

Operator Augmentation for Model-based Policy Evaluation

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Abstract

In model-based reinforcement learning, the transition matrix and reward vector are often estimated from random samples subject to noise. Even if the estimated model is an unbiased estimate of the true underlying model, the value function computed from the estimated model is biased. We introduce an operator augmentation method for reducing the error introduced by the estimated model. When the error is in the residual norm, we prove that the augmentation factor is always positive and upper bounded by $1 + O(1/n)$, where n is the number of samples used in learning each row of the transition matrix. We also propose a practical numerical algorithm for implementing the operator augmentation.

1 Introduction

Reinforcement learning (RL) has received much attention following recent successes, such as AlphaGo and AlphaZero [25, 26]. One of the fundamental problems of RL is policy evaluation [29]. When the transition dynamics are unknown, one learns the dynamics model from observed data in model-based RL. However, even if the learned model is an unbiased estimate of the true dynamics, the policy evaluation under the learned model is biased. The question of interest in this paper is whether one can increase the accuracy of the policy evaluation given an estimated dynamics model.

We consider a discounted Markov decision process (MDP) $\mathcal{M} = (\mathbb{S}, \mathbb{A}, P, r, \gamma)$ with discrete state space \mathbb{S} and discrete action space \mathbb{A} . $|\mathbb{S}|$ and $|\mathbb{A}|$ are used to denote the size of \mathbb{S} and \mathbb{A} , respectively. P is a third-order tensor where, for each action $a \in \mathbb{A}$, $P^a \in \mathbb{R}^{|\mathbb{S}| \times |\mathbb{S}|}$ is the transition matrix between the states. r is a second-order tensor that $r_{s,a}$ is the reward at state $s \in \mathbb{S}$ if action $a \in \mathbb{A}$ is taken. Finally, $\gamma \in (0, 1)$ is the discount factor. A policy π is a second-order tensor, where for each state $s \in \mathbb{S}$, π_s represents the probability distribution over \mathbb{A} . At each time step t , one observes a state $s_t \in \mathbb{S}$ and takes an action $a_t \in \mathbb{A}$ according to the policy π_{s_t} . The environment returns the next state s_{t+1} according to the distribution $P_{s_t}^{a_t}$, and an associated reward r_{s_t, a_t} . The state value function $v^\pi \in \mathbb{R}^{|\mathbb{S}|}$ is the expected discounted cumulative reward if one starts from an initial state s and follows a policy π , i.e., the s -th component is

$$v_s^\pi = \mathbb{E}_{\substack{a_t \sim \pi_{s_t} \\ s_{t+1} \sim P_{s_t}^{a_t}}} \left[\sum_{t \geq 0} \gamma^t r_{s_t, a_t} \mid s_0 = s \right].$$

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Given a policy π , the goal of policy evaluation in MDP is to solve for v^π . Let $b^\pi \in \mathbb{R}^{|\mathcal{S}|}$, $P^\pi \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{S}|}$ be the reward vector and the transition matrix under policy π , i.e.,

$$b^\pi = \sum_a r_{sa} \pi_s^a, \quad P^\pi = \sum_a P_{ss'}^a \pi_s^a. \quad (1.1)$$

The value function v^π satisfies the Bellman equation [29] $(I - \gamma P^\pi) v^\pi = b^\pi$. For notational simplicity, we drop the dependency on π and write this system as

$$(I - \gamma P)v = b. \quad (1.2)$$

In practice, the true transition matrix P and the reward vector b are often inaccessible. In the model-based RL, one approximates the transition matrix P and the reward vector b by the empirical data \hat{P} and \hat{b} estimated from samples, respectively [16, 6, 28, 31, 22]. A naive approach is to solve

$$(I - \gamma \hat{P}) \hat{v} = \hat{b}. \quad (1.3)$$

Even if \hat{P} and \hat{b} are unbiased estimates for P and b , $\hat{v} = (I - \gamma \hat{P})^{-1} \hat{b}$ is a biased estimate for v , i.e., $\mathbb{E}_{\hat{P}, \hat{b}} \hat{v} \neq v$.

The operator augmentation idea was introduced in [10, 9] to address this issue. The paper [10] considers the noisy symmetric elliptic systems, while the follow-up paper [9] addresses the asymmetric setting under the assumption that \hat{b} is isotropic, i.e., $\mathbb{E}[\hat{b}\hat{b}^\top] = I$. However, this isotropic condition often fails to hold in RL. In this paper, we extend the operator augmentation framework to general MDPs of form (1.2). When applying this framework to the MDP setting, we add an appropriately chosen matrix \hat{K} to the operator $(I - \gamma \hat{P})^{-1}$ so that the augmented estimate $\tilde{v} = \left[(I - \gamma \hat{P})^{-1} - \beta \hat{K} \right] \hat{b}$ is a better estimate than \hat{v} in the sense that,

$$\mathbb{E}_{\hat{P}, \hat{b}} \|\tilde{v} - v\|^2 < \mathbb{E}_{\hat{P}, \hat{b}} \|\hat{v} - v\|^2 \quad (1.4)$$

for a certain norm $\|\cdot\|$.

Contributions. We derive a stable augmented operator for model-based policy evaluation without assumptions on the underlying transition dynamics or reward vectors. When the approximated transition matrix \hat{P} follows the multinomial distribution and n samples are used to learn each row of the transition matrix P ,

- we prove that the optimal augmentation factor is always positive and upper bounded by $1 + O(\frac{1}{n})$ for any P and b , which guarantees the stability of the augmented operator, and
- we propose a numerical algorithm to find the optimal augmentation factor, which is more efficient and accurate than the bootstrapping method proposed in [10].

Related work. Our problem is a special instance of the larger field of uncertainty quantification (UQ). In most UQ problems, one assumes that the operator (linear or non-linear) and the source term are generated from known distributions, and the task is to estimate certain quantities (such as moments, tail bounds) of the distribution of the solution. A large variety of numerical methods have been developed in UQ for this purpose in the last two

decades [11, 13, 15, 33, 23, 8, 27, 17], including Monte-Carlo and quasi Monte-Carlo methods [20, 18, 4, 7, 12], stochastic collocation methods [1, 21, 34, 3], stochastic Galerkin methods [2, 35, 5, 19], and etc. The problem that we face is somewhat different: since the true P and b are unknown, one does not know the distributions of the empirical data \hat{P} or \hat{b} . As a result, the solution relies more on statistical techniques such as shrinkage [14] rather than the traditional UQ techniques.

Contents. Section 2 derives the oracle estimators and proves their lower and upper bounds. Section 3 proposes a practical estimator and demonstrates its performance with a few numerical examples. Section 4 contains all the proofs of the main results.

2 Operator Augmentation for Policy Evaluation

2.1 Problem setup

As mentioned above, P and b are the *unknown* underlying transition matrix and reward vector, while \hat{P} and \hat{b} are unbiased estimates for P and b , respectively. For notational convenience, we introduce A and \hat{A}

$$A = (I - \gamma P), \quad \hat{A} = (I - \gamma \hat{P}). \quad (2.1)$$

Since the transition dynamics is not symmetric in general, both P and A are non-symmetric in general. The norm of interest is a slightly generalized version of the residual norm

$$\|x\|_M^2 = x^\top A^\top M A x, \quad (2.2)$$

where M is a symmetric positive definite matrix. This paper mainly discusses two cases: (1) $M = I$, which means $\|\cdot\|_M$ is the usual residual norm, and (2) $M = A^{-\top} A^{-1}$, which means $\|\cdot\|_M$ is the l_2 norm.

In this paper, we choose the augmentation matrix $\hat{K} = \hat{A}^{-1}$, which implies that the augmented estimate is $(1 - \beta) \hat{A}^{-1} \hat{b}$. By using $\varepsilon = (1 - \beta)$ instead as the augmentation parameter, one can write the above estimate as $\tilde{v}_\varepsilon \equiv \varepsilon \hat{A}^{-1} \hat{b}$, and the objective is to minimize the following mean square error over ε ,

$$\text{MSE}(\varepsilon) \equiv \mathbb{E}_{\hat{P}, \hat{b}} \|v - \tilde{v}_\varepsilon\|_M^2. \quad (2.3)$$

The minimizer ε^* is referred as the *optimal augmentation factor*.

Since (2.3) is a quadratic minimization, one can explicitly write out the optimal augmentation factor ε^* :

$$\varepsilon^* = \frac{\mathbb{E}_{\hat{P}, \hat{b}} [b^\top M A \hat{v}]}{\mathbb{E}_{\hat{P}, \hat{b}} [\hat{v}^\top A^\top M A \hat{v}]}, \quad \text{where } \hat{v} = \hat{A}^{-1} \hat{b}. \quad (2.4)$$

The oracle estimate (2.4) is not easy to work with as it depends on the unknown matrix A . Our immediate goal is to derive a closed-form approximation of ε^* , which is accurate and allows for efficient implementation. To achieve this, we introduce a second-order approximation ε° to ε^* . We show that ε° takes a simple closed-form without approximating any expectations under the following mild assumption:

Assumption 1: The i -th row \hat{P}_i of \hat{P} is an independent random variable $\frac{1}{n_i}X_i$, where n_i is the number of samples for state i and X_i follows the multinomial distribution with $\mathbb{E}[X_i] = n_i P_i$. The i -th entry of \hat{b} is an average of observed reward at state i .

The part of Assumption 1 on the estimation of P is equivalent to that \hat{P}_i follows the normalized multinomial distribution, which holds when a tabular maximum likelihood model [28] is used to estimate the transition dynamics P . That is, one generates sufficiently many transitions according to P and lets $\hat{P}_{ii'} = n_{ii'}/n_i$, where $n_{ii'}$ denotes the number of transitions observed from i to i' , and $n_i = \sum_{i'} n_{ii'}$.

Throughout this paper, we assume for simplicity that the number of samples n_i of each state is the same, i.e., for any $i \in \mathbb{S}$, $n_i \equiv n$. The sample size n plays an important role in determining the magnitude of the operator augmentation factor ε^* and the performance of the operator augmentation algorithm. If the value of n_i depends on $i \in \mathbb{S}$, all the theoretical results still hold with slight modification (see Remark 2.3 for details).

