OPERATOR AUGMENTATION FOR GENERAL NOISY MATRIX SYSTEMS

PHILIP A. ETTER \(^*\) AND LEXING YING \(^\dagger\)

Abstract. In the computational sciences, one must often estimate model parameters from data subject to noise and uncertainty, leading to inaccurate results. In order to improve the accuracy of models with noisy parameters, we consider the problem of reducing error in a linear system with the operator corrupted by noise. To address this problem, we extend the elliptic operator augmentation framework [4] to the general nonsymmetric matrix case. We show that under the conditions of right-hand-side isotropy and noise symmetry that the optimal operator augmentation factor for the residual error is always positive, thereby making the framework amenable to a necessary bootstrapping step. While the above conditions are unnecessary for positive optimal augmentation factor in the elliptic case, we provide counter-examples that illustrate their necessity when applied to general matrices. When the noise in the operator is small, however, we show that the condition of noise symmetry is unnecessary. Finally, we demonstrate through numerical experiments on Markov chain problems that operator augmentation can significantly reduce error in noisy matrix systems — even when the aforementioned conditions are not met.

Key words. Operator Augmentation, Random Matrices, Monte Carlo, Polynomial Expansion, Nonsymmetric Matrices.

AMS subject classifications. Linear and multilinear algebra; matrix theory. Statistics. Computer Science.

1. Introduction. There are a plethora of different situations in the natural, mathematical, and computer sciences that necessitate computing the solution to a linear system of equations given by

\[(1.1) \quad Ax = b,\]

where \(A \in \mathbb{R}^{n \times n}\) and \(x, b \in \mathbb{R}^n\) for \(n \in \mathbb{N}\). When both the matrix \(A\) and \(b\) are known, there are many decades of research on how to solve the system (1.1) efficiently. Unfortunately, for a variety of reasons, it is often the case that the true matrix \(A\) is not known exactly, and must be estimated from data (see [9, 8]). In this situation, there is a sampling error between the unobserved true matrix \(A\) and the matrix \(A^{\hat{}}\) one constructs from data. The discrepancy between \(A\) and \(A^{\hat{}}\) is often referred to as model uncertainty, as it stems from incomplete or inaccurate information about the underlying system. This model uncertainty means that with naive application of the inverse of the observed matrix \(A^{\hat{}}\), one is not solving the desired system (1.1), but rather, the system

\[(1.2) \quad A^{\hat{}} x = b,\]

where \(x = A^{-1} b \in \mathbb{R}^n\) is the solution we observe when we solving the observed system naively. Often, we will write

\[(1.3) \quad \hat{A} = A + \hat{Z},\]

where one can think of the matrix \(\hat{Z}\) as constituting the noise or sampling error in our measurements of the system (1.1). Hence, the sampling error \(Z\) between \(A\) and \(A^{\hat{}}\) translates into sampling error between the true solution \(x\) and the naively estimated solution \(\hat{x}\).

The question of interest in this paper is whether one can increase the accuracy of the solution \(\hat{x}\) vis-à-vis the true solution \(x\) by modifying the sampled operator \(A^{\hat{}}\). The paper [4] proposes the operator augmentation framework; whereby one augments the operator \(A^{\hat{}}^{-1}\) by an appropriately chosen augmentation matrix \(K\),

\[(1.4) \quad A^{\hat{}}^{-1} - \beta K.\]

Solving the system of equations with this augmented inverse operator instead of the naive operator \(A^{-1}\), yields an augmented estimate \(x_\beta\) of \(x\),

\[(1.5) \quad \hat{x}_\beta = (A^{-1} - \beta K)b.\]

\(^*\)Institute for Computational and Mathematical Engineering, Stanford University (paetter@stanford.edu)

\(^\dagger\)Department of Mathematics, Stanford University (lexing@stanford.edu)
Once \( \hat{K} \) has been chosen, obtaining an optimal value \( \beta^* \) for the augmentation factor \( \beta \) involves solving the quadratic optimization problem,

\[
\beta^* = \arg \min_{\beta} \mathbb{E} \| \hat{x}_\beta - x \|^2_B = \arg \min_{\beta} \mathbb{E} \| (\hat{A}^{-1} - \beta \hat{K}) b - A^{-1} b \|^2_B,
\]

for some positive definite norm matrix \( B \). Of course, the true value of \( \beta^* \) is not possible to obtain, by virtue of the fact that we do not have access to the matrix \( A \). Therefore, operator augmentation attempts to bootstrap \( \beta^* \) by substituting \( \hat{A} \) for \( A \) and instead solving

\[
\hat{\beta}^* = \arg \min_{\beta} \mathbb{E} \| (\hat{A}_h^{-1} - \beta \hat{K}) b - \hat{A}^{-1} b \|^2_B,
\]

where now the expectation \( \mathbb{E} \) is over a bootstrapped noisy matrix \( \hat{A}_h \), sampled from a distribution we estimate from \( \hat{A} \). This minimization problem can now be solved with Monte Carlo, although one might opt to use specially truncated Taylor expansions of \( \hat{A}_h^{-1} \) about \( \hat{A}^{-1} \) to accelerate computation [4].

When \( A \) is a positive definite symmetric operator, one can prove for several choices of augmentation matrix \( \hat{K} \), that, under a wide range of norms and noise distributions satisfying \( \mathbb{E}[\hat{A}] \preceq A \), the optimal augmentation factor \( \beta^* \) will always be positive [4]. In effect, optimal operator augmentation always shrinks the noisy matrix \( \hat{A}^{-1} \) towards some appropriate base point. The intuition behind this comes from Jensen’s inequality (see Figure 1.1). Matrix inversion operation is a convex function (wrt. the Löwner Order) on the set of positive definite matrices \( S(\mathbb{R}^n)_+ \). This means that naively inverting an unbiased estimator \( \hat{A} \) for \( A \) will always overshoot the true goal \( A^{-1} \). One can think of operator augmentation as correcting for this overshooting effect. This is similar to the intuition behind Stein estimation [5], which makes the observation that in high dimensions, the standard Pitman estimator is always inadmissible because appropriately shrinking the Pitman estimate towards the origin produces an estimator with strictly better risk. The guarantee that \( \beta^* > 0 \) is desirable because amplifying the noise in the matrix \( \hat{A} \) could potentially produce unstable results, particularly because \( \hat{\beta}^* \) is estimated from a bootstrap.

However, while [4] provides theory and numerical experiments for the space of elliptic operators \( S(\mathbb{R}^n)_+ \), it does not provide any theory or experiments for general matrix systems in \( GL(\mathbb{R}^n) \). In this paper, we attempt to fill this gap by studying the operator augmentation algorithm on the full generality of nonsingular matrices in \( GL(\mathbb{R}^n) \). Immediately, the theoretical task of analyzing the algorithm is made more difficult by the fact that \( GL(\mathbb{R}^n) \) doesn’t have the same convexity structure relative to the matrix inversion operation \( A^{-1} \) that the SPD matrices \( S(\mathbb{R}^n)_+ \) do. Despite this obstacle, we are able to provide error reduction guarantees in the

---

\[1\]The general linear group over \( \mathbb{R}^n \)
residual norm under the conditions of noise symmetry and right-hand-side isotropy — and we provide proofs of these guarantees in section 4. Furthermore, we show the existence of adversarial examples that demonstrate the necessity of the aforementioned conditions and thereby lead us to a better understanding of the phenomena that may cause operator augmentation to fail in the nonsymmetric case. We provide these case studies in section 5. Fortunately, the noise symmetry assumption can be discarded if one is willing to assume a small noise regime, as we demonstrate in section 6. Finally, we examine more general forms of operator augmentation and anisotropic right-hand-side in section 7.

To complete our discussion about nonsymmetric operator augmentation, we benchmark the technique on value function estimation problems for Markov Decision Processes (MDPs), and show that despite the limitations of the nonsymmetric setting, operator augmentation still achieves a substantial reduction in error. We give an overview of our benchmark problems and numerical results in section 9.

2. Related Work. As we discussed earlier, the operator augmentation framework for elliptic problems was originally proposed and analyzed in [4]. However, the paper [4] only considers the elliptic case and does not study the general matrix case.

