parametric transition probability matrix $P = \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix}$, where p and q are the parameters to be identified. The aim of the project is to estimate p and q based on a finite number of traces (N) of finite length (n), using different parameter inference techniques. In what follows, we assume the initial distribution over the states to be known (e.g. *uniformly distributed*), thus we focus on the estimation of the transition probabilities only.

1.2 Methodology

We explore two different approaches for parameter inference:

- **Maximum Likelihood Estimation (MLE):** this method estimates the parameters by maximizing the likelihood of the observed data.
- **Bayesian Inference:** this method estimates the posterior distribution of parameters, given a prior distribution and the observed data.

1.2.1 Maximum Likelihood Estimation (MLE)

In order to estimate the parameters p and q using MLE, we derive the likelihood function based on the observed traces. Given a single trace $\sigma_i = s_1 s_2 \dots s_n$ of length n , its likelihood is given by the following expression:

$$\begin{aligned} L(\sigma_i | p, q) &= P(s_1) \prod_{j=1}^{n-1} P(s_{j+1} | s_j) \propto \prod_{j=1}^{n-1} P(s_{j+1} | s_j) \\ &= \prod_{j=1}^{n-1} [\mathbb{1}_{\{s_j=s_A, s_{j+1}=s_A\}}(1-p) \cdot \\ &\quad \mathbb{1}_{\{s_j=s_A, s_{j+1}=s_B\}}p \cdot \\ &\quad \mathbb{1}_{\{s_j=s_B, s_{j+1}=s_A\}}q \cdot \\ &\quad \mathbb{1}_{\{s_j=s_B, s_{j+1}=s_B\}}(1-q)] \end{aligned}$$

Let N_{ij} be the number of transitions from state s_i to s_j in the trace. An alternative formulation of the likelihood is:

$$L(\sigma_i | p, q) = (1-p)^{N_{AA}} p^{N_{AB}} q^{N_{BA}} (1-q)^{N_{BB}}$$

and the corresponding log-likelihood:

$$l(\sigma_i | p, q) = N_{AA} \log(1-p) + N_{AB} \log(p) + N_{BA} \log(q) + N_{BB} \log(1-q)$$

To obtain the Maximum Likelihood estimates, we need to maximize the log-likelihood function with respect to the parameters p and q . Since the two parameters are independent and depend only on the counts of transitions,

we can maximize the log-likelihood function separately for each parameter.

$$\begin{cases} \frac{\partial l}{\partial p} = \frac{N_{AB}}{p} - \frac{N_{AA}}{1-p} = 0 & \Rightarrow \hat{p} = \frac{N_{AB}}{N_{AA} + N_{AB}} \\ \frac{\partial l}{\partial q} = \frac{N_{BA}}{q} - \frac{N_{BB}}{1-q} = 0 & \Rightarrow \hat{q} = \frac{N_{BA}}{N_{BA} + N_{BB}} \end{cases}$$

We observe that these estimates are nothing but the relative frequencies of transitions from state s_A to state s_B and from state s_B to state s_A , respectively.

In terms of consistency, the ML estimates converge to the true parameters as the number of traces N increases. Let p_{ij}^0 be the true transition probabilities, and keep the same notation as above. Recall that $\hat{p}_{ij} = \frac{N_{ij}}{\sum_j N_{ij}}$, with $N_{ij} = \sum_{i=1}^{n-1} \mathbb{1}_{s=i}(s_t) \mathbb{1}_{s=j}(s_{t+1})$. It holds that:

$$\begin{aligned} \frac{N_{ij}}{n-1} &= \frac{1}{n-1} \sum_{t=1}^{n-1} \mathbb{1}_{s=i}(s_t) \mathbb{1}_{s=j}(s_{t+1}) \\ &\rightarrow_{n \rightarrow \infty} \mathbb{E} [\mathbb{1}_{s=i}(s_t) \mathbb{1}_{s=j}(s_{t+1})] \end{aligned}$$

Moreover, we can express:

$$\mathbb{E} [\mathbb{1}_{s=i}(s_t) \mathbb{1}_{s=j}(s_{t+1})] = P(X_t = i, X_{t+1} = j) = p_i^0 p_{ij}^0$$

with p_i^0 the long-run probability of being in state s_i . Thus, we derive that $\frac{N_{ij}}{n-1} \rightarrow p_i^0 p_{ij}^0$ as $n \rightarrow \infty$. We further note that $\sum_j N_{ij} = \sum_{i=1}^{n-1} \mathbb{1}_{s=i}(s_t)$. Putting everything together and applying the same reasoning as above:

$$\hat{p}_{ij} = \frac{\frac{N_{ij}}{n-1}}{\sum_j \frac{N_{ij}}{n-1}} \rightarrow \frac{p_i^0 p_{ij}^0}{p_i^0} = p_{ij}^0$$