2.2 Second-order approximation for ε^*

To simplify the discussion, we introduce \hat{Z} and \hat{Y}

$$\hat{Z} = A - \hat{A} = \gamma(P - \hat{P}), \quad \hat{Y} = \hat{Z}A^{-1} = (A - \hat{A})A^{-1}. \quad (2.5)$$

where A and \hat{A} are defined in (2.1). Some basic algebraic manipulations lead to the following lemma.

Lemma 2.1. *When $\mathbb{E}[\hat{b}] = b$, the optimal augmentation factor ε^* defined in (2.4) has the form*

$$\varepsilon^* = \frac{\mathbb{E}_{\hat{P}} \left[b^\top M (I - \hat{Y})^{-1} b \right]}{\mathbb{E}_{\hat{P}} \left[b^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} b \right] + \mathbb{E}_{\hat{P}} \left[\text{tr} \left(\text{cov}[\hat{b}] (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \right) \right]}, \quad (2.6)$$

where \hat{Y} is defined in (2.5). Moreover, if the values of the reward at state s and s' (i.e. \hat{b}_s and $\hat{b}_{s'}$) are uncorrelated, the matrix $\text{cov}[\hat{b}]$ is diagonal.

Next, we approximate the value of ε^* using a Neumann expansion of the matrix $(I - \hat{Y})^{-1}$

$$(I - \hat{Y})^{-1} = I + \hat{Y} + \hat{Y}^2 + O\left(\frac{\rho(\hat{Y})^3}{1 - \rho(\hat{Y})}\right), \quad (2.7)$$

when the spectral radius $\rho(\hat{Y}) < 1$. In fact, a modest requirement on n guarantees $\rho(\hat{Y}) < 1$ with high probability, as shown in Appendix A. The denominator term in (2.6) admits the approximation

$$(I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \approx M + M(\hat{Y} + \hat{Y}^2) + (\hat{Y}^\top + (\hat{Y}^\top)^2)M + \hat{Y}^\top M \hat{Y}. \quad (2.8)$$

Assumption 1 implies $\mathbb{E}[\hat{Y}] = \mathbb{E}[\hat{Y}^\top] = 0$ as a simple consequence of \hat{P} being an unbiased estimator. Therefore, after taking an expectation, the first order terms of \hat{Y} in (2.7) and (2.8) disappear.

We can further approximate the augmentation factor ε^* by expanding $(I - \hat{Y})^{-1}$ in the numerator and denominator of (2.6) up to the second order in \hat{Y} . When Assumption 1 holds and $\rho(\hat{Y}) < 1$, the approximated optimal augmentation factor ε^* defined in (2.4) has a second-order approximation

$$\varepsilon^* \approx \varepsilon^\circ \equiv \frac{\mathbb{E}_{\hat{P}} \left[b^\top (M + \frac{M\hat{Y}^2 + (\hat{Y}^\top)^2 M}{2}) b \right]}{\mathbb{E}_{\hat{P}} \left[b^\top (M + \hat{Y}^\top M \hat{Y} + M\hat{Y}^2 + (\hat{Y}^\top)^2 M) b + \text{tr} \left(\text{cov} [\hat{b}] (M + \hat{Y}^\top M \hat{Y} + M\hat{Y}^2 + (\hat{Y}^\top)^2 M) \right) \right]}. \quad (2.9)$$

The derivation of (2.9) is deferred to Section 4.2.

Under Assumption 1, this second-order approximation can be written in a form without explicit expectation. This expectation-free form depends on the transition matrix P , the expected reward b , and the reward covariance $\text{cov} [\hat{b}]$. Let \hat{p}_i be random vectors corresponding to the i -th row of \hat{P} and $p_i = \mathbb{E}[\hat{p}_i]$, i.e., $\{\hat{p}_i\}_{i=1}^{|\mathcal{S}|}$ and $\{p_i\}_{i=1}^{|\mathcal{S}|}$ are the row vectors of \hat{P} and P , respectively:

$$\hat{P} = \begin{bmatrix} \hat{p}_1^\top \\ \dots \\ \hat{p}_{|\mathcal{S}|}^\top \end{bmatrix}, \quad P = \begin{bmatrix} p_1^\top \\ \dots \\ p_{|\mathcal{S}|}^\top \end{bmatrix}. \quad (2.10)$$

Theorem 2.2. *The second-order approximation ε° in (2.9) admits the expectation-free form*

$$\varepsilon^\circ = \theta(b, P) \equiv \frac{b^\top (M + H/2) b}{b^\top (M + G + H) b + \text{tr} \left(\text{cov} [\hat{b}] (M + G + H) \right)}, \quad (2.11)$$

where

$$\begin{cases} B_i = \frac{1}{n} (\text{diag} (p_i) - p_i p_i^\top); \\ G = \mathbb{E}_{\hat{P}} [\hat{Y}^\top M \hat{Y}] = \gamma^2 A^{-\top} \left(\sum_{i=1}^{|\mathcal{S}|} [M]_{ii} B_i \right) A^{-1}; \\ H = \mathbb{E}_{\hat{P}} \left[(\hat{Y}^\top)^2 M + M \hat{Y}^2 \right] \\ = \gamma^2 \left[\sum_{i=1}^{|\mathcal{S}|} A^{-\top} B_i A^{-1} \text{diag} (e_i) \right] M + \gamma^2 M \left[\sum_{i=1}^{|\mathcal{S}|} \text{diag} (e_i) A^{-\top} B_i A^{-1} \right]. \end{cases} \quad (2.12)$$

Here $\text{diag}(e_i) \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{S}|}$ is a matrix with elements 0 except for 1 on the (i, i) -th entry, p_i are row vectors of P as defined in (2.10), and the matrices A and \hat{Y} depend on P .

The proof of the above theorem is given in Section 4.2.

Remark 2.3. *Theorem 2.2 still holds under conditions weaker than Assumption 1. Assuming the row of \hat{P} and entries for \hat{b} are independent unbiased estimators, then the second-order approximation in (2.9) is still valid. Moreover, the expectation-free form in (2.11) holds when one replaces the definition of B_i in (2.12) by $B_i = \text{cov} [\hat{p}_i]$. This slightly more general statement is presented in Lemma 4.1, from which Theorem 2.2 is derived as a special case. In particular, if the state i receives n_i samples, then (2.11) will still hold with B_i in (2.12) replaced by $\frac{1}{n_i} (\text{diag} (p_i) - p_i p_i^\top)$.*

Theorem 2.2 also proves that the choice of ε° is asymptotically as powerful as ε^* with $n \rightarrow \infty$. For $\text{MSE}(\varepsilon)$ defined in (2.3), the following estimation holds, with the proof deferred to Section 4.3.

Lemma 2.4. *The MSE in (2.3) can be approximated by*

$$\text{MSE}(\varepsilon) = (1 - \varepsilon)^2 \|b\|_M^2 + (g + h + t)\varepsilon^2 - h\varepsilon + O\left(n^{-\frac{3}{2}}\right), \quad (2.13)$$

where $g = b^\top Gb$, $h = b^\top Hb$, $t = \text{tr}\left(\text{cov}\left[\hat{b}\right](M + G + H)\right)$ with all symbols defined in Theorem 2.2. In addition,

$$\varepsilon^* - \varepsilon^\circ = O\left(n^{-\frac{3}{2}}\right). \quad (2.14)$$

2.3 Lower and upper bounds for ε°

In this section, we demonstrate that operator augmentation usually means shrinking the original solution \hat{v} . That is, we aim to provide bounds to show that ε° will approximately fall in the $(0, 1)$ range. Throughout this subsection, we conduct the analysis in the residual norm, which is the case with $M = I$. We first present an upper bound and a lower bound for ε° in Theorem 2.5, where both bounds are independent of the state size $|\mathbb{S}|$. The relevant parameters are n and γ , which are the number of samples per state and the discount factor, respectively. Later, a tighter upper bound for certain types of transition matrices and reward vectors are given in Theorem 2.7. These two theorems state that the approximation of the optimal augmentation factor ε° cannot deviate much from the desired range $(0, 1)$.

Theorem 2.5. *If $n \geq 8\frac{\gamma^2}{(1-\gamma)^2}$ and $\forall b \neq 0$, then*

$$\varepsilon^\circ(b, P) > 0.$$

Moreover, if $n \geq 16\frac{\gamma^2}{(1-\gamma)^2}$,

$$\varepsilon^\circ(b, P) \leq 1 + 8\frac{\gamma^2}{(1-\gamma)^2} \frac{1}{n}. \quad (2.15)$$

Remark 2.6. *The analysis made here is for the worst case. Hence, the constant in (2.15) is quite pessimistic. Nevertheless, in practice, for nearly all numerical examples we encountered, it suffices to take $n = 1$ and $|\mathbb{S}| > 5$ for ε° to be positive. As for an upper bound of ε° , we observe consistently that $\varepsilon^\circ < 1$ for practical cases.*

One can improve the constant of the upper bound in Theorem 2.5 when b or P is far from sparse. The reward vector b is *spread* if $\frac{\max_i |b_i|}{\|b\|_2} \sim O\left(|\mathbb{S}|^{-1/2}\right)$. Similarly, the transition matrix P is *spread* if $\max P_{ij} \sim o\left(|\mathbb{S}|^{-1/2}\right)$. One common case for $\frac{b_M}{\|b\|_2}$ being spread is that the reward b is discretized from a smooth function. For the transition matrix P , if the transition dynamics are evenly distributed, then $\max P_{ij} \sim O\left(|\mathbb{S}|^{-1}\right)$.

The following bound comes from an entirely different technique, where we explicitly use the spectral structure of the covariance matrix of a multinomial distribution and a tight bound for $(I - \gamma P)^{-1}b$.