The spirit of operator augmentation derives from Stein Estimation [5]. In their seminal paper, James and Stein consider the high dimensional problem of estimating a parameter corrupted by noise and show that the standard Pitman estimator is always inadmissible because appropriately shrinking the Pitman estimate towards the origin produces an estimator with strictly better risk. At a fundamental level, one can frame our work as taking this idea and applying it to the novel setting of matrices corrupted by noise.

A pertinent area of the literature related to our work is model uncertainty. Quantifying and representing model uncertainty is important in many different fields of computational science, ranging from structural dynamics [9] to weather and climate prediction [8]. However, work relating to model or parameter uncertainty is usually domain specific and focuses more on establishing a model for uncertainty than it does on trying to reduce error in the resulting predictions. In contrast, our work focuses entirely on reducing error, rather than quantifying it. Our work is also not restricted to a particular domain, class of problems, or randomness structure, as long as those problems are linear.

We note that our setting shares some similarities with the problem of uncertainty quantification (UQ). However, the problem we face here is different from the standard uncertainty quantification setting in a subtle but very important way. In UQ, one is usually given a distribution $\mathcal{P}$ and a map $T$ and asked to estimate statistics about the pushforward distribution $T_*\mathcal{P}$ (i.e., expectation, standard error, etc.). Practitioners typically accomplish this task via Monte Carlo techniques [7] or some form of stochastic Galerkin projection [12] or collocation method [11]. In contrast, in our setting we have a distribution $\mathcal{P} = D_{\omega^*}$ and our goal is to accurately compute the image under $T$ of a statistic of $\mathcal{P}$, rather than a statistic of the push-forward of $\mathcal{P}$ under $T$. Here $T(\cdot)$ is matrix inversion and the statistic we are interested in is the true matrix $s(D_{\omega^*}) = A$.

Indeed, the issue that $E[\tilde{A}^{-1}]$ and $E[\hat{A}]^{-1}$ are significantly different is at the core of our paper, as we are (in the unbiased case) interested in $E[\hat{A}]^{-1}$, and not $E[\tilde{A}]^{-1}$. What does, however, fall into the purview of uncertainty quantification is the question of evaluating how well one does of estimating $E[\hat{A}]^{-1}$; but this is ultimately an orthogonal discussion.

The central problem in this paper is also not dissimilar to the setting of matrix completion seen in [2, 6]. In matrix completion, one usually seeks to recover a low-rank ground truth matrix $M_{ij}$ from observations that have been corrupted by additive noise, e.g., $N = M + Z$. If $\mathcal{P}_\Omega$ denotes the subset sampling operator on matrix space, then one is trying to recover $M$ from

$$P_\Omega(N) = P_\Omega(M) + P_\Omega(Z) .$$

However, the operator augmentation and matrix completion settings are subtly different. The matrix completion analogue of $A$ is the actual linear operator $P_\Omega$, and not the matrix $M$. Morally, one may think of the matrix competition problem as solving the under-determined linear system

$$P_\Omega(M) = P_\Omega(N)$$
by assuming a low-rank regularity on M. The randomness in this problem lies completely in the right-hand-side N, and not in the actual linear operator P_Ω.

We also draw attention to the related field of perturbation matrix analysis. In this setting, one is usually interested in proving results about how various properties of matrices change under a perturbation to the elements of the matrix. A seminal example of work in this field is the Davis-Kahan Theorem [3], which quantifies the extent to which the invariant sub-spaces of a matrix change under perturbations. In a similar vein, work in backward stability analysis revolves around understanding the behavior of the solution of a linear system under perturbations to the matrix. However, backward stability analysis typically adopts a worst-case mentality in analysis. In contrast, we care about average case error — and more importantly, how one can reduce it.

We should briefly mention that the mathematical branch of random matrix theory (RMT) studies the spectral properties of random matrix ensembles [1, 10]. However, RMT results usually apply only when the entries of the random matrices are independent and in the large matrix limit. Studies of the spectral properties of random matrix ensembles typically adopt a low-rank regularity on M. However, backward stability analysis typically adopts a worst-case mentality in analysis.

In conclusion, we do not believe that the setting we introduce in this paper, where the operator is noisy, has been studied in the proposed fashion before. There is little precedent in the literature for the operator augmentation method beyond the original paper [4].

3. Probabilistic Model and Problem Formalism. To provide mathematical clarity to the underlying setting, we briefly devote time to explaining the formalism of the operator augmentation setting. Formally, we model this process by assuming that there exists an underlying parameter space Ω (with sigma algebra Σ), where the parameters ω ∈ Ω contain a description of the system that produces the matrices above (e.x., ω may be measurements of a scattering background, edge weights, vertex positions, etc.). The relationship between parameters and matrices is given by a Borel-measurable mapping M : Ω → GL(ℝ^n), where GL(ℝ^n) denotes the group of non-singular matrices in ℝ^{n×n}. For example, ω ∈ Ω may be a weighted graph, and M(ω) may denote a minor of its Laplacian. We suppose that there exist some unobserved true system parameters ω∗ ∈ Ω that produce the true matrix A = M(ω∗). We also suppose that there exists a known family of distributions P_ω over Ω indexed by ω ∈ Ω that describes the observed randomness in the system if ω were to be the true system parameters. It is this the relationship between ω∗ and the distribution P_ω∗ that we assume is known as part of the model (but not the true system parameters ω∗ themselves). Once this family has been specified, the distribution of A is given by M_∗P_ω∗, where M_∗ denotes the pushforward. For shorthand, we will denote D_ω∗ = M_∗P_ω∗.

Finally, we formally state our problem as follows: suppose that we observe exactly one sample ω ∼ P_ω∗. Given b or a distribution from which b is sampled, we wish to build an inverse operator A^−1 β so that ˜x = A^−1 β b produces a better estimate of x = A^−1 b than x = A^−1 b. In our case, we take

$$\hat{A}^−1 β \equiv \hat{A}^−1 - β\hat{K},$$

for some β ∈ ℝ, $\hat{K} \in ℝ^{n×n}$ to be specified later. For ease of understanding, we present flow-chart of the above probabilistic setting together with the operator augmentation framework in Figure 3.1.

4. Provable Error Reduction Guarantees. In order to provide a theory for nonsymmetric operator augmentation that mirrors the theory for symmetric operator augmentation, we focus on the semi-Bayesian error as defined for symmetric operator augmentation. For semi-Bayesian error, we assume that the right-hand-side b in the equation

$$Ax = b,$$

is drawn at random from a prior distribution P. For a given value of augmentation factor β, we are interested in the error between the operator augmentation ˜x_β and the true solution x, averaged over both the matrix noise distribution $\hat{A} ∼ D_ω∗$ as well as the prior P for b:

$$\mathcal{E}^\text{Bayes}_β(\hat{x}_β) \equiv \mathbb{E}_P\mathbb{E}_{D_ω∗} \left[\|\hat{x}_β - x\|^2_B\right].$$

$$D_ω∗ \equiv \mathbb{E}_ω P(ω) \mathbb{E}_{\hat{A} | ω} \|\hat{A} - A\|^2,$$
Note that the formulation of this error is meant to include cases where \( P \) is supported at a single point (i.e., \( b \) is deterministic). Viewing the problem in terms of operators, the error can equivalently be written in terms of the operators \( \hat{A} \), \( A \) and right-hand-side \( b \),

\[
\mathcal{E}_\text{Bayes}(\hat{A}_\beta) = \mathbb{E}_P \mathbb{E}_{D^*} \left[ \| \hat{A}_\beta^{-1}b - A^{-1}b \|^2_B \right].
\]

Letting \( R \) be the auto-correlation matrix of \( b \), i.e., \( R = \mathbb{E}_P[bb^T] \), one can transform this into a definition purely in terms of operators. Define the semi-norm

\[
\|A\|_{B,R}^2 = \langle A, A \rangle_{B,R} \equiv \text{tr}(R^{1/2}A^TBR^{1/2}) \geq 0.
\]

Note that, in the isotropic-\( L_2 \) case where \( B = R = I \), \( \| \cdot \|_{B,R} \) is the well-known Frobenius norm. When the prior \( P \) for \( b \) has non-degenerate auto-correlation \( R \), the semi-norm \( \| \cdot \|_{B,R} \) is a proper norm, as \( R^{1/2}A^TBR^{1/2} \) is a symmetric positive definite matrix. Nonetheless, using the linearity and cyclic properties of the trace on (4.3), one obtains that

\[
\mathcal{E}_B(\hat{A}_\beta) = \mathbb{E}_{D^*} \left[ \| \hat{A}_\beta^{-1} - A^{-1} \|^2_{B,R} \right].
\]

Therefore, the problem of finding a more accurate estimate \( \hat{x}_\beta \) of the solution \( x \) in the \( \| \cdot \|_B \) norm can equivalently be seen as finding an estimator \( \hat{A}_\beta^{-1} \) so that the inverse \( \hat{A}_\beta^{-1} \) is closer to \( A^{-1} \) in the \( \| \cdot \|_{B,R} \) semi-norm.