Besides point estimates, we consider also their Confidence Intervals, in order to provide a measure of uncertainty on the estimates. In the case of a DTMC with two states only, we can model the probability of changing state as a Bernoulli distribution, with parameter being the transition probability. Assuming a large number of total transitions $N(n-1)$, we can apply the Central Limit Theorem to the binomial distribution and get a normal approximation of the confidence intervals for the MLE estimates, as follows:

$$\hat{p}_{ij} \pm z_{1-\frac{\alpha}{2}} \sqrt{\frac{\hat{p}_{ij}(1-\hat{p}_{ij})}{N_i}}$$

where $z_{1-\frac{\alpha}{2}}$ is the quantile of the standard normal distribution with confidence level α , and $N_i = \sum_j N_{ij}$ is the total number of transitions from state s_i . Notice that the quantity N_i highly impacts the width of the confidence interval. It is also interesting to note that the width does directly depend neither on the length of the sample, nor on the number of traces, but rather on the total number of transitions from state s_i .

1.2.2 Bayesian Inference

In order to estimate the parameters p and q using Bayesian inference, we should define a prior distribution for the parameters and compute the posterior distribution given the observed traces. As we are working with a two-state DTMC, we consider the process of changing state as a Bernoulli process, and we can use a Beta distribution as a (conjugate) prior for the parameters p and q . Specifically:

$$p \sim \text{Beta}(\alpha_p, \beta_p)$$

$$q \sim \text{Beta}(\alpha_q, \beta_q)$$

Analogously to the MLE case, we can define the likelihood function based on the observed traces. Being Beta the conjugate prior for a Bernoulli distribution, we can compute the posterior distribution in a closed form:

$$p \mid \sigma_i \sim \text{Beta}(\alpha_p^{\text{post}} = \alpha_p + N_{AB}, \beta_p^{\text{post}} = \beta_p + N_{AA})$$

$$q \mid \sigma_i \sim \text{Beta}(\alpha_q^{\text{post}} = \alpha_q + N_{BA}, \beta_q^{\text{post}} = \beta_q + N_{BB})$$

From the posterior distributions, we can compute both point estimates (as maximum a posteriori) and credibility intervals for the parameters. In particular:

$$\hat{p} = \frac{\alpha_p + N_{AB}}{\alpha_p + \beta_p + N_{AA} + N_{AB}}$$

$$\hat{q} = \frac{\alpha_q + N_{BA}}{\alpha_q + \beta_q + N_{BA} + N_{BB}}$$

while the γ -level credibility intervals can be obtained from the quantile function of the posterior distribution:

$$\left[F_{\text{Beta}}^{-1}\left(\frac{\gamma}{2}, \alpha_p^{\text{post}}, \beta_p^{\text{post}}\right), F_{\text{Beta}}^{-1}\left(1 - \frac{\gamma}{2}, \alpha_p^{\text{post}}, \beta_p^{\text{post}}\right) \right]$$

$$\left[F_{\text{Beta}}^{-1}\left(\frac{\gamma}{2}, \alpha_q^{\text{post}}, \beta_q^{\text{post}}\right), F_{\text{Beta}}^{-1}\left(1 - \frac{\gamma}{2}, \alpha_q^{\text{post}}, \beta_q^{\text{post}}\right) \right]$$

1.3 Results

To validate the theoretical results presented above, we tested our estimation techniques on a simulated DTMC with known parameters. Results are presented in the figures below.

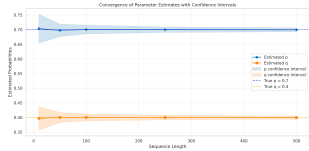


Figure 1: Convergence of the MLE estimates for p and q with increasing size of traces (number of traces fixed to 100)

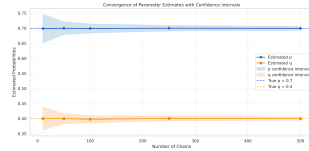


Figure 2: Convergence of the MLE estimates for p and q with increasing number of traces (length of traces fixed to 100)

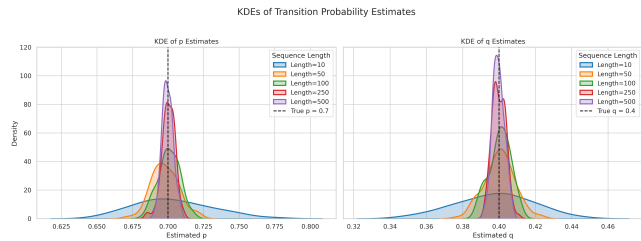


Figure 3: Distribution of the MLE estimates for p and q with increasing size of traces (length of traces fixed to 100)

The number of observations highly impacts the quality of the results, both in terms of point estimates and confidence of the estimates. Bayesian estimates are more stable and less affected by the number of observations, as they are able to adapt to the observed data and provide a more robust estimate of the parameters.