Theorem 2.7. *Let $p_M = \max P_{i,j}$ and $b_M = \max_i |b_i|$. If $\frac{p_M}{n} \frac{\gamma^2}{(1-\gamma)^2} \left((1-\gamma) + \gamma \frac{\sqrt{|\mathbb{S}|} b_M}{\|b\|_2} \right)^2 \leq \frac{1}{2}$, then ε° is upper bounded by*

$$\varepsilon^\circ \leq 1 + \frac{p_M}{n} \frac{\gamma^2}{(1-\gamma)^2} \left((1-\gamma) + \gamma \frac{\sqrt{|\mathbb{S}|} b_M}{\|b\|_2} \right)^2.$$

Since the upper bound in Theorem 2.7 is $1 + O\left(|\mathbb{S}|^{1/2} \frac{\rho_M}{n} \frac{b_M}{\|b\|_2}\right)$, it is tighter than the one stated in Theorem 2.5 when the reward vector b or the transition matrix P is spread. When both the transition matrix P and the reward vector b are sparse, one should refer to the upper bound in Theorem 2.5, which guarantees the stability of the augmented operator when n is sufficiently large.

3 Practical algorithm

3.1 Algorithm

In practice, we do not have direct access to P or b . Therefore, the second-order estimate ε° derived in (2.11) is an oracle estimator. One can address this issue by bootstrapping the distribution of \hat{P} . More specifically, let P be a transition matrix and denote $\mathcal{M}_n(P)$ as the normalized multinomial distribution that the estimated transition matrix \hat{P} follows according to Assumption 1. Since one only has access to a single observation \hat{P} , $\mathcal{M}_n(P)$ is approximated by $\mathcal{M}_n(\hat{P})$ in the numerical implementation. In the usual bootstrapping procedure, one needs to simulate i.i.d. samples $\{\tilde{P}_{(j)}\}_{j=1}^l \sim \mathcal{M}_n(\hat{P})$. By setting $\tilde{Y}_{(j)} = (\tilde{P}_{(j)} - \hat{P})\hat{A}^{-1}$ and following the form in Theorem 2.4, one can approximate ε° in (2.9) by replacing the expectation with an empirical mean:

$$\varepsilon^\circ \approx \frac{\hat{b}^\top (M + \tilde{H}/2)\hat{b}}{\hat{b}^\top (M + \tilde{G} + \tilde{H})\hat{b} + \text{tr}(\tilde{\Sigma} (M + \tilde{G} + \tilde{H}))}, \quad (3.1)$$

with

$$\begin{cases} \tilde{G} = \frac{1}{l} \sum_{j=1}^l \tilde{Y}_{(j)}^\top M \tilde{Y}_{(j)} \approx \mathbb{E}_{\hat{P}} [\hat{Y}^\top M \hat{Y}] = G; \\ \tilde{H} = \frac{1}{l} \sum_{j=1}^l M \tilde{Y}_{(j)}^2 + (\tilde{Y}_{(j)}^\top)^2 M \approx \mathbb{E}_{\hat{P}} [M \hat{Y}^2 + (\hat{Y}^\top)^2 M] = H; \\ \tilde{\Sigma} \approx \text{cov}[\hat{b}]. \end{cases} \quad (3.2)$$

However, there is a major drawback to this scheme. In addition to the error caused by the difference between $\mathcal{M}_n(\hat{P})$ and $\mathcal{M}_n(P)$, the scheme introduces additional errors due to the empirical mean in place of the expectation. The empirical mean errors $\tilde{G} - G$ and $\tilde{H} - H$ are of order $O(l^{-1/2})$. In addition, the procedure in (3.1) has a computational cost of order $O(l|\mathbb{S}|^3)$.

Plug-in estimate. Luckily in our case, Assumption 1 (i.e., \hat{P} follows the normalized multinomial distribution) allows for a direct formula for ε° , which automatically removes the error in the empirical mean. We can simply set

$$\tilde{\varepsilon}^\circ := \theta(\hat{b}, \hat{P}), \quad (3.3)$$

where $\theta(b, P)$ is defined in Theorem 2.2. The complete numerical algorithm is presented in Algorithm 1. The right-hand side of (3.1) converges to $\theta(\hat{b}, \hat{P})$ as $l \rightarrow \infty$. In addition, the computational cost is reduced from $O(l|\mathbb{S}|^3)$ to $O(|\mathbb{S}|^3)$. This complete removal of empirical mean error is what sets the multinomial MDP case apart from general operator augmentation. Moreover, since both ε° in (2.11) and $\tilde{\varepsilon}^\circ$ in (3.3) share the same functional form, the lower and upper bounds in Section 2.3 automatically apply to both ε° and $\tilde{\varepsilon}^\circ$. In all the following numerical examples, we use the approximated factor $\tilde{\varepsilon}^\circ$, which does not rely on oracle access.

Algorithm 1 Operator Augmentation for estimating MDP (Multinomial)

Outputs the bootstrapped $\hat{\varepsilon}^\circ = \theta(\hat{b}, \hat{P})$. The function can also output the true value by $\varepsilon^\circ = \theta(b, P)$ if one has oracle access to P, b .

Require: \hat{P} : Estimated transition matrix

Require: \hat{b} : Estimated expected reward

Require: n : Sample data size per state

Require: $\hat{\Sigma}$: Estimated covariance matrix of \hat{b}

Require: γ : Discount factor

Require: M : The chosen norm matrix

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1: function  $\theta(\hat{P}, \hat{b})$ 
2:    $\hat{C}, \hat{D} \leftarrow \text{zeros}(|\mathbb{S}|)$  ▷ zeros( $n$ ): A zero matrix of size  $n$ 
3:   for  $i \leftarrow 1$  to  $|\mathbb{S}|$  do
4:      $\hat{p}_i \leftarrow \hat{P}^\top e_i$  ▷ Get the  $i$ -th row of  $\hat{P}$ 
5:      $\hat{B}_i \leftarrow \frac{1}{n} (\hat{p}_i \hat{p}_i^\top - \text{diag}(\hat{p}_i))$  ▷ Estimate covariance
6:      $\hat{C} \leftarrow \hat{C} + \hat{B}_i \hat{A}^{-1} \text{diag}(e_i)$ 
7:      $\hat{D} \leftarrow \hat{D} + [M]_{ii} \hat{B}_i$ 
8:   end for
9:    $\hat{C} \leftarrow \gamma^2 \hat{A}^{-\top} \hat{C}$  ▷ Approximate  $\mathbb{E}[(\hat{Y}^\top)^2]$ 
10:   $\hat{G} \leftarrow \gamma^2 \hat{A}^{-\top} \hat{D} \hat{A}^{-1}$  ▷ Approximate  $\mathbb{E}[\hat{Y}^\top M \hat{Y}]$ 
11:   $\hat{H} \leftarrow \hat{C} M + M \hat{C}^\top$  ▷ Approximate  $\mathbb{E}[(\hat{Y}^\top)^2 M + M \hat{Y}^2]$ 
12:   $\hat{\varepsilon}^\circ \leftarrow \frac{\hat{b}^\top (M + \hat{H}/2) \hat{b}}{\hat{b}^\top (M + \hat{G} + \hat{H}) \hat{b} + \text{tr}(\hat{\Sigma} (M + \hat{G} + \hat{H}))}$ 
13:  return  $\hat{\varepsilon}^\circ$ 
14: end function

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3.2 Examples

Policy evaluation of an MDP over a circle. We first consider an MDP over a discrete state space $\mathbb{S} = \{k\}_{k=0}^{N-1}$ with $N = 64$ and $\gamma = 0.9$. The transition dynamics are given as below,

$$s_{t+1} \leftarrow s_t + (1 + Z_t) a_t,$$

$$r_{s_t, a_t} = \sin\left(\frac{2\pi s_t}{N}\right) + a_t \cos\left(\frac{2\pi s_t}{N}\right) / 10 + X_t,$$

where $a_t \in \{\pm 1\}$ is drawn from a policy $\pi(a_t | s_t) = \frac{1}{2} + \frac{1}{5} a_t \sin\left(\frac{2\pi s_t}{N}\right)$, and $X_t \sim N(0, \delta)$ with $\delta \in \{0, 0.1, 0.2\}$. When $\delta = 0$, the reward is deterministic. Here Z_t is a random integer taking values in the set $\{-\sigma, \dots, \sigma\}$ with equal probability, where $\sigma \in \{1, 2, 4\}$. A larger σ means each state could transit to more neighboring states under one step.

Figure 1 illustrates the case where $\delta = 0.2$ and $\sigma = 4$. The red line for the augmented solution is more concentrated around the ground truth. As shown in Figure 2, for all configurations of δ and σ values, applying the operator augmentation method will significantly reduce the error.

We now explain how the performance of operator augmentation changes under different configurations of δ, σ . A larger σ means that a state can transit to more neighboring states in one step, thus causing more sampling errors with the same n . A larger error of $\hat{A}^{-1} \hat{b} - A^{-1} b$

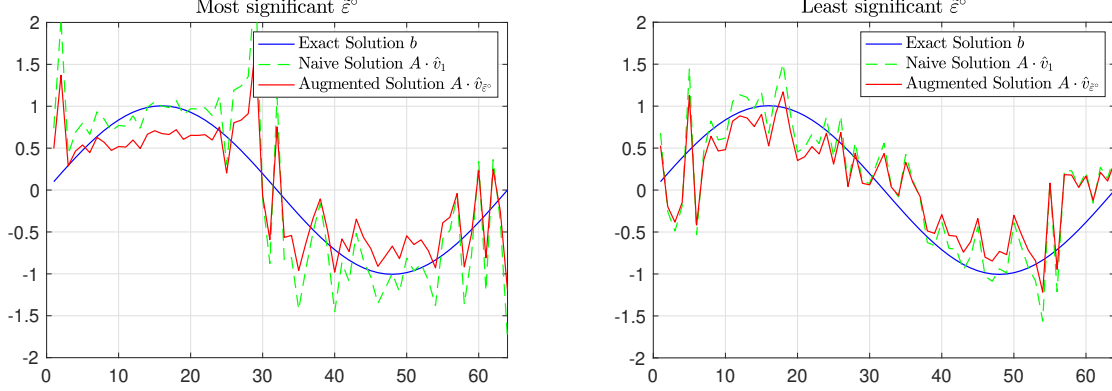


Figure 1: Comparison of the naive solution, the operator augmentation solution, and the ground truth solution, multiplied by A from the left. $n = 8$, $\delta = 0.2$, and $\sigma = 4$. Among the 60 random realizations, the plots show the two samples with the largest and smallest ε° values, i.e., the two cases where the solution is altered the most (left) and the least (right). In both cases, the operator augmentation solution is closer to the ground truth.