In the elliptic case, the choice of augmentation matrix \( \hat{K} \) is usually a function of \( \hat{A} \) – as the intent is to move the sampled matrix \( \hat{A} \) closer to some base-point matrix. For example, the
choice $\hat{K} = \hat{A}$ moves our estimated operator $\hat{A}_\beta$ closer to the zero matrix $0$. Because of this, it is important to establish that the optimal $\beta^*$ is greater than zero – if this is not the case, then our method is essentially amplifying the noise in $\hat{A}$ rather than diminishing it. This is potentially dangerous when paired with the need to bootstrap the quantity $\beta^*$.

A simple calculation gives that

$$\beta^* = \frac{E_{D,\omega} \langle \hat{K}, \hat{A}^{-1} - A^{-1} \rangle_{B,R}}{E_{D,\omega} \|\hat{K}\|_{B,R}}$$

hence the sign of $\beta^*$’s sign is equivalent to the sign of $E_{D,\omega} \langle \hat{K}, \hat{A}^{-1} - A^{-1} \rangle_{B,R}$, and we would therefore like an augmentation method to exhibit $E_{D,\omega} \langle \hat{K}, \hat{A}^{-1} - A^{-1} \rangle_{B,R} \geq 0$. We will begin by studying the simplest choice of operator augmentation,

$$(4.7) \quad \hat{K} = \hat{A}^{-1}.$$  

The overshooting effect demonstrated in Figure 1.1 gives one reason to believe that this choice of augmentation is a reasonable one, as it involves shrinks the inverse operator towards zero.

4.1. Conditions. Unlike in the symmetric case, to prove a rigorous statement about the sign of $\beta^*$ for (4.7) in the nonsymmetric case, one must place a number of additional conditions on the constituent components of the model. We will discuss the necessity of these conditions in more detail in section 5 – in short, each of these conditions has an adversarial example associated with it that causes the theory to fail when the conditions are not assumed.

In order to prove positivity of $\beta^*$, we introduce the following constraints:

1. **Unbiased Noise**: We assume that the noise matrix $\hat{Z}$ is unbiased, i.e., $E[\hat{A}] = A$.
2. **Isotropy**: We assume that $R = E_p[bb^T] = I$. This means that there is no preferred direction in which we care about the accuracy of the estimator $\hat{A}_\beta^{-1}$.
3. **Noise Symmetry**: We assume that the distribution of the matrix $\hat{A}$ is symmetric about its mean, namely that $\hat{Z}$ has the same distribution as $-\hat{Z}$.
4. **Residual Norm**: We specifically choose our norm of interest $B$ to be the residual norm $B = A^T A$. The residual norm is often used as an objective in nonsymmetric iterative methods.

We note that for the theory of elliptic operator augmentation, items (2) through (4) are not necessary – and so their apparent necessity in the nonsymmetric case is a curious mathematical phenomenon of the group $GL(\mathbb{R}^n)$.

4.2. Proof. With the conditions outlined above, we proceed to prove the positivity of the augmentation factor $\beta^*$.

**Theorem 4.1.** Let $\hat{A}$ be a random matrix, invertible almost everywhere, such that $E[\hat{A}^{-2}]$ exists. Under the conditions outlined in subsection 4.1, the optimal augmentation factor is always nonnegative.

**Proof.** We must verify:

$$E(\hat{A}^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A, I} \geq 0.$$  

Expanding,

$$E(\hat{A}^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A, I} = \text{tr} E \left[ \hat{A}^{-T} A^T A (\hat{A}^{-1} - A^{-1}) \right],$$

Since $A$ is invertible and $\hat{A}$ is invertible almost everywhere, let us define the matrix $\hat{Y}$,

$$\hat{Y} = \hat{A} A^{-1} - I = \hat{Z} A^{-1}.$$  

Note that this definition implies that $E[\hat{Y}] = 0$ as well as that the distribution of $\hat{Y}$ is symmetric, since the distribution of $\hat{Z}$ is symmetric by condition (3).
One can rearrange to obtain an expression for $\hat{A}^{-1}$,

$$\hat{A}^{-1} = A^{-1}(I + \hat{Y})^{-1}.$$  \hfill (4.11)

And we substitute the above expression into (4.9),

$$\mathbb{E}(\hat{A}^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A, I} = \text{tr}\left[(I + \hat{Y})^{-T}(I + \hat{Y})^{-1} - (I + \hat{Y})^{-T}\right].$$  \hfill (4.12)

Since the distribution of $\hat{Y}$ is symmetric, it suffices to verify that

$$\text{tr}\left[(I + Y)^{-T}(I + Y)^{-1} - (I + Y)^{-T}\right] + \text{tr}\left[(I - Y)^{-T}(I - Y)^{-1} - (I - Y)^{-T}\right] \geq 0,$$  \hfill (4.13)

or alternatively,

$$\text{tr}\left[(I + Y)^{-T}(I + Y)^{-1} + (I - Y)^{-T}(I - Y)^{-1}\right] \geq \text{tr}\left[(I + Y)^{-T} + (I - Y)^{-T}\right],$$  \hfill (4.14)

for all matrices $Y$ for which $I + Y$ and $I - Y$ are nonsingular.

In order to verify (4.14), we begin by considering the matrix,

$$(I - Y)^{-T} - (I + Y)^{-1}(I - Y)^{-1} - (I + Y)^{-T} \geq 0.$$  \hfill (4.15)

Since this matrix is positive definite (by virtue of the fact that it has the form $M^T M$), it follows that the trace of the above matrix is positive,

$$\text{tr}\left[((I + Y)^{-T} - (I - Y)^{-1})(I + Y)^{-1} - (I - Y)^{-T}\right] \geq 0.$$  \hfill (4.16)

The above inequality can be rearranged,

$$\text{tr}\left[(I + Y)^{-T}(I + Y)^{-1} + (I - Y)^{-T}(I - Y)^{-1}\right] \geq \text{tr}\left[(I - Y^2)^{-T} + (I - Y^2)^{-1}\right].$$  \hfill (4.17)

Note that, by the cyclic property of the trace, that the left hand sides of both (4.14) and (4.17) are identical. Therefore, it suffices to prove that

$$\text{tr}\left[(I - Y^2)^{-T} + (I - Y^2)^{-1}\right] = \text{tr}\left[(I + Y)^{-T} + (I - Y)^{-T}\right],$$  \hfill (4.18)

from which (4.14) will follow.

To prove (4.18), we note that

\begin{align*}
\text{tr}\left[(I + Y)^{-T} + (I - Y)^{-T}\right] \\
= \text{tr}\left[(I + Y)^{-T} (I - Y)^{-T} + (I + Y)^{-T} (I - Y)^{-T}\right] \\
= \text{tr}\left[(I + Y)^{-T} (I - Y) + (I + Y) (I - Y)^{-T}\right] \\
= 2 \text{tr}\left[(I + Y)^{-T} (I - Y)^{-T}\right] \\
= 2 \text{tr}\left[(I - Y^2)^{-T}\right] \\
= \text{tr}\left[(I - Y^2)^{-T} + (I - Y^2)^{-1}\right].
\end{align*}  \hfill (4.19)

We remark that the critical step that requires isotropy is the assertion that the left hand sides of both (4.14) and (4.17) are equal, namely that

$$\text{tr}\left[(I - Y)^{-1} (I - Y)^{-T}\right] = \text{tr}\left[(I - Y)^{-T} (I - Y)^{-1}\right].$$  \hfill (4.20)

This is no longer necessarily true if we replace the isotropic trace operator $\text{tr}(\cdot)$ with an anisotropic operator $\text{tr}(R^{1/2}(\cdot)R^{1/2})$ for general $R$.