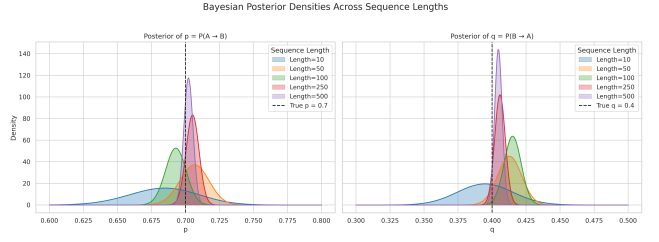


Figure 4: Distribution of the Bayesian estimates for p and q with increasing size of traces (length of traces fixed to 100)

1.4 Conclusions and considerations

From our simulations, we conclude that ML estimation is very efficient, as the solution can be found analytically, but suffers in terms of precision when the number of samples is low (≤ 10000 samples). A Bayesian approach using conjugate priors may be more appropriate, as it allows the estimates to adapt dynamically to new observations (online learning framework). This method becomes particularly effective when prior knowledge about the process parameters is available, guiding the inference towards faster convergence.

In a more general framework of a DTMC with $|S|$ states, ML estimates are given by:

$$\hat{p}_{ij} = \frac{N_{ij}}{N_i} \quad \forall i, j = 1, \dots, |S|$$

where N_{ij} is the number of transitions from state s_i to state s_j , and $N_i = \sum_j N_{ij}$ is the total number of transitions from state s_i . This simple generalization makes this approach very efficient, as the ML estimates can be computed in linear time with respect to the number of states and transitions.

Concerning confidence intervals, however, the approach is not that straight-forward. Goodman et al [3] showed that a general form of the ML confidence interval can be obtained when describing the DTMC changes of state with a Multinomial distribution. The following expression holds $\forall i, j = 1, \dots, |S|$:

$$\left[\frac{\chi_{\frac{1-\gamma}{|S|}, |S|-1}^2 + 2N_{ij} - c}{2(N_i + \chi_{\frac{1-\gamma}{|S|}, |S|-1}^2)} \leq \hat{p}_{ij} \leq \frac{\chi_{\frac{1-\gamma}{|S|}, |S|-1}^2 + 2N_{ij} + c}{2(N_i + \chi_{\frac{1-\gamma}{|S|}, |S|-1}^2)} \right]$$

with $c = \sqrt{\chi_{\frac{1-\gamma}{|S|}, |S|-1}^2 \left(\chi_{\frac{1-\gamma}{|S|}, |S|-1}^2 + 4N_{ij} \frac{(N_i - N_{ij})}{N_i} \right)}$, and $\chi_{\frac{1-\gamma}{|S|}, |S|-1}^2$ being the Chi-Squared quantile with $|S| - 1$ degrees of freedom and confidence level $\frac{1-\gamma}{|S|}$.

From a Bayesian perspective, conjugate prior families can still be leveraged when analytical tractability is desired. Modeling state transitions with a Categorical distribution pairs naturally with the Dirichlet distribution as a conjugate prior, allowing for closed-form posterior updates. However, alternative modeling strategies that do not rely on conjugate relationships (such as more flexible prior specifications or more complex hierarchical structures) may necessitate approximate inference methods such as Markov Chain Monte Carlo (MCMC) or Variational Inference.

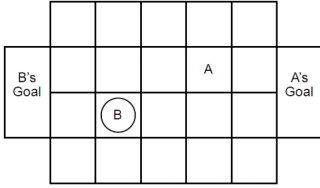
2 Multi-Agent Reinforcement Learning on Stochastic Game

In this section, we present the design and implementation of a multi-agent reinforcement learning (MARL) algorithm in a two-player zero-sum stochastic game setting. The environment is based on the simplified soccer game, originally proposed by Littman in [4].

2.1 Environment

The environment consists of a 4x5 grid populated by two players, each of whom can choose to move up, down, left, right, or remain stationary at each step. Ball possession is initially assigned at random. Both players select their actions simultaneously, which are then executed in a randomly determined order. Ball possession plays a central role in the game dynamics: when a player attempts to move into the square currently occupied by the opponent, possession is transferred to the invaded player, while the invading player's move is canceled. A player scores by reaching the opponent's goal area when in possession of the ball, receiving a reward of +1 (the opponent incurs a penalty of -1 instead). At the beginning of each match, the players are positioned as shown in Figure 5, with ball possession assigned randomly.