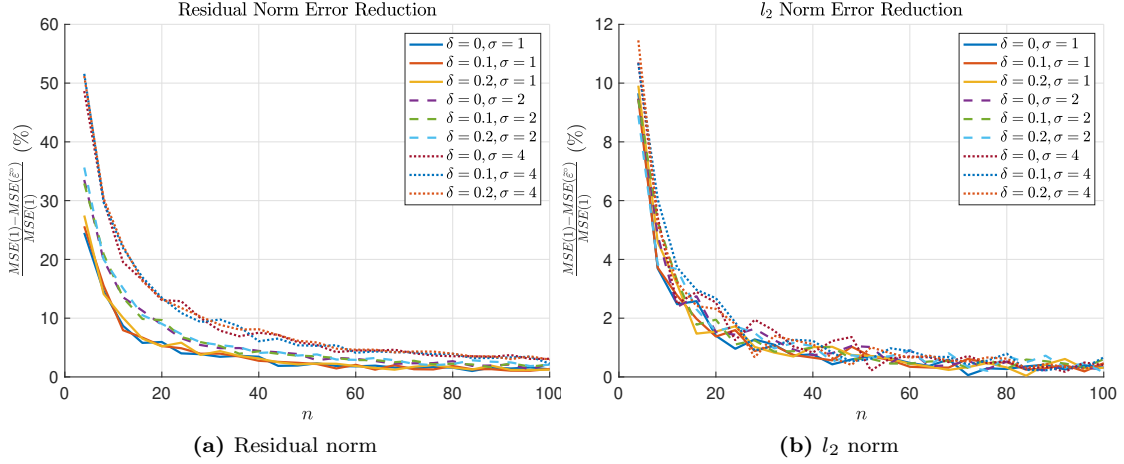


Figure 2: 1D circle example. Error reduction as a function of n for the residual norm (left) and the l_2 norm (right). The y -axis is the error reduction rate in MSE, relative to the error of the naive solution. The error reduction rate is inversely proportional to n across different choices of σ and δ . For the residual norm case, the error reduction is heavily influenced by the choice of parameters, where a larger σ or δ implies a larger reduction in error.

usually means a greater benefit from applying operator augmentation. A larger δ means more variance on the reward, which implies that the denominator of ε° in (2.11) becomes larger, and thus the value of ε° becomes smaller. Since ε° is always smaller than 1 empirically, smaller ε° means the augmented operator has more significant shrinkage effect on the solution. Overall, larger σ and δ tend to improve the performance of operator augmentation.

The relative error reduction factor $\eta \equiv \frac{\text{MSE}(1) - \text{MSE}(\varepsilon^\circ)}{\text{MSE}(1)}$, with MSE representing the mean square error defined in (2.3), is a useful measure for improvements. Below is a corollary of Lemma 2.4 regarding η .

Corollary 3.1. *The relative error reduction factor $\eta \equiv \frac{\text{MSE}(1) - \text{MSE}(\varepsilon^\circ)}{\text{MSE}(1)}$ decays as follows*

$$\eta = O(1/n), \quad (3.4)$$

where MSE is defined in (2.3).

The proof is given in Section 4.3. The numerical results also verify the relationship in the above Corollary.

One can also bootstrap to reduce the l_2 error. Specifically, the l_2 error refers to the case when $M = A^{-\top}A^{-1}$ in the norm $\|\cdot\|_M$ defined in (2.2). Despite a lack of access to A , one can use $M = \hat{A}^{-\top}\hat{A}^{-1}$ for l_2 error minimization, which works well empirically. The error reduction trend remains the same (see Figure 2 for details). Overall, the error reduction for l_2 norm is less significant than the residual norm, though it is still significant for small n .

In the following examples, we focus on the results for the residual norm.

Policy Evaluation for MDPs generated by random graphs. To test the robustness of Algorithm 1, here we apply the operator augmentation method to different underlying transition matrices. For consistency, we set $|\mathbb{S}| = 64$.

As discussed in the 1D circle case, the randomness in \hat{b} usually boosts the performance of the operator augmentation method. Here we take out the randomness in the reward and instead let \hat{b} be deterministic, i.e., $\hat{b} = b$ and $\text{cov}[\hat{b}] = 0$. To test different b , we assume that b is randomly generated according to $\mathcal{N}(0, I)$. The transition matrix P corresponds to the random walk on a directed random graph $G = (V, E, w)$, where $V = \mathbb{S}$ is the vertex set, E is the edge set, and the edge weight is $w : E \rightarrow \mathbb{R}_{\geq 0}$.

Two types of random graphs are considered. In the first *dense* case, the graph G is considered to be fully connected, and the weight $w(e)$ on each edge e is an i.i.d. random variable following $w(e) \sim \mathcal{U}(0, 1)$. In the second *sparse* case, a sparse graph is considered. In order to generate a random sparse graph, one initializes with a graph containing an empty edge set,

$$G \leftarrow G_0 := (V = \mathbb{S}, E = \emptyset).$$

For each vertex $v \in V$, two vertices v_1, v_2 are randomly selected from the set $\mathbb{S} \setminus \{v\}$ that excludes v itself with equal probability, and then

$$E \leftarrow E \cup \{(v_1, v), (v, v_2)\}.$$

After enumerating over all vertices, one then assigns a weight of one to all existing edges in G . This construction ensures that none of the vertices is a well or sink node, that is, each vertex has at least one indegree and one outdegree, but the transition matrix is still quite sparse.

Figure 3 shows that the same MSE reduction pattern holds in the random directed graph cases. The operator augmentation solution still consistently outperforms the naive solution.

Policy evaluation of an MDP over a torus. We now consider an MDP with a discrete state space $\mathbb{S} = \{s_{ij} = (i, j)\}_{i,j=0}^{N-1}$ with $N = 8$ and $\gamma = 0.9$. Note that the size of the state space $|\mathbb{S}|$ is still 64. Let $(s)_k$ stand for the first or second entry of the vector s with $k = 1$ or 2. The

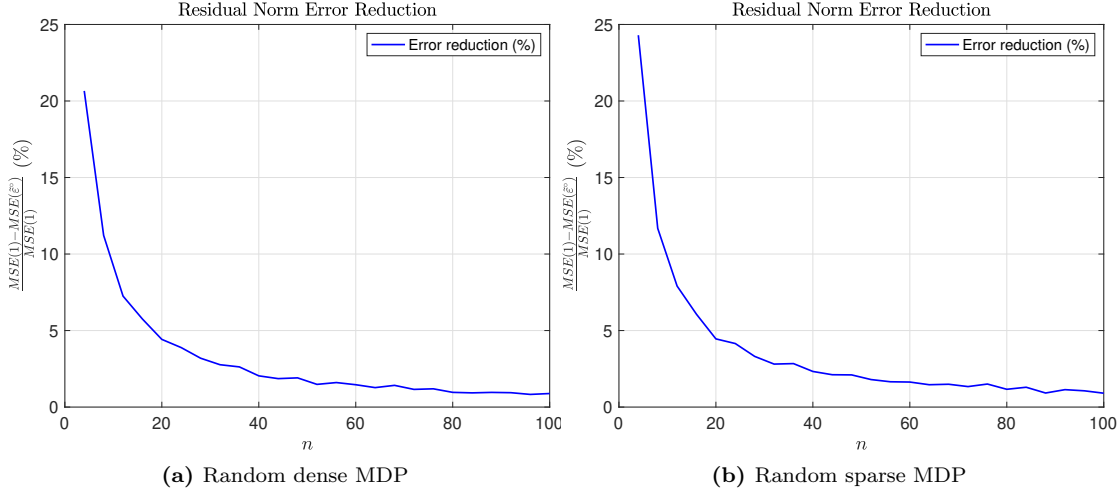


Figure 3: Random directed graphs. Error reduction as a function of sample size n . Left: the random dense graph. Right: the random sparse graph.

transition dynamics and reward are given by

$$\begin{aligned}
 s_{t+1} &\leftarrow s_t + (1 + Z_t)a_t, \\
 r_{s_t, a_t} &\leftarrow 2 + \sin\left(\frac{2\pi(s_t)_1}{N}\right) + \cos\left(\frac{2\pi(s_t)_2}{N}\right) + X_t,
 \end{aligned}$$

where $a_t \in \mathbb{A} = \{(\pm 1, 0), (0, \pm 1)\}$, $X_t \sim N(0, \delta)$ with $\delta \in \{0, 0.1, 0.2\}$. Here Z_t is a random integer taking values in the set $\{-\sigma, \dots, \sigma\}$ with equal probability, where $\sigma \in \{1, 2, 4\}$. We use the policy

$$\pi(a_t = (a_1, a_2) | s_t) = \frac{1}{4} + \frac{1}{20} \left(a_1 \cos\left(\frac{2\pi(s_t)_1}{N}\right) + a_2 \sin\left(\frac{2\pi(s_t)_2}{N}\right) \right). \quad (3.5)$$

Figure 4 summarizes the performance and exhibits a similar error reduction trend. Contrary to the role of the parameters in the 1D circle case, different choices of σ and δ do not change the performance of the operator augmentation method.

Summary of numerical experiments. Figure 5 plots the normalized MSE of the naive solution against the operator augmentation solution. In the torus and circle cases, the data points are obtained by varying the sample size n , the reward variance δ , and the transition parameter σ . In the randomly generated MDP case, the data points are obtained by sampling random MDPs and varying the value of the sample size n . The vast majority of the data points are below the diagonal line, suggesting that operator augmentation consistently reduces the MSE.

We consistently observe $\varepsilon^\circ \in (0, 1)$ even when n is as small as 4. The sample size requirements in Theorems 2.5 and 2.7 are the worst-case analysis. In practice, ε° almost always falls in the $(0, 1)$ range, even for small n .