5. The Necessity of Conditions. In this section, we provide adversarial examples of how violating the conditions in subsection 4.1 can lead to situations where the optimal augmentation factor $\beta^*$ for $K = \hat{A}^{-1}$ is negative. This provides a concrete lens of how the group $GL(\mathbb{R}^n)$ differs from the symmetric positive definite cone $S(\mathbb{R}^n)_+$, as such situations are not possible in the SPD case. These examples demonstrate how one might use the structure of $GL(\mathbb{R}^n)$ to construct situations where increasing the “noise” in our estimator can actually lead to more accurate results.
5.1. The Necessity of Isotropy. First, we investigate the necessity of the isotropy condition. Suppose that $A = I$ and $Z$ has two-atom distribution with atoms:

$Z_1 = \begin{bmatrix} 0 & k \\ 0 & -k \end{bmatrix}, \quad Z_2 = \begin{bmatrix} 0 & -k \\ 0 & k \end{bmatrix},$

where each atom occurs with equal probability, and $k \gg 1$. Clearly in this situation, the error distribution of $\hat{Z}$ is symmetric and has mean zero. Therefore, all of the other conditions in subsection 4.1 are met. The augmented operator $\tilde{A}^{-1}$ is given by $\tilde{A}^{-1}_{\beta} = (1 - \beta)A^{-1}$ and the random matrix $\hat{A}$ has two outcomes with equal probability,

$A_1 = \begin{bmatrix} 1 & k \\ 0 & -k + 1 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 1 & -k \\ 0 & k + 1 \end{bmatrix}.$

These outcomes have inverses

$A_1^{-1} = \begin{bmatrix} 1 & 1/k \\ 0 & 1/(k-1) \end{bmatrix}, \quad A_2^{-1} = \begin{bmatrix} 1 & 1/k \\ 0 & 1/(k+1) \end{bmatrix}.$

This means that in either case, we have

$\hat{A}^{-1} = \begin{bmatrix} 1 & 1/k \\ 0 & 1/(k-1) \end{bmatrix} + O(1/k).$

With this matrix ensemble, we can take the prior $P$ to be deterministic, such that

$\mathbf{b} = \begin{bmatrix} 2 \\ -1 \end{bmatrix}.$

This immediately makes the problem with this setup evident, as

$\hat{A}^{-1}\mathbf{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + O(1/k), \quad A^{-1}\mathbf{b} = \begin{bmatrix} 2 \\ -1 \end{bmatrix}.$

It is therefore clear that the minimum of the objective

$E_{A_{\beta}}^{\text{Bayes}}(\hat{A}_{\beta}) = E_{A_{\beta}}^{\text{Bayes}}(\hat{A}_{\beta}) = E\| (1 - \beta)\hat{A}^{-1}\mathbf{b} - A^{-1}\mathbf{b}\|_2^2$

must achieve its minimum at

$\beta^* = -1 + O(1/k).$

One might initially conclude that the ability of this example to undermine Theorem 4.1 has something to do with the assumption that $k$ is very large. This is not the case. The largeness of $k$ is assumed only for illustrative purposes. One can verify numerically (see Figure 5.1) for the above choice of $\hat{A}$, that $E[\hat{A}^{-T}\hat{A}^{-1} - A^{-T}]$ has a negative eigenvalue for all $k \neq \pm 1, 0$. Therefore, for any $k \neq \pm 1, 0$, one can find a $\mathbf{b}$ such that $\beta^*$ is negative.

In particular, one should note that without a requirement of positive definiteness, it is possible to create a situation where $\hat{A}$ is always “larger” than $A$. This runs counter to the intuition behind operator augmentation in the symmetric positive definite case [4], where such a situation is not possible.

5.2. Outlier Masking and the Importance of Noise Symmetry. The second condition that one needed to prove the results in section 4 is the presence of symmetry in the noise distribution. In this section, we will see how if this is not required, it is possible to construct an adversarial example where $\beta^* < 0$ for the augmentation (4.7). For this example, we take $A = I$ and let $\hat{Z}$ have a distribution of three equally probable atoms, given by

$Z_1 = I, \quad Z_2 = kI, \quad Z_3 = -(k+1)I,$
where $k \gg 1$. Note that this distribution is mean zero. Computing the atoms of the distribution $\tilde{A}^{-1}$,

\begin{equation}
A_1^{-1} = \frac{1}{2} I, \quad A_2^{-1} = \frac{1}{k+1} I, \quad A_3^{-1} = -\frac{1}{k} I.
\end{equation}

Now, note that in order to minimize the quantity

\begin{equation}
\mathcal{E}_{\text{Bayes}}^{\text{A}\text{T}A}(\tilde{A}_\beta) = \mathbb{E}\|\tilde{A}_\beta^{-1} - I\|_F^2 = \frac{2}{3}\left(\frac{1 - \beta}{2} - 1\right)^2 + \frac{2}{3}\left(\frac{1 - \beta}{k+1} - 1\right)^2 + \frac{2}{3}\left(-\frac{1 - \beta}{k} - 1\right)^2,
\end{equation}

one can verify by taking the derivative and setting it to zero that

\begin{equation}
\beta^* = -1 + O(1/k).
\end{equation}

Therefore, the optimal augmentation will grow the inverse operator instead of shrinking it.

The message of this example is that outliers in the matrix noise can mask distribution imbalances in the region near $A$ that can cause $\mathbb{E}[\tilde{A}^{-1}]$ to both lie in the direction of $A^{-1}$ while at the same time being dominated by $A^{-1}$. Indeed, we have that $\mathbb{E}[\tilde{A}^{-1}] \approx \frac{1}{2} I \approx I = A^{-1}$ (it bears repeating that such a feat is impossible in the symmetric positive definite setting where $\mathbb{E}[\tilde{A}^{-1}] \succeq A^{-1}$ [4]). The importance of noise symmetry is that it forces the distribution of $\tilde{Z}$ to be balanced in the region around $A$, even if the distribution contains large outliers.

5.3. The Importance of Conditioning and a Counter-Example for the L2 Norm. Our final counter-example concerns the use of the $L_2$ norm in the objective (4.5) rather than the residual norm. In the symmetric positive definite case, one can prove the positivity of the optimal augmentation factor for a large range of different objective norms [4]. However, as we will see in this section, there are adversarial ways to break norms other than the residual norm in the nonsymmetric case. We will focus here on giving an example that shows how if using the $L_2$ norm instead of the residual norm makes it possible to have a negative optimal augmentation factor for the augmentation (4.7).