Figure 5: Game scheme



2.2 Learning algorithm

The implemented approach is a belief-based joint action learning algorithm that employs behavioral strategies. *Behavioral* refers to the fact that actions are sampled from a probability distribution, rather than being selected via a deterministic policy. The *belief* component indicates that, over the course of the game, each player continuously updates an estimate of the opponent's action distribution. The learning process extends the standard version of Q-learning with the following update steps (w.r.t one of the two agents):

Q-value update

$$Q_{t+1}(s_t, a_t, o_t) = (1 - \alpha_t)Q_t(s_t, a_t, o_t) + \alpha_t (r_t + \gamma V_t(s_{t+1}))$$

Policy update (using linear programming)

$$\pi_{t+1}(s_t) = \arg \max_{\pi_t(s_t)} \sum_{a_t, o_t} \pi_t(s_t)[a_t] B_{t+1}(s_t, o_t) Q_{t+1}(s_t, a_t, o_t)$$

Utility update

$$V_{t+1}(s_t) = \max_{a_t} \sum_{a_t, o_t} \pi_{t+1}(s_t)[a_t] B_{t+1}(s_t, o_t) Q_{t+1}(s_t, a_t, o_t)$$

where s_t is the joint current state of the game, a_t is the action taken by the agent, o_t is the opponent's action.

As a belief function, we use a probability distribution over the opponent's actions conditioned on the current state. This distribution is updated in an online fashion throughout the game, incorporating the opponent's observed actions to refine the estimate over time.

2.3 Experiments & Results

The learning task was carried out under two settings: (i) against a random opponent, and (ii) in self-play against another learner of identical design. In both cases, training lasted for 10^6 steps using the following parameters:

$$\alpha_0 = 1$$

$$\alpha_{t+1} = \alpha_t \cdot 10^{\log_{10}(\frac{0.01}{10^6})}$$

$$\gamma = 0.9$$

$$\epsilon = 0.2$$

After training, the learned strategies were evaluated over 10^5 test steps. Besides standard testing, an additional setting was considered in which the game could terminate early at each step with probability $1 - \gamma = 0.1$, resulting in a draw (zero reward to both players) and immediate reset of the environment. This mechanism emulates the effect of the discount factor γ during evaluation. Due to the stochastic nature of the process, the entire training and testing routine was repeated 10 times for robustness. Performance metrics are reported as 95% confidence intervals. Results are summarized in Tables 1 and 2, with the following legend on the settings: "random" and "belief" refer to the opponent's strategy while training, while "dummy" refers to a fixed strategy that always perform a random action.

Setting	Home Win %	Matches	Avg. Len.
random-dummy	94.51 \pm 0.67%	8351.40 \pm 432.02	12.03 \pm 0.65
belief _A -belief _B	53.51 \pm 4.08%	8454.60 \pm 1071.30	12.20 \pm 1.69
belief _A -dummy	89.42 \pm 1.33%	4422.20 \pm 472.39	23.03 \pm 2.28
dummy-belief _B	12.12 \pm 1.08%	3824.30 \pm 390.25	26.57 \pm 2.40

Table 1: Results without early termination

Setting	Home Win %	Matches	Avg. Len.
random-dummy	97.74 \pm 0.36%	6343.10 \pm 542.92	7.44 \pm 0.45
belief _A -belief _B	56.87 \pm 7.67%	5886.50 \pm 1276.90	8.42 \pm 1.17
belief _A -dummy	95.21 \pm 1.02%	3304.30 \pm 720.17	9.72 \pm 1.31
dummy-belief _B	6.61 \pm 1.18%	2581.90 \pm 513.34	10.79 \pm 1.03

Table 2: Results with early termination

2.4 Conclusion

The belief-based joint action learning algorithm exhibits strong adaptive capabilities across diverse opponent strategies in the stochastic soccer domain. The algorithm is able to learn a good strategy against a random opponent, achieving an expected win rate percentage of 94.51 ± 0.67 and an expected average match length of 12.03 ± 0.65 steps. When training is performed via self-play, the win rate against a random opponent slightly decreases (89.42 ± 1.33), while the average match length increases (23.03 ± 2.28). This phenomenon might be likely due to the lack of strategy in the random opponent, which can lead to atypical scenarios that were underrepresented during learning, challenging the trained agent. Moreover, the near perfect equilibrium achieved in self-play, with a win rate of 53.51 ± 4.08 , provides strong empirical evidence of convergence to an optimal strategy for both the agents.

Lastly, the sensitivity of estimates to early termination reveals important considerations about the role of temporal horizons. The marked improvement in performance against a random opponent, coupled with the stable results against a belief-based opponent, suggests that the effective discount factor plays a crucial role in shaping the learning dynamics by enhancing the agent's preference for shorter and more decisive actions.

References

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