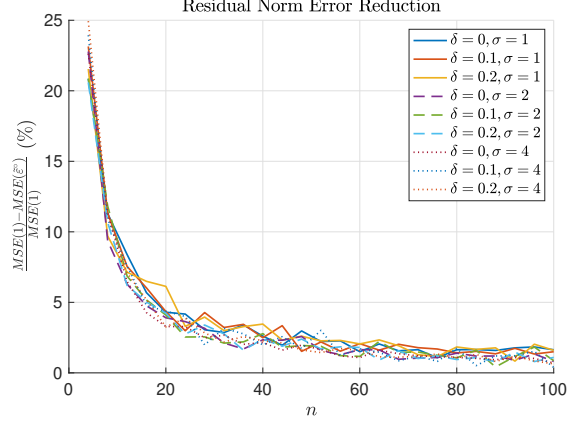


Figure 4: 2D torus example. Error reduction as a function of sample size n .

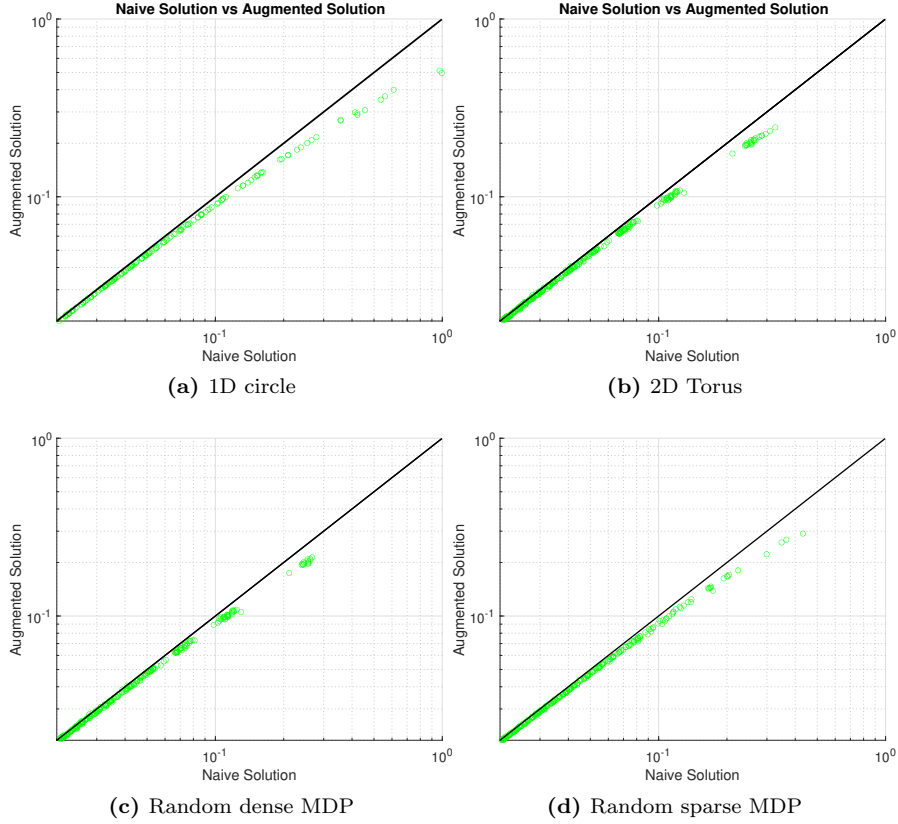


Figure 5: The normalized MSE of the operator augmentation solution is plotted against that of the naive solution. All data points are below or close to the diagonal, showing that the operator augmentation solution outperforms the naive solution in all data points collected.

4 Proofs

4.1 Proof for Lemma 2.1

Proof. From (2.5), $(I - \hat{Y})A\hat{v} = (\hat{A}A^{-1})A\hat{v} = \hat{A}\hat{v} = \hat{b}$ and

$$A\hat{v} = \left(I - \hat{Y}\right)^{-1} \hat{b}.$$

Hence (2.4) can be written as

$$\varepsilon^* = \frac{\mathbb{E}_{\hat{P}, \hat{b}} \left[b^\top M (I - \hat{Y})^{-1} \hat{b} \right]}{\mathbb{E}_{\hat{P}, \hat{b}} \left[\hat{b}^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \hat{b} \right]}.$$

From Assumption 1, $\mathbb{E}[\hat{b}] = b$. Moreover, it follows from Assumption 1 that \hat{P} is independent to \hat{b} . Hence one can write the numerator as

$$\mathbb{E}_{\hat{P}, \hat{b}} \left[b^\top M (I - \hat{Y})^{-1} \hat{b} \right] = \mathbb{E}_{\hat{P}} \left[b^\top M (I - \hat{Y})^{-1} b \right],$$

and the denominator as

$$\begin{aligned} & \mathbb{E}_{\hat{P}, \hat{b}} \left[\hat{b}^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \hat{b} \right] \\ &= \mathbb{E}_{\hat{P}} \left[b^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} b \right] + \mathbb{E}_{\hat{P}, \hat{b}} \left[(b - \hat{b})^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} (b - \hat{b}) \right]. \end{aligned}$$

One can rewrite the second term in terms of the variance of \hat{b} by the trace property

$$\mathbb{E}_{\hat{P}, \hat{b}} \left[(b - \hat{b})^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} (b - \hat{b}) \right] = \mathbb{E}_{\hat{P}} \left[\text{tr} \left(\text{cov} [\hat{b}] (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \right) \right],$$

The entries of \hat{b} are uncorrelated because as defined in (1.1),

$$\mathbb{P}(b_{s_1} = r_{s_1}^{a_1}, b_{s_2} = r_{s_2}^{a_2}) = \pi_{s_1, a_2} \pi_{s_1, a_2} = \mathbb{P}(b_{s_1} = r_{s_1}^{a_1}) \mathbb{P}(b_{s_2} = r_{s_2}^{a_2}).$$

As a result, $\text{cov} [\hat{b}]$ is a diagonal matrix as claimed. ■

4.2 Proof for Theorem 2.2 and derivation of (2.9)

Derivation of (2.9) We first show the derivation of (2.9). First one inserts the truncated Neumann series into the definition of ε^* in (2.6). According to (2.7),

$$(I - \hat{Y})^{-1} \approx I + \hat{Y} + \hat{Y}^2.$$

One has the following series of approximations by truncating out terms beyond order two

$$M (I - \hat{Y})^{-1} \approx M + M\hat{Y} + M\hat{Y}^2,$$

$$(I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \approx M + M(\hat{Y} + \hat{Y}^2) + (\hat{Y}^\top + (\hat{Y}^\top)^2)M + \hat{Y}^\top M\hat{Y}.$$

Note that $\mathbb{E}[\hat{P}] = P$ due to Assumption 1. Thus $\mathbb{E}[\hat{Y}] = 0$. Therefore, taking expectation of the above two terms gives

$$\mathbb{E}_{\hat{P}} \left[M (I - \hat{Y})^{-1} \right] \approx M + M\mathbb{E}_{\hat{P}} [\hat{Y}^2], \quad (4.1)$$

$$\mathbb{E}_{\hat{P}} \left[(I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \right] \approx M + M\mathbb{E}_{\hat{P}} [\hat{Y}^2] + \mathbb{E}_{\hat{P}} [(\hat{Y}^\top)^2] M + \mathbb{E}_{\hat{P}} [\hat{Y}^\top M\hat{Y}]. \quad (4.2)$$

Plugging (4.1) and (4.2) into (2.6) leads to

$$\begin{aligned} \varepsilon^* &= \frac{\mathbb{E}_{\hat{P}} \left[b^\top M (I - \hat{Y})^{-1} b \right]}{\mathbb{E}_{\hat{P}} \left[b^\top (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} b \right] + \mathbb{E}_{\hat{P}} \left[\text{tr} \left(\text{cov} [\hat{b}] (I - \hat{Y})^{-\top} M (I - \hat{Y})^{-1} \right) \right]} \\ &\approx \frac{\mathbb{E}_{\hat{P}} \left[b^\top (M + M\hat{Y}^2) b \right]}{\mathbb{E}_{\hat{P}} \left[b^\top (M + \hat{Y}^\top M \hat{Y} + M\hat{Y}^2 + (\hat{Y}^\top)^2 M) b + \text{tr} \left(\text{cov} [\hat{b}] (M + \hat{Y}^\top M \hat{Y} + M\hat{Y}^2 + (\hat{Y}^\top)^2 M) \right) \right]}, \end{aligned}$$

where the numerator term can be symmetrized so as to get (2.9).

Proof of Theorem 2.2 Let $N = |\mathbb{S}|$. Denote by $\{\hat{p}_i\}_{i=1}^N$ and $\{p_i\}$ the row vectors of \hat{P} and P , respectively:

$$\hat{P} = \begin{bmatrix} \hat{p}_1^\top \\ \dots \\ \hat{p}_N^\top \end{bmatrix}, \quad P = \begin{bmatrix} p_1^\top \\ \dots \\ p_N^\top \end{bmatrix}.$$

To show that ε° follows the formula in Theorem 2.2, it suffices to prove the following auxiliary lemma:

Lemma 4.1. *Assume the following two conditions hold.*

- (a): \hat{P}, \hat{b} are unbiased estimators of P, b .
- (b): X_i is independent to X_j whenever $i \neq j$.

Then one has

$$\mathbb{E} \left[\hat{Y}^\top M \hat{Y} \right] = \gamma^2 A^{-\top} \left(\sum_{i=1}^N [M_{ii} \text{cov}[\hat{p}_i]] \right) A^{-1}, \quad (4.3)$$

$$\mathbb{E} \left[\hat{Y}^2 \right] = \gamma^2 \sum_{i=1}^N \text{diag} (e_i) A^{-\top} \text{cov}[\hat{p}_i] A^{-1}, \quad (4.4)$$

$$\mathbb{E} \left[(\hat{Y}^\top)^2 \right] = \gamma^2 \sum_{i=1}^N A^{-\top} \text{cov}[\hat{p}_i] A^{-1} \text{diag} (e_i), \quad (4.5)$$

where \hat{p}_i is the random vector corresponding to the i -th row of \hat{P} .

Both conditions in Lemma 4.1 are satisfied under Assumption 1. In Theorem 2.2, one has $X_i \sim \text{multinomial}(n, p_i)$ with the following covariance structure

$$\text{cov}[\hat{p}_i] = \frac{1}{n} [\text{diag} (p_i) - p_i p_i^\top] = B_i. \quad (4.6)$$

Plugging in (4.6) in Lemma 4.1 immediately gives the expectation-free form in Lemma 2.1, which proves Theorem 2.2.