To begin, consider the ground truth matrix

\begin{equation}
A = \begin{bmatrix} 1 & -\epsilon \\ \epsilon & 0 \end{bmatrix},
\end{equation}

where $0 < \epsilon \ll 1$. For the noise $\tilde{Z}$, we reuse the noise distribution from subsection 5.1 — consider a two-atom distribution with atoms

\begin{equation}
Z_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad Z_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},
\end{equation}

where each atom has equal probability. Note that this distribution is symmetric and mean zero. Since $\epsilon$ is extremely small, this means that the distribution of $\tilde{A}$ will have two atoms whose inverses
are approximately
\begin{equation}
A_1^{-1} \approx \left[ \begin{array}{cc} 1 & 1 \\ -1 & 0 \end{array} \right]^{-1} = \left[ \begin{array}{cc} 0 & 1 \\ -1 & 1 \end{array} \right], \quad A_2^{-1} \approx \left[ \begin{array}{cc} 1 & -1 \\ 1 & 0 \end{array} \right]^{-1} = \left[ \begin{array}{cc} 0 & -1 \\ 1 & 1 \end{array} \right].
\end{equation}

Note that the inverses of these atoms have the same Frobenius norm the atoms themselves. In sharp contrast, the ill-conditioning of $A$ means that $A^{-1}$ is an order of magnitude larger than $A$,
\begin{equation}
A^{-1} = \left[ \begin{array}{cc} 0 & -\epsilon^{-1} \\ \epsilon^{-2} & \epsilon^{-1} \end{array} \right].
\end{equation}

Immediately, we see that in order for $\beta^*$ to minimize
\begin{equation}
E_1^{Bayes}(\beta_\beta) = \frac{1}{2} \| (1 - \beta)A_1^{-1} - A^{-1} \|_F^2 + \frac{1}{2} \| (1 - \beta)A_2^{-1} - A^{-1} \|_F^2,
\end{equation}
One must therefore have $\beta^* \sim -\epsilon^{-2}$, for which $E_1^{Bayes}(\beta_\beta) \sim \epsilon^{-1}$. For other growth orders of $\beta$, one has $E_1^{Bayes}(\beta_\beta) = \omega(\epsilon^{-1})$. It is therefore clear that for $\epsilon$ small enough, $\beta^*$ will be negative.

In contrast to the $L_2$ norm, note that the residual norm for this problem is given by
\begin{equation}
A^T A = \left[ \begin{array}{cc} 1 + \epsilon^2 & \epsilon \\ \epsilon & 0 \end{array} \right],
\end{equation}
Therefore, we see that the reason why Theorem 4.1 holds in the residual norm but not in the $L_2$ norm is because the residual norm places significantly less weight on the part of the matrix $A^{-1}$ that contributes to the ill-conditioning of $A$ in a way that the $L_2$ norm does not.

This example therefore also demonstrates the importance of conditioning in the ground truth matrix $A$. It is perfectly possible that $A$ lies close to a singular matrix, while the outcomes of $\tilde{A}$ are moved away from singularity by the noise imparted by $\tilde{Z}$. If this is the case, $E[\tilde{A}^{-1}]$ will be small in magnitude compared to $A^{-1}$ and shrinking the operator $\tilde{A}^{-1}$ further will not reduce average error in the Frobenius sense.

Note that symmetric positive definite setting [4] avoids this issue, since if $\tilde{A}$ is symmetric positive definite everywhere, it is impossible for $E[\tilde{A}]$ to be close to the origin without a significant chunk of the probability distribution also lying close to the origin. This ensures that $E[\tilde{A}^{-1}]$ will always spectrally dominate $\tilde{A}^{-1}$, and shrinking the operator $\tilde{A}^{-1}$ will reduce error.

6. The Small Noise Regime Allows for Nonsymmetric Noise. As we saw in subsection 5.2, the presence of large adversarial outliers can completely mask local imbalances in the noise distribution near $A$. These local imbalances can be severe enough to invalidate Theorem 4.1. Naturally, the example presented in subsection 5.2 is quite extreme, so one might ask if the issue inherent is not necessarily the symmetry of the noise, but rather the magnitude of the noise. To answer this question, we consider the small noise regime, where deviations in $\tilde{Y}$ are very small relative to $E[\tilde{Y}] = I$. It turns out, that if one assumes that terms of order $O(E[\tilde{Y}^3])$ are negligible — what we term the small noise regime — then the symmetry assumption is unnecessary, as we will see momentarily.

For this discussion, we duplicate the setting of Theorem 4.1, except we replace the condition that the noise distribution is symmetric with the condition that noise terms of the order $O(E[\tilde{Y}^3])$ are negligible. Recall that the statement necessary for Theorem 4.1 to be true was
\begin{equation}
E(\tilde{A}^{-1}, \tilde{A}^{-1} - A^{-1}) A^T A_1 = \text{tr} E \left[ (I + \tilde{Y})^{−T}(I + \tilde{Y})^{-1} - (I + \tilde{Y})^{-T} \right] \geq 0.
\end{equation}

We define the function $f$,
\begin{equation}
f(\tilde{Y}) \equiv \text{tr} \left[ (I + \tilde{Y})^{−T}(I + \tilde{Y})^{-1} - (I + \tilde{Y})^{-T} \right].
\end{equation}
Taking a second order Taylor expansion of $f$ about $\mathbf{Y} = \mathbf{0}$, we obtain
\begin{equation}
\label{eq:6.3}
f(\hat{\mathbf{Y}}) = f(\mathbf{0}) + \delta f(\hat{\mathbf{Y}}) + \delta^2 f(\hat{\mathbf{Y}}) + O(\hat{\mathbf{Y}}^3).
\end{equation}
Note that $f(\mathbf{0}) = 0$ and that $\delta f(\hat{\mathbf{Y}})$ is linear in $\mathbf{Y}$. Hence, in expectation, both of these terms vanish,
\begin{equation}
\label{eq:6.4}
E[f(\hat{\mathbf{Y}})] = E[\delta^2 f(\hat{\mathbf{Y}})] + O(\hat{\mathbf{E}}^3).
\end{equation}
A calculation of $\delta^2 f$ gives
\begin{equation}
\label{eq:6.5}
E[\delta^2 f(\hat{\mathbf{Y}})] = E \left[ 2 \mathbf{Y}^T \mathbf{Y}^T + 2 \mathbf{Y}^T \mathbf{Y} + 2 \mathbf{Y} \mathbf{Y}^T - 2 \mathbf{Y}^T \mathbf{Y}^T \right]
= 2 E \left[ \mathbf{Y}^T \mathbf{Y} + \mathbf{Y} \mathbf{Y}^T \right]
= E \left[ \mathbf{Y}^T \mathbf{Y}^T + \mathbf{Y}^T \mathbf{Y} + \mathbf{Y}^T \mathbf{Y} - \mathbf{Y}^2 \right]
= E \left[ (\mathbf{Y} + \mathbf{Y}^T)^T (\mathbf{Y} + \mathbf{Y}^T) \right] \geq 0.
\end{equation}
Indeed, if $\mathbf{Y}$ not zero almost everywhere, then the above is in fact a strict inequality, meaning that (6.1) must be true to second order.

7. More General Augmentations and Anisotropic Priors. In the elliptic case [4], one can prove a reduction in error for a variety of different augmentations. In particular, the energy norm in the elliptic augmentation setting has an extensive theory regarding the approximation of $\beta^*$ via truncated Taylor expansions that is valid for augmentations of the form
\begin{equation}
\label{eq:7.1}
\hat{\mathbf{K}} \equiv \hat{\mathbf{A}}^{-1} \mathbf{C},
\end{equation}
where $\mathbf{C}$ is a symmetric positive definite matrix that commutes with the auto-correlation of $\mathbf{b}$, i.e., $[\mathbf{C}, \mathbf{R}] = 0$. Part of this theory states that $\beta^*$ must always be positive.

In the analysis in [4], adding this $\mathbf{C}$ term effectively just changes the autocorrelation matrix from $\mathbf{R}$ to $\mathbf{RC}$ in the analysis. Note that $\mathbf{RC}$ remains symmetric positive definite by virtue of the condition that $[\mathbf{C}, \mathbf{R}] = 0$. This therefore begs the question: do augmentations of the form (7.1) retain their nice properties in the nonsymmetric augmentation setting — where the residual norm plays the role of the energy norm in the elliptic augmentation setting? Subsection 5.1 provides a definitive answer to this question: it is not possible unless the modified auto-correlation is isotropic — that is, unless $\mathbf{RC} = \mathbf{I}$.

Nonetheless, while the wide number of choices regarding norms and augmentations do not translate to the nonsymmetric augmentation setting, the operator augmentation framework does provide a way for handling anisotropic right-hand-side $\mathbf{b}$ with $E[\mathbf{bb}^T] = \mathbf{R} \neq \mathbf{I}$. Namely, one chooses the operator augmentation
\begin{equation}
\label{eq:7.2}
\hat{\mathbf{K}} \equiv \hat{\mathbf{A}}^{-1} \mathbf{R}^{-1}.
\end{equation}
It is immediate that the results of Theorem 4.1 hold for this choice of augmentation — as the $\mathbf{R}^{-1}$ will cancel the $\mathbf{R}$ in the error objective. We restate this conclusion into the main theorem of this paper:

**Theorem 7.1.** Let $\hat{\mathbf{A}} \sim D_{\omega^*}$ be a random matrix, invertible almost everywhere, such that $E[\hat{\mathbf{A}}^{-2}]$ exists. Suppose that the distribution of $\hat{\mathbf{A}}$ is symmetric about its mean, and that $E[\hat{\mathbf{A}}] = \mathbf{A}$. Let $\mathbf{b} \sim P$ with nonsingular auto-correlation matrix $E[\mathbf{bb}^T] = \mathbf{R}$. Under these assumptions, consider the semi-Bayesian residual error:
\begin{equation}
\label{eq:7.3}
E_{\hat{\mathbf{A}}^T \mathbf{A}}^{Bayes} (\hat{\mathbf{A}}_\beta) = E_{P} E_{D_{\omega^*}} \left[ \| \hat{\mathbf{A}}_\beta^{-1} \mathbf{b} - \mathbf{A}^{-1} \mathbf{b} \|^2_{\hat{\mathbf{A}}^T \mathbf{A}} \right] = E_{D_{\omega^*}} \left[ \| \hat{\mathbf{A}}_\beta^{-1} - \mathbf{A}^{-1} \|_{\hat{\mathbf{A}}^T \mathbf{A} \mathbf{R}}^2 \right].
\end{equation}
Consider the operator augmentation:
\begin{equation}
\label{eq:7.4}
\hat{\mathbf{A}}^{-1} = \hat{\mathbf{A}}^{-1} - \beta \hat{\mathbf{A}}^{-1} \mathbf{R}^{-1}.
\end{equation}
Then the optimal $\beta^*$ with respect to the semi-Bayesian error is always nonnegative.
The condition (7.5) is therefore equivalent to
\[
E(\hat{A}^{-1}R^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A} \geq 0.
\]

But note, by definition in (4.4) and symmetry of \( R \), that
\[
(\hat{A}^{-1}R^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A} = (\hat{A}^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A, I}.
\]

The condition (7.5) is therefore equivalent to
\[
E(\hat{A}^{-1}, \hat{A}^{-1} - A^{-1})_{A^T A, I} \geq 0,
\]
which we proved in Theorem 4.1. \( \square \)

8. Monte Carlo Estimation. To build an algorithm from this theory, we attempt to estimate the optimal augmentation factor with bootstrap Monte Carlo. The quantity of interest is
\[
\beta^* = \frac{E_{D_{\omega^*}}(K, \hat{A}^{-1} - A^{-1})_{A^T A}}{E_{D_{\omega^*}}\|K\|^2_{A^T A}}.
\]

Obviously, it is not possible to compute this quantity directly, since we only have a single sample \( A \) and we do not have access to the ground truth \( A \) or its distribution \( D_{\omega^*} \). We must therefore try to approximate these quantities as best as possible with the available information. Suppose that \( \hat{\omega} \in \Omega \) is the parameter instance that generates the matrix \( \hat{A} = M(\hat{\omega}) \). To bootstrap (8.1), we replace all instances of \( A \) with \( \hat{A} \) and draw random instances from \( D_{\hat{\omega}} \) instead of \( D_{\omega^*} \). We get
\[
\hat{\beta} = \frac{E_{D_{\hat{\omega}}}(K_b, \hat{A}_b^{-1} - A^{-1})_{A^T A, I}}{E_{D_{\hat{\omega}}}\|K_b\|^2_{A^T A}},
\]
where \( K_b \) and \( \hat{A}_b \) are drawn from \( D_{\hat{\omega}} \). This can then be discretized with Monte Carlo:
\[
\hat{\beta} = \frac{\sum_{i=1}^{m} b_i^T K_{b,i}^T \hat{A}^T \hat{A}^{-1} - A^{-1})_{A^T A} b_i}{\sum_{i=1}^{m} b_i^T K_{b,i}^T \hat{A} b_i}, \quad b_i \sim P \text{ i.i.d.}, \quad \hat{A}_{b,i} \sim D_{\hat{\omega}} \text{ i.i.d.}.
\]

If one opts to use the augmentation provided by (7.2), the expression simplifies to
\[
\hat{\beta} = 1 - \frac{\sum_{i=1}^{m} b_i^T \hat{A}_{b,i}^{-T} \hat{A}^T b_i}{\sum_{i=1}^{m} q_i^T \hat{A}_{b,i}^{-T} \hat{A} \hat{A}_{b,i}^{-1} q_i}, \quad b_i \sim \mathcal{N}(0, I) \text{ i.i.d.}, \quad q_i \sim \mathcal{N}(0, \hat{A}^{-1}) \text{ i.i.d.}, \quad \hat{A}_{b,i} \sim D_{\hat{\omega}} \text{ i.i.d.}.
\]

Note that \( b_i \) and \( q_i \) do not necessarily have to be normal – they must just have the same autocorrelation as the normal distributions specified. For good measure, one might also threshold the above expression to guarantee \( \hat{\beta} \geq 0 \). Finally, one can now estimate the true solution to the system (1.1) via
\[
\tilde{x}_\beta = \hat{A}^{-1} b = (\hat{A}^{-1} - \hat{\beta} \hat{A}^{-1} R^{-1}) b = \hat{A}^{-1} (b - \hat{\beta} R^{-1} b).
\]

8.1. Approximation via Taylor Expansion. Note that every Monte Carlo sample in (8.4) requires inverting a matrix system. There are times where this may be too computationally expensive to be feasible. However, if we are in the small noise regime, one may take a Taylor expansion of \( \hat{A}^{-1} \) about \( A^{-1} \) — as this means one only has the factorize an operator once for the whole estimation process. The expansion to second order is given by
\[
\hat{A}^{-1} = A^{-1} - A^{-1} \hat{Z} A^{-1} + 2A^{-1} \hat{Z} A^{-1} \hat{Z} A^{-1} + O(\hat{Z}^3).
\]
Inserting this expression into (8.4) yields

\[ \hat{\beta} \approx 1 - \frac{\text{tr}(I) + \frac{1}{m} \sum_{j=1}^{m} b_j^T (\hat{Z}_{b,i} \hat{A}^{-1})^2 b_i}{\text{tr}(R^{-1}) + \frac{1}{m} \sum_{j=1}^{m} \|Z_{b,i} \hat{A}^{-1} q_i\|^2 + \frac{1}{m} \sum_{j=1}^{m} q_j^T (\hat{Z}_{b,i} \hat{A}^{-1})^2 q_i}, \]

note that we have omitted linear terms, because terms linear in $\hat{Z}$ will be zero in expectation, by virtue of the fact that $\mathbb{E}[\hat{Z}] = 0$. It is possible that higher orders of truncation may produce better results; however, unlike the elliptic augmentation setting [4], it is difficult to prove guarantees about the quality of these truncated expansions.

9. Numerical Experiments. To confirm our theoretical results, we will examine the asymmetric operator augmentation algorithm applied to the problem of more accurately computing a value function for a Markov chain whose probability transition function must be estimated from data.

9.1. Background. For context, a discrete Markov chain is a stochastic process $X_i$ for $i \in \mathbb{Z}_{\geq 0}$ on a finite state set $V$ in a process that satisfies the Markov property

\[ \mathbb{P}(X_i = v_i \mid X_{i-1} = v_{i-1}, \ldots, X_1 = v_1) = \mathbb{P}(X_i = v_i \mid X_{i-1} = v_{i-1}). \]

A discrete Markov chain is time homogeneous if the right-hand-side of (9.1) does not depend on the time $i$. In this situation, the Markov chain is completely characterized by its probability transition matrix

\[ P_{v,u} = \mathbb{P}(X_i = u \mid X_{i-1} = v), \]

as well as a distribution $\mathbb{P}(X_0 = v)$ of the initial state $X_0$. There are countless examples of such Markov chains from the fields of probability, statistics, reinforcement learning, and physics.