Proof. (of Lemma 4.1) We first calculate $\mathbb{E} \left[\hat{Y}^\top M \hat{Y} \right]$. To do this, we must rely on the Markov structure of the problem, i.e., the i -th row \hat{p}_i is independent to \hat{p}_j whenever $i \neq j$. As a consequence, the rows of \hat{Z} are independent. Then, for any matrix M , one has

$$\mathbb{E} \left[\hat{Y}^\top M \hat{Y} \right] = \mathbb{E} \left[A^{-\top} \hat{Z}^\top M \hat{Z} A^{-1} \right] = A^{-\top} \mathbb{E} \left[\hat{Z}^\top M \hat{Z} \right] A^{-1}.$$

By denoting the rows of \hat{Z} by $\hat{z}_1^\top, \dots, \hat{z}_N^\top$,

$$\hat{Z}^\top M \hat{Z} = \begin{bmatrix} \hat{z}_1 & \dots & \hat{z}_N \end{bmatrix} M \begin{bmatrix} \hat{z}_1^\top \\ \dots \\ \hat{z}_N^\top \end{bmatrix} = \sum_{i,j=1}^N \hat{z}_i M_{ij} \hat{z}_j^\top$$

By taking the expectation, the only non-zero terms are the ones with $i = j$. Hence,

$$\mathbb{E} \left[\hat{Z}^\top M \hat{Z} \right] = \sum_{i=1}^N M_{ii} \mathbb{E} \left[\hat{z}_i \hat{z}_i^\top \right]$$

Then by definition of \hat{Z} one has

$$\mathbb{E} \left[\hat{z}_i \hat{z}_i^\top \right] = \gamma^2 \mathbb{E} \left[(\hat{p}_i - \mathbb{E}[\hat{p}_i]) (\hat{p}_i - \mathbb{E}[\hat{p}_i])^\top \right] = \gamma^2 \text{cov}[\hat{p}_i] \quad (4.7)$$

Hence one can get the first part of Lemma 4.1, which is

$$\mathbb{E} \left[\hat{Y}^\top M \hat{Y} \right] = A^{-\top} \mathbb{E} \left[\hat{Z}^\top M \hat{Z} \right] A^{-1} = \gamma^2 A^{-\top} \left(\sum_{i=1}^N M_{ii} \text{cov}[\hat{p}_i] \right) A^{-1}.$$

Now we move on to proving the form of $\mathbb{E} \left[\hat{Y}^2 \right]$. Writing out \hat{Y}^2 explicitly

$$\hat{Y}^2 = \hat{Z} A^{-1} \hat{Z} A^{-1} = \begin{bmatrix} \hat{z}_1^\top A^{-1} \\ \dots \\ \hat{z}_N^\top A^{-1} \end{bmatrix} \begin{bmatrix} \hat{z}_1^\top \\ \dots \\ \hat{z}_N^\top \end{bmatrix} A^{-1} = \sum_{i=1}^N \sum_{j=1}^N \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top A^{-1} \\ \dots \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ \dots \\ \hat{z}_j^\top \\ \dots \\ 0 \end{bmatrix} A^{-1}.$$

After the expectation, the only non-zero terms are $i = j$. Thus one has

$$\mathbb{E} \left[\hat{Y}^2 \right] = \sum_{i=1}^N \mathbb{E} \left[\begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top A^{-1} \\ \dots \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top \\ \dots \\ 0 \end{bmatrix} \right] A^{-1},$$

with

$$\left(\begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top A^{-1} \\ \dots \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top \\ \dots \\ 0 \end{bmatrix} \right)_{jk} = \begin{cases} \sum_{l=1}^N \hat{Z}_{il} A_{li}^{-1} \hat{Z}_{ik} & j = i \\ 0 & j \neq i. \end{cases}$$

For the matrix $A^{-\top} \hat{z}_i \hat{z}_i^\top$, note that

$$\left[A^{-\top} \hat{z}_i \hat{z}_i^\top \right]_{jk} = (A^{-\top} \hat{z}_i)_j (\hat{z}_i^\top)_k = \sum_{l=1}^N A_{jl}^{-\top} \hat{Z}_{il} \hat{Z}_{ik} = \sum_{l=1}^N A_{lj}^{-1} \hat{Z}_{il} \hat{Z}_{ik}$$

Applying $j = i$ leads to

$$\left[\text{diag}(e_i) A^{-\top} \hat{z}_i \hat{z}_i^\top \right]_{jk} = \begin{cases} \sum_{l=1}^N \hat{Z}_{il} A_{li}^{-1} \hat{Z}_{ik} & j = i \\ 0 & j \neq i \end{cases}.$$

Hence we have

$$\begin{aligned}\mathbb{E}[\hat{Y}^2] &= \sum_{i=1}^N \mathbb{E} \left[\begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top A^{-1} \\ \dots \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top \\ \dots \\ 0 \end{bmatrix} \right] A^{-1} = \sum_{i=1}^N \mathbb{E} \left[\text{diag}(e_i) \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top A^{-1} \\ \dots \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ \dots \\ \hat{z}_i^\top \\ \dots \\ 0 \end{bmatrix} \right] A^{-1} \\ &= \sum_{i=1}^N \mathbb{E} [\text{diag}(e_i) A^{-\top} \hat{z}_i \hat{z}_i^\top] A^{-1} = \sum_{i=1}^N \text{diag}(e_i) A^{-\top} \mathbb{E} [\hat{z}_i \hat{z}_i^\top] A^{-1}.\end{aligned}$$

Taking transpose results in

$$\mathbb{E}[(\hat{Y}^\top)^2] = \sum_{i=1}^N A^{-\top} \mathbb{E}[\hat{z}_i \hat{z}_i^\top] A^{-1} \text{diag}(e_i).$$

■

4.3 Proof of Lemma 2.4 and Corollary 3.1

Proof of Lemma 2.4 Going back to the original quadratic optimization problem, one has

$$\mathbb{E}_{\hat{P}, \hat{b}} \|b - \varepsilon A \hat{v}\|_M^2 = \varepsilon^2 \mathbb{E}_{\hat{P}, \hat{b}} \|A \hat{v}\|_M^2 - 2\varepsilon \mathbb{E}_{\hat{P}, \hat{b}} [b^\top M A \hat{v}] + \|b\|_M^2. \quad (4.8)$$

Using Lemma 2.1 and the second-order approximation in equation (2.9), we have

$$\mathbb{E}_{\hat{P}, \hat{b}} [b^\top M A \hat{v}] = \mathbb{E}_{\hat{P}} \left[b^\top \left(M + \frac{M \hat{Y}^2 + (\hat{Y}^\top)^2 M}{2} \right) b \right] + h.o.t.,$$

and

$$\begin{aligned}\mathbb{E}_{\hat{P}, \hat{b}} \|A \hat{v}\|_M^2 &= \mathbb{E}_{\hat{P}} \left[b^\top (M + \hat{Y}^\top M \hat{Y} + M \hat{Y}^2 + (\hat{Y}^\top)^2 M) b \right] \\ &\quad + \mathbb{E}_{\hat{P}} \left[\text{tr} \left(\text{cov}[\hat{b}] (M + \hat{Y}^\top M \hat{Y} + M \hat{Y}^2 + (\hat{Y}^\top)^2 M) \right) \right] + h.o.t.,\end{aligned}$$

where *h.o.t.* stands for high order terms.

We now show that *h.o.t.* = $O(n^{-\frac{3}{2}})$. The expectation of the third order or higher terms in \hat{Y} is computed by moments of third order or higher in \hat{Z} . Under Assumption 1, rows of \hat{Z} are independent, and hence moments of \hat{Z} are linear combinations of moments in multinomial distribution. Each row of matrix \hat{Z} is an average of n random variables with mean zero, which is why its moments of third order or higher decay at the rate of at least $O(n^{-\frac{3}{2}})$ by use of the Marcinkiewicz-Zygmund inequality.

One can then plug in the explicit formula from Lemma 4.1 and (4.6), leading to

$$\mathbb{E}_{\hat{P}, \hat{b}} [b^\top M A \hat{v}] = \|b\|_M^2 + b^\top H b / 2 + O(n^{-\frac{3}{2}}) = \|b\|_M^2 + h/2 + O(n^{-\frac{3}{2}}).$$

and

$$\begin{aligned}\mathbb{E}_{\hat{P}, \hat{b}} \|A \hat{v}\|_M^2 &= \|b\|_M^2 + b^\top G b + b^\top H b + \text{tr} \left(\text{cov}[\hat{b}] (M + G + H) \right) + O(n^{-\frac{3}{2}}) \\ &= \|b\|_M^2 + h + g + t + O(n^{-\frac{3}{2}}).\end{aligned}$$

Plugging it into (4.8) results in (2.13).

We now move to prove (2.14). From (4.8) and the results before, one has

$$\varepsilon^* = \frac{\|b\|_M^2 + h/2 + O\left(n^{-\frac{3}{2}}\right)}{\|b\|_M^2 + h + g + t + O\left(n^{-\frac{3}{2}}\right)}.$$

Note that the choice of ε° in Theorem 2.2 essentially optimizes for the approximate objective

$$\widetilde{\text{MSE}}(\varepsilon) = (1 - \varepsilon)^2 \|b\|_M^2 + (g + h + t)\varepsilon^2 - h\varepsilon.$$

Thus

$$\varepsilon^\circ = \frac{\|b\|_M^2 + h/2}{\|b\|_M^2 + h + g + t}. \quad (4.9)$$

From Theorem 2.2, it follows that $G, H, \text{cov}[\hat{b}] \propto \frac{1}{n}$, and therefore $g, h, t \propto \frac{1}{n}$. Hence (2.14) holds and ε° is asymptotically optimal.