One is often interested in computing or approximating functionals of the process $X_i$. For example, one may think of $X_i$ as an agent navigating through the set $V$ via the means of some fixed policy, where the agent obtains a fixed reward $r(v)$ whenever it transitions from the state $v$. In many situations in reinforcement learning, one is often interested in the average discounted reward $Q(v)$ the agent obtains over its life-cycle when beginning at $X_0 = v$, namely,

\[ Q(v) = \mathbb{E} \left[ \sum_{i=0}^{\infty} \gamma^i r(X_i) \mid X_0 = v \right]. \]

$Q(v)$ is typically referred to as the value function of $X_i$ with respect to reward function $r(v)$. It is used to gauge the quality of the agent’s policy at maximizing the discounted reward it receives over its life-time. One notes that the function $Q$ is linear in $r$. One may use first transition analysis to express the relationship between $Q$ and $r$ in matrix form. Isolating the first term in the infinite sum (9.3) gives

\[ Q(v) = r(v) + \gamma \sum_u \mathbb{P}(X_1 = u \mid X_0 = v)Q(u). \]

Alternatively,

\[ q = r + \gamma Pq, \]

where $q$ is the vector with entries $q_v = Q(v)$ and $r$ is the vector with entries $r_v = r(v)$. This finally produces a linear system for the value function,

\[ Aq \equiv (I - \gamma P)q = r. \]

However, there are many situations where the transition matrix $P$ may not be known exactly. In reinforcement learning, for example, one does not have access to $P$ itself, but rather a number
of finite realizations of the process $X_i$ as it traverses the state space. Therefore, instead of having access to the ground truth $P$, one usually has access to a noisy version $\hat{P}$ thereof. A naive solve will give

$$ (I - \gamma P) \hat{q} = r. $$

We will see how operator augmentation can be used to reduce the average error between our estimate $\hat{q}$ and the ground truth $q$ in the residual norm.

### 9.2. Noise Model

One popular way to approximate a Markov chain’s probability transition matrix from a sample $X_0, X_1, \ldots, X_t$ of the Markov chain is to approximate the probability $P(X_t = v | X_{t-1} = u)$ by examining the fraction of times $X_i$ transitions to $v$ from $u$ out of the total number of times $X_i$ transitions from $u$, i.e.,

$$ P(X_t = v | X_{t-1} = u) = \frac{\mathbb{P}(X_t = v \land X_{t-1} = u)}{\mathbb{P}(X_{t-1} = u)} \approx \frac{\#\{i \mid X_i = v \land X_{i-1} = u\}}{\#\{i \mid X_i = u \land i \geq 1\}}. $$

But while this estimator is commonly used — it is difficult to ensure coverage of the state space in a way that is natural, as one must take care to ensure that $\#\{i \mid X_i = u \land i \geq 1\}$ is positive for every $u$.

Therefore, to model the uncertainty in a Markov chain constructed from data, we assume that, instead of observing the first $t$ states of the Markov chain $X_i$, we instead observe the first $N$ transitions of the Markov chain $X_i$ out of every state $v$. We denote the first $N$ transitions out of a state $v$ as $\hat{Y}_{v,1}, \hat{Y}_{v,2}, \ldots, \hat{Y}_{v,N}$. If the Markov chain is irreducible, $\hat{Y}_{v,1}, \hat{Y}_{v,2}, \ldots, \hat{Y}_{v,N}$ are well-defined almost surely, and have distribution

$$ \hat{Y}_{v,1}, \hat{Y}_{v,2}, \ldots, \hat{Y}_{v,N} \sim \mathbb{P}(X_i \mid X_{i-1} = v), \quad \text{i.i.d.} $$

One may then easily estimate the probability transition matrix by using the empirical distribution of $\mathbb{P}(X_i \mid X_{i-1} = v)$ to construct each row of $\hat{P}$,

$$ \hat{P}_{v,u} = \frac{\#\{\hat{Y}_{v,i} = u\}}{N} \approx \mathbb{P}(X_i = u \mid X_{i-1} = v) = P_{v,u}. $$

Note that $\hat{P}$ is unbiased and hence that

$$ \mathbb{E}[\hat{A}] = A. $$

We pose the question: is it possible to use operator augmentation to increase the accuracy of the naive estimate of the value function $Q$? Our numerical results suggest that the answer to this question is yes.

### 9.3. Numerical Results

To test the theory, we consider 3 different Markov chains on 1D, 2D, and 3D grids respectively. For our experiments, we use the operator augmentation $\bar{K} = \hat{A}$,

$$ \bar{A}^{-1} = \hat{A}^{-1} - \beta \hat{K} = (1 - \beta) \hat{A}^{-1} = (1 - \beta)(I - \gamma \hat{P})^{-1}, $$

where we use the Taylor expanded Monte Carlo approximation $\hat{\beta}$ from (8.7). We compute our augmented solution via

$$ \tilde{q} = \bar{A}^{-1}r. $$

#### 9.3.1. Random Walk with Drift on a 1D Grid

For this example, we consider the Markov chain of a lazy random walk with drift on a 1D periodic grid graph. We let the state space $V$ be the set of integers $\{1, 2, \ldots, K\}$ where $K = 16$ and take the probability transition matrix to be

$$ \mathbb{P}_{\ell, r}^{(1D)}(X_t = u \mid X_{t-1} = v) = \begin{cases} \ell & u = v - 1 \mod K \\ 1 - \ell - r & u = v \mod K \\ r & u = v + 1 \mod K \\ 0 & \text{o.w.} \end{cases} $$

where $\ell$ and $r$ are drift parameters.
We test a handful of different values for \((\ell, r)\) as well as a handful of different values for the sample count \(N\) that determines the “noise” in the matrix \(\hat{P}\) (higher \(N\) means less noise). For the reward function — we consider two cases: for the first, we consider deterministic reward function given by

\begin{equation}
(9.15) \quad r^{(1D)}(v) = \sin(4\pi v/K).
\end{equation}

For the second, we consider a random isotropic reward vector prior where \(r^{(1D)} \sim \mathcal{N}(0, I)\).

In addition to the above collection of transition matrices, we also consider random walks with the ability to skip a vertex in the grid,

\begin{equation}
(9.16) \quad \mathbb{P}_{\ell_1, \ell_2, r_1, r_2}^{(1D)}(X_i = u \mid X_{i-1} = v) = \begin{cases} 
\ell_1 & u = v - 2 \mod K \\
\ell_2 & u = v - 1 \mod K \\
1 - \ell_1 - \ell_2 - r_1 - r_2 & u = v \mod K \\
r_1 & u = v + 1 \mod K \\
r_2 & u = v + 2 \mod K \\
0 & \text{o.w.}
\end{cases}
\end{equation}

as well as transition matrices corresponding to a random walk on a complete graph,

\begin{equation}
(9.17) \quad \mathbb{P}_{\text{complete}}^{(1D)}(X_i = u \mid X_{i-1} = v) = \frac{1}{K}.
\end{equation}

For these 1D experiments, we use discount factor

\begin{equation}
(9.18) \quad \gamma^{(1D)} = 0.99.
\end{equation}

We present the results of our numerical experiments for the specified reward vectors in Table 9.1 as well as for isotropic reward vectors in Table 9.2.