Proof of Corollary 3.1 Without loss of generality, assume that $\|b\|_M^2 = 1$. When $\varepsilon = 1$, one is using the solution without any operator augmentation, and the MSE error in (2.13) is thus equal to

$$\text{MSE}(1) = (g + t) + o(1/n) = O(1/n), \quad (4.10)$$

where the last equality is due to $g, t \propto \frac{1}{n}$. By some algebra, one can see that

$$\text{MSE}(1) - \text{MSE}(\varepsilon^\circ) = \frac{(g + h/2 + t)^2}{1 + (g + h + t)} + o\left(\frac{1 - \varepsilon^\circ}{n}\right). \quad (4.11)$$

We first deal with the nuisance term $o\left(\frac{1 - \varepsilon^\circ}{n}\right)$, note that by simple algebra from (4.9), one has

$$1 - \varepsilon^\circ = \frac{g + t + h/2}{1 + g + h + t} \quad (4.12)$$

From Theorem 2.2, it follows that $G, H, \text{cov}[\hat{b}] \propto \frac{1}{n}$, and therefore $g, h, t \propto \frac{1}{n}$. Thus one has from (4.12) that $1 - \varepsilon^\circ = O(1/n)$. Therefore, the nuisance term $o\left(\frac{1 - \varepsilon^\circ}{n}\right) = o(1/n^2)$. Also due to $g, h, t \propto \frac{1}{n}$, the first term in the right hand side of (4.11) is $O(1/n^2)$. Thus we've proved

$$\text{MSE}(1) - \text{MSE}(\varepsilon^\circ) = O(1/n^2).$$

The relative error reduction is $O(1/n)$. Hence by (4.10) and (4.11), it follows that

$$\eta = \frac{\text{MSE}(1) - \text{MSE}(\varepsilon^\circ)}{\text{MSE}(1)} = O(1/n).$$

4.4 Proof of Theorem 2.5

Proof. We define a new term

$$H_k = \mathbb{E}_{\hat{P}} [Y^2 + (Y^\top)^2 | n = k].$$

Using the result in Theorem 2.2 and $M = I$, one can write H_k explicitly

$$H_k = \frac{\gamma^2}{k} \left[\sum_{i=1}^{|\mathcal{S}|} A^{-\top} (\text{diag}(p_i) - p_i p_i^\top) A^{-1} \text{diag}(e_i) + \sum_{i=1}^{|\mathcal{S}|} \text{diag}(e_i) A^{-\top} (\text{diag}(p_i) - p_i p_i^\top) A^{-1} \right].$$

Since A and p_i are independent of k , $H_k = \frac{1}{k}H_1$. The proof depends on the following bound

$$H_1 \succeq -8 \frac{\gamma^2}{(1-\gamma)^2} I. \quad (4.13)$$

Assuming (4.13) is true, one has the following bound for general H

$$H = H_n \succeq -\frac{8}{n} \frac{\gamma^2}{(1-\gamma)^2} I. \quad (4.14)$$

Thus in this case it suffices to take $n \geq 8 \frac{\gamma^2}{(1-\gamma)^2}$ to ensure $I + H$ is a SPD matrix. By the same bound the matrix $I + H/2$ can be shown to be SPD. Since G is already a SPD matrix, (2.11) leads to $\varepsilon^\circ \geq 0$.

To prove the upper bound (4.13), we introduce $h = b^\top H b$. Without loss of generality, we can assume $b^\top b = 1$. Since both $b^\top G b$ and the term involving trace are positive,

$$\varepsilon^\circ \leq \frac{1 + h/2}{1 + h}.$$

From (4.14), $h \geq -\frac{8}{n} \frac{\gamma^2}{(1-\gamma)^2}$. By introducing $\omega = 4 \frac{\gamma^2}{(1-\gamma)^2}$, we can bound by

$$\varepsilon^\circ \leq \frac{1 - \omega/n}{1 - 2\omega/n} = 1 + \frac{\omega/n}{1 - 2\omega/n}.$$

Under the condition that $n \geq 16 \frac{\gamma^2}{(1-\gamma)^2}$, one has $1 - 2\omega/n > 1/2$ and hence

$$\varepsilon^\circ \leq 1 + 2\omega/n = 1 + 8 \frac{\gamma^2}{(1-\gamma)^2} \frac{1}{n}.$$

It remains to prove (4.13). We use the fact that each row of a transition matrix only has non-negative entries and sums to one. Therefore one has $\|P\|_\infty = 1$ for any transition matrix. Similarly, $\|A^{-1}\|_\infty = \frac{1}{1-\gamma}$. Then by basic matrix norm inequality one has

$$\left\| \hat{Y}^2 + (\hat{Y}^\top)^2 \right\|_2 = \rho \left(\hat{Y}^2 + (\hat{Y}^\top)^2 \right) \leq \rho(\hat{Y}^2) + \rho \left((\hat{Y}^\top)^2 \right) = 2\rho \left(\hat{Y}^2 \right) \leq 2 \left\| \hat{Y} \right\|_\infty^2.$$

One can further bound $\left\| \hat{Y} \right\|_\infty \leq \left\| \hat{Z} \right\|_\infty \|A^{-1}\|_\infty = \frac{\gamma}{1-\gamma} \|P - \hat{P}\|_\infty$. By triangle inequality, $\left\| P - \hat{P} \right\|_\infty \leq \|P\|_\infty + \left\| \hat{P} \right\|_\infty = 2$. From these two bounds, we have

$$\left\| \hat{Y}^2 + (\hat{Y}^\top)^2 \right\|_2 \leq 2 \frac{\gamma^2}{(1-\gamma)^2} \left\| P - \hat{P} \right\|_\infty^2 \leq 8 \frac{\gamma^2}{(1-\gamma)^2}.$$

Hence, regardless of n , $H = \mathbb{E}_{\hat{P}} \left[\hat{Y}^2 + (\hat{Y}^\top)^2 \right] \succeq -8 \frac{\gamma^2}{(1-\gamma)^2} I$. In particular, when $n = 1$, one has $H_1 \succeq -8 \frac{\gamma^2}{(1-\gamma)^2} I$. ■

4.5 Proof of Theorem 2.7

To prove Theorem 2.7, one first finds a tight bound for $A^{-1}b$ and $A^{-1}\text{diag}(e_i)b$. The tight upper and lower bounds for $A^{-1}b$ are stated in Lemma 4.2. Then, the upper bounds for $\|A^{-1}b\|^2$ and $\sum_i \|A^{-1}\text{diag}(e_i)b\|^2$ are listed in Corollary 4.4. Finally, based on Corollary 4.4, we derive the upper bound for ε° in Theorem 2.7.

Lemma 4.2. For any transition matrix $P \in \mathbb{R}^{|\mathbb{S}| \times |\mathbb{S}|}$, vector $b \in \mathbb{R}^{|\mathbb{S}|}$ and $\gamma \in (0, 1)$,

$$b + \frac{\gamma}{1-\gamma} b_m \mathbf{1} \leq (I - \gamma P)^{-1} b \leq b + \frac{\gamma}{1-\gamma} b_M \mathbf{1},$$

where $b_m = \min_s b_s, b_M = \max_s b_s$.

Proof. Let $x = (I - \gamma P)^{-1} b$, and $s = \operatorname{argmin}_i x_i$, then the s -th row of $(I - \gamma P)x = b$ is

$$b_s = x_s - \gamma \sum_t P_{st} x_t \leq x_s - \gamma \sum_t P_{st} x_s = (1 - \gamma) x_s,$$

which implies

$$x_s \geq \frac{b_s}{1-\gamma} \geq \frac{b_m}{1-\gamma}, \quad (4.15)$$

where $b_m = \min_s b_s$. For $\forall j \neq s$, one has

$$b_j = x_j - \gamma \sum_t P_{jt} x_t \leq x_j - \gamma \sum_t P_{st} x_s = x_j - \gamma x_s \leq x_j - \gamma \frac{b_m}{1-\gamma},$$

which yields,

$$x_j \geq b_j + \frac{\gamma}{1-\gamma} b_m. \quad (4.16)$$

Combining (4.15) and (4.16) gives

$$x = (I - \gamma P)^{-1} b \geq b + \frac{\gamma}{1-\gamma} b_m \mathbf{1}.$$

On the other hand, let $l = \operatorname{argmax}_i x_i$, then the l -th row of $(I - \gamma P)x = b$ is

$$b_l = x_l - \gamma \sum_t P_{lt} x_t \geq x_l - \gamma \sum_t P_{lt} x_l = (1 - \gamma) x_l,$$

which implies

$$x_l \leq \frac{b_l}{1-\gamma} \leq \frac{b_M}{1-\gamma}, \quad (4.17)$$

where $b_M = \max_s b_s$. For $\forall j \neq l$, one has

$$b_j = x_j - \gamma \sum_t P_{jt} x_t \geq x_j - \gamma \sum_t P_{jt} x_l = x_j - \gamma \frac{b_M}{1-\gamma},$$

which yields,

$$x_j \leq b_j + \frac{\gamma}{1-\gamma} b_M. \quad (4.18)$$

Combining (4.17) and (4.18) gives

$$x = (I - \gamma P)^{-1} b \leq b + \frac{\gamma}{1-\gamma} b_M \mathbf{1},$$

which completes the proof. ■

Lemma 4.3. For any transition matrix P , vector $b \in \mathbb{R}^{|\mathbb{S}|}$ and $\gamma \in (0, 1)$,

$$|(I - \gamma P)^{-1} b| \leq (I - \gamma P)^{-1} |b|.$$

Proof. Let $x = (I - \gamma P)^{-1}b$ and denote by b_+, b_- the positive and negative parts of b , respectively. That is, $(b_+)_i = b_i \mathbb{1}_{b_i > 0}$ and $(b_-)_i = b_i \mathbb{1}_{b_i < 0}$. Applying the bound in Lemma 4.2 gives,

$$(I - \gamma P)^{-1}b_+ \geq \mathbf{0}, \quad (I - \gamma P)^{-1}b_- \leq \mathbf{0}.$$

Since $x = (I - \gamma P)^{-1}b_+ + (I - \gamma P)^{-1}b_-$, one has $x \leq (I - \gamma P)^{-1}b_+ - (I - \gamma P)^{-1}b_-$ and $-x \leq (I - \gamma P)^{-1}b_+ - (I - \gamma P)^{-1}b_-$. Hence

$$|x| \leq (I - \gamma P)^{-1}b_+ - (I - \gamma P)^{-1}b_- = (I - \gamma P)^{-1}|b|.$$