### 9.3.2. Random walk with Drift on 2D and 3D Grids.

Now let us consider the Markov chain of a lazy random walk with non-uniform drift on a 2D periodic grid graph. We let the state space \(V\) be the set of tuples \(\{1, 2, ..., K\} \times \{1, 2, ..., K\}\) where \(K = 16\) and we consider two probability transition matrices, the first a standard uniform random walk:

\begin{equation}
(9.19) \quad \mathbb{P}_{\text{unif}}^{(2D)}(X_i = u \mid X_{i-1} = v) = \begin{cases} 
1/4 & |u - v| = 1 \\
0 & \text{o.w.}
\end{cases}
\end{equation}

and the second a random walk with a non-uniform drift:

\begin{equation}
(9.20) \quad \mathbb{P}_{\text{nonunif}}^{(2D)}(X_i = u \mid X_{i-1} = v) = \begin{cases} 
\frac{1}{4} \pm \frac{1}{8} \sin(2\pi v_x/K) & u = v \mp (1, 0) \\
\frac{1}{4} \pm \frac{1}{8} \sin(2\pi v_y/K) & u = v \mp (0, 1) \\
0 & \text{o.w.}
\end{cases}
\end{equation}

For the reward function, we consider both a deterministic reward

\begin{equation}
(9.21) \quad r^{(2D)}(v) = -\sin(2\pi v_x/K) \sin(2\pi v_y/K),
\end{equation}

as well as an isotropic reward vector prior where \(r^{(2D)} \sim \mathcal{N}(0, I)\). For these 2D experiments, we use discount factor

\begin{equation}
(9.22) \quad \gamma^{(2D)} = 0.99.
\end{equation}

We can define similar transition matrices on 3D periodic grid graphs, where \(V = \{1, ..., K\}^3\) and \(K = 8\):

\begin{equation}
(9.23) \quad \mathbb{P}_{\text{unif}}^{(3D)}(X_i = u \mid X_{i-1} = v) = \begin{cases} 
1/6 & |u - v| = 1 \\
0 & \text{o.w.}
\end{cases}
\end{equation}
as well as an analogous 3D random walk with a non-uniform drift:

\[
P_{\text{nonunif}}^{(3D)}(X_1 = u \mid X_{i-1} = v) = \begin{cases} 
\frac{1}{2} \pm \frac{1}{8} \sin(2\pi v / K) & u = v \mp (1,0,0) \\
\frac{1}{2} \pm \frac{1}{8} \sin(2\pi v / K) & u = v \mp (0,1,0) \\
\frac{1}{2} \pm \frac{1}{8} \sin(2\pi v / K) & u = v \mp (0,0,1) \\
0 & \text{o.w.}
\end{cases}
\]

For the reward function, we consider both a deterministic reward

\[
r^{(3D)}(v) = -\sin(2\pi v_x / K) \sin(2\pi v_y / K) \sin(2\pi v_z / K),
\]

as well as an isotropic reward vector prior where \( r^{(3D)} \sim \mathcal{N}(0, I) \). For these 3D experiments, we use discount factor

\[
\gamma^{(3D)} = 0.9.
\]

We present the results of our numerical experiments for the specified reward vectors in Table 9.1 as well as for isotropic reward vectors in Table 9.2.

9.4. Discussion. As we see in Table 9.1 and Table 9.2, operator augmentation can provide significant reductions in error for a variety of different Markov chain problems, measured both in the reduction of residual norm error for deterministic right-hand-side (Table 9.1). As predicted by the theory, the method also reduces the error in isotropic residual matrix norm, as seen in (Table 9.2), but these improvements seem are more marginal. This behavior is present for all different levels of sample count \( N \) we tested. Therefore, while there are theoretical limitations in the non-symmetric case of operator augmentation that make the theory less powerful than the symmetric positive definite case, operator augmentation still functions quite well on the Markov chain problems we’ve tested it on.

Note that the confidence intervals for the 2D and 3D problems in the isotropic setting seen in Table 9.2 are quite large. This is despite the fact that we use a very large number of samples (256,000 for 2D, and 25,600 for 3D) to estimate the isotropic error. However, the theory tells us that the naive isotropic error will always be greater than the augmented isotropic error, so this chart is provided more-so as a way to gauge the magnitude of the error reduction, rather than existence of an error reduction.

10. Conclusion. We conclude this paper by noting that we have accomplished two main goals. First, we have investigated the extent to which the symmetric positive definite operator augmentation theory of [4] can be applied to the general non-symmetric matrix case. We have found that under the assumptions of noise symmetry and right-hand-side isotropy, the optimal augmentation factor is always positive. This means that the act of bootstrapping is relatively safe, as operator augmentation will damp noise rather than amplify it. We have also shown that there are pathological situations that make our assumptions necessary in general. However, in the small noise regime, the noise symmetry assumption can be discarded.

Second, we have shown empirically that operator augmentation can still reduce error for noisy Markov chain problems, even when the aforementioned theoretical assumptions are not satisfied. This holds true across a number of different Markov chains and for both deterministic and isotropic right-hand-side.

One may continue this work by attempting to apply some form of operator augmentation to real problems – for example, in control theory or reinforcement learning, where the underlying Markov decision process may not be fully known and must be estimated from data. Another more theoretical possibility would be to investigate if the operator augmentation framework can be applied to optimization to create optimization algorithms that are less vulnerable to noise in the objective function, as is common in many real world applications.

REFERENCES
[1] G. W. Anderson, A. Guionnet, and O. Zeitouni, An introduction to random matrices, vol. 118, Cambridge university press, 2010.
[2] E. J. Candès and Y. Plan, Matrix completion with noise, Proceedings of the IEEE, 98 (2010), pp. 925–936.
[3] C. Davis and W. M. Kahan, The rotation of eigenvectors by a perturbation. iii, SIAM Journal on Numerical Analysis, 7 (1970), pp. 1–46.
[4] P. A. Etter and L. Ying, Operator augmentation for noisy elliptic systems, arXiv preprint arXiv:2010.09656, (2020).
[5] W. James and C. Stein, Estimation with quadratic loss, in Breakthroughs in statistics, Springer, 1992, pp. 443–460.
[6] R. Keshavan, A. Montanari, and S. Oh, Matrix completion from noisy entries, in Advances in neural information processing systems, 2009, pp. 952–960.
[7] Y. Marzouk, T. Moselhy, M. Parno, and A. Spantini, An introduction to sampling via measure transport, arXiv preprint arXiv:1602.05023, (2016).
[8] T. Palmer, G. Shutts, R. Hagedorn, F. Doblas-Reyes, T. Jung, and M. Leutbecher, Representing model uncertainty in weather and climate prediction, Annu. Rev. Earth Planet. Sci., 33 (2005), pp. 163–193.
[9] C. Soize, A comprehensive overview of a non-parametric probabilistic approach of model uncertainties for predictive models in structural dynamics, Journal of sound and vibration, 288 (2005), pp. 623–652.
[10] T. Tao, Topics in random matrix theory, vol. 132, American Mathematical Soc., 2012.
[11] D. Xiu and J. S. Hesthaven, High-order collocation methods for differential equations with random inputs, SIAM Journal on Scientific Computing, 27 (2005), pp. 1118–1139.
[12] D. Xiu and G. E. Karniadakis, The wiener–askey polynomial chaos for stochastic differential equations, SIAM journal on scientific computing, 24 (2002), pp. 619–644.
| Chain                | Samples (N) | Naive Error ±2σ | Augmented Error ±2σ |
|---------------------|-------------|-----------------|---------------------|
| $P^{1D}_{1/4,1/4}$  | 16          | 166% ±13.5%     | 53.5% ±1.35%        |
|                     | 32          | 48.8% ±1.50%    | 30.1% ±0.53%        |
|                     | 64          | 20.1% ±0.45%    | 16.0% ±0.27%        |
| $P^{1D}_{1/6,2/6}$  | 16          | 115% ±10.2%     | 42.2% ±1.57%        |
|                     | 32          | 31.7% ±1.11%    | 20.8% ±0.47%        |
|                     | 64          | 12.7% ±0.31%    | 10.4% ±0.20%        |
| $P^{1D}_{0,1/2}$    | 16          | 11.7% ±1.06%    | 8.70% ±0.67%        |
|                     | 32          | 4.02% ±0.12%    | 3.49% ±0.04%        |
|                     | 64          | 1.75% ±0.04%    | 1.63% ±0.03%        |
| $P^{1D}_{1/8,1/8,1/8}$ | 16      | 55.2% ±2.61%    | 29.9% ±0.59%        |
|                     | 32          | 19.5% ±0.44%    | 15.0% ±0.24%        |
|                     | 64          | 8.55% ±0.15%    | 7.55% ±0.12%        |
| $P^{1D}_{\text{complete}}$ | 16 | 6.63% ±0.18%    | 6.09% ±0.09%        |
|                     | 32          | 3.25% ±0.05%    | 3.10% ±0.04%        |
|                     | 64          | 1.43% ±0