■

Corollary 4.4. For any transition matrix P , vector $b \in \mathbb{R}^{|\mathbb{S}|}$ and $\gamma \in (0, 1)$, one has,

$$\left\| (I - \gamma P)^{-1}b \right\|_2 \leq \|k\|_2, \quad \sum_i \left\| (I - \gamma P)^{-1} \text{diag}(\cdot) e_i b \right\|_2^2 \leq \|k\|_2^2, \quad \sum_i \left\| (I - \gamma P)^{-1} \text{diag}(\cdot) e_i b \right\|_2 \leq \sqrt{|\mathbb{S}|} \|k\|_2,$$

where $k = \frac{1}{1-\gamma} ((1-\gamma)|b| + \gamma b_M)$ with $b_M = \max_i |b_i|$ and

$$\|k\|_2^2 = \frac{1}{(1-\gamma)^2} \left((1-\gamma)^2 \|b\|_2^2 + |\mathbb{S}| \gamma^2 b_M^2 + 2\gamma(1-\gamma) b_M \|b\|_1 \right).$$

Proof. First, Lemmas 4.2 and 4.3 lead to

$$\left| (I - \gamma P)^{-1}b \right| \leq (I - \gamma P)^{-1}|b| \leq k = \frac{1}{1-\gamma} ((1-\gamma)|b| + \gamma b_M),$$

where $b_M = \max_i |b_i|$, which is the first inequality in the corollary. The second inequality is because

$$\sum_i \left\| (I - \gamma P)^{-1} \text{diag}(e_i) b \right\|_2^2 \leq \left\| \sum_i \left| (I - \gamma P)^{-1} \text{diag}(e_i) b \right| \right\|_2^2 \leq \left\| (I - \gamma P)^{-1}|b| \right\|_2^2 \leq \|k\|_2^2.$$

The third inequality is due to

$$\sum_i \left\| (I - \gamma P)^{-1} \text{diag}(e_i) b \right\|_2 \leq \sqrt{|\mathbb{S}|} \left\| \sum_i \left| (I - \gamma P)^{-1} \text{diag}(e_i) b \right| \right\|_2 \leq \sqrt{|\mathbb{S}|} \left\| (I - \gamma P)^{-1}|b| \right\|_2 \leq \sqrt{|\mathbb{S}|} \|k\|_2.$$

■

Now we are ready to proof Theorem 2.7.

Proof of Theorem 2.7 Since B_i is the covariance matrix, $B_i \succeq 0$. By the definition of G, H in Theorem 2.2, one has $\text{tr} \left(\text{cov} \left[\hat{b} \right] (I + G + H) \right) \geq 0$. By letting $a_i = (I - \gamma P)^{-1} \text{diag}(e_i) b$ and $d = (I - \gamma P)^{-1} b$,

$$\begin{aligned} \varepsilon^\circ &\leq \frac{\frac{1}{\gamma^2} b^\top b + \sum_i a_i^\top B_i d}{\frac{1}{\gamma^2} b^\top b + \sum_i d^\top B_i d + 2 \sum_i a_i^\top B_i d} = 1 - \frac{\sum_i d^\top B_i d + \sum_i a_i^\top B_i d}{\frac{1}{\gamma^2} b^\top b + \sum_i d^\top B_i d + 2 \sum_i a_i^\top B_i d} \\ &= 1 + \frac{\frac{1}{2} \sum_i a_i^\top B_i a_i - \frac{1}{2} \sum_i (a_i + d)^\top B_i (a_i + d) - \frac{1}{2} \sum_i d^\top B_i d}{\frac{1}{\gamma^2} b^\top b + \sum_i (a_i + d)^\top B_i (a_i + d) - \sum_i a_i^\top B_i a_i} \end{aligned} \quad (4.19)$$

The numerator of the second term in (4.19) can be bounded by

$$\frac{1}{2} \sum_i a_i^\top B_i a_i - \frac{1}{2} \sum_i (a_i + d)^\top B_i (a_i + d) - \frac{1}{2} \sum_i d^\top B_i d \leq \frac{1}{2} \lambda_M \sum_i \|a_i\|_2^2,$$

where λ_M is the largest eigenvalue of B_i for $\forall i$.

Suppose that $\frac{\lambda_M \|k\|_2^2}{\frac{1}{\gamma^2} b^\top b} \leq \frac{1}{2}$. Then the denominator of the second term of (4.19) can be lower bounded by

$$\frac{1}{\gamma^2} b^\top b + \sum_i (a_i + d)^\top B_i (a_i + d) - \sum_i a_i^\top B_i a_i \geq \frac{1}{\gamma^2} b^\top b - \lambda_M \|k\|_2^2 > 0,$$

where $\sum_i \|a_i\|_2^2 \leq \|k\|_2^2$ from Corollary 4.4 is used. Therefore, (4.19) can be bounded by

$$\varepsilon^\circ \leq 1 + \frac{\frac{1}{2} \lambda_M \|k\|_2^2}{\frac{1}{\gamma^2} b^\top b - \lambda_M \|k\|_2^2} \leq 1 + \frac{\lambda_M \|k\|_2^2}{\frac{1}{\gamma^2} b^\top b}.$$

Note that

$$\begin{aligned} \frac{\|k\|_2^2}{\frac{1}{\gamma^2} \|b\|_2^2} &\leq \frac{\gamma^2 \left((1-\gamma)^2 \|b\|_2^2 + n\gamma^2 b_M^2 + 2\gamma(1-\gamma) b_M \|b\|_1 \right)}{(1-\gamma)^2 \|b\|_2^2} \\ &\leq \frac{\gamma^2 \left((1-\gamma)^2 + n\gamma^2 \frac{b_M^2}{\|b\|_2^2} + 2\gamma(1-\gamma) \sqrt{n} \frac{b_M}{\|b\|_2} \right)}{(1-\gamma)^2} = \frac{\gamma^2}{(1-\gamma)^2} \left((1-\gamma) + \gamma \frac{\sqrt{n} b_M}{\|b\|_2} \right)^2. \end{aligned} \quad (4.20)$$

where $\|b\|_1 \leq \sqrt{n} \|b\|_2$ is used in the above inequality. The largest eigenvalue λ_M of B_i defined in (2.12) is smaller than $\lambda_M < \frac{p_M}{n}$, where $p_M = \max_{i,j} P_{i,j}$ is the maximum probability of the transition matrix P [30]. This implies that

$$\frac{\lambda_M \|k\|_2^2}{\frac{1}{\gamma^2} \|b\|_2^2} \leq \frac{p_M}{n} \frac{\gamma^2}{(1-\gamma)^2} \left((1-\gamma) + \gamma \frac{\sqrt{n} b_M}{\|b\|_2} \right)^2 \leq \frac{1}{2}$$

by assumption. Therefore,

$$\varepsilon^\circ \leq 1 + \frac{p_M}{n} \frac{\gamma^2}{(1-\gamma)^2} \left((1-\gamma) \gamma \frac{\sqrt{n} b_M}{\|b\|_2} \right)^2,$$

which completes the proof.

Appendices

A Condition for Convergence of Neumann Series

The spectral radius $\rho(\hat{Y})$ of \hat{Y} can be bounded by the size of state space $|\mathbb{S}|$, the number of samples n used to learn the model P and the number of possible transitions. We define κ as the largest number of transitions among all states,

$$\kappa = \max_{s \in \mathbb{S}} \{k : k = \|P_s\|_0, P_s \text{ is the } s\text{-th row of } P\}. \quad (\text{A.1})$$

The following lemma gives the condition for $\rho(\hat{Y}) < 1$ with high probability. The proof relies on the concentration inequality of l_1 -norm of the multinomial distribution.

Lemma A.1. *Under Assumption 1, for any $C > 0$ and any positive integer $q > 1$, if $n \geq \frac{2C^2\gamma^2\kappa}{(1-\gamma)^2} \log(2|\mathbb{S}|^q)$,*

$$\mathbb{P} \left[\rho(\hat{Y}) < \frac{1}{C} \right] \geq 1 - \frac{1}{|\mathbb{S}|^{q-1}}.$$

Proof. We have

$$\rho(\hat{Y}) \leq \|\hat{Y}\|_\infty \leq \|\hat{Z}\|_\infty \|A^{-1}\|_\infty = \frac{\gamma}{1-\gamma} \|P - \hat{P}\|_\infty.$$

By the concentration inequality in [32, 24], for arbitrary $r \in [0, 1]$

$$\mathbb{P} \left[\left\| e_i^\top (\hat{P} - P) \right\|_1 \geq \frac{\sqrt{2\kappa \log 2/r}}{\sqrt{n}} \right] \leq r. \quad (\text{A.2})$$

Taking union bound and setting $r = \frac{1}{|\mathbb{S}|^q}$ leads to

$$\mathbb{P} \left[\left\| P - \hat{P} \right\|_\infty \geq \frac{\sqrt{2\kappa \log 2 |\mathbb{S}|^q}}{\sqrt{n}} \right] \leq 1 - (1 - 1/|\mathbb{S}|^q)^{|\mathbb{S}|} \leq 1/|\mathbb{S}|^{q-1},$$

where the second inequality is by Bernoulli's inequality: for $r \geq 1$ and $x \leq 1$,

$$(1-x)^r \geq 1 - rx.$$

The proof is completed by noticing

$$\frac{\sqrt{2\kappa \log 2 |\mathbb{S}|^q}}{\sqrt{n}} \leq \frac{1}{C} \iff n \geq \frac{2C^2\gamma^2\kappa}{(1-\gamma)^2} \log(2|\mathbb{S}|^q)$$

■

Remark A.2. *In particular, our goal is to show a bound of n to ensure that $\rho(\hat{Y}) < 1$ with high probability. In this case, the sample size requirement is*

$$n \geq \frac{2\gamma^2\kappa}{(1-\gamma)^2} \log(2|\mathbb{S}|^q).$$

The requirement of sample size n only grows at the rate of $O(\kappa \log(|\mathbb{S}|))$. Even though κ may grow proportionally to $|\mathbb{S}|$, one can generally assume that κ grows sublinearly with respect to $|\mathbb{S}|$. In practice, the numerical examples are more well-behaved if κ is large, and usually the convergence of the Taylor series needs only $n = 1$. The bound on the spectral radius is intended for ill-behaved MDP with small κ .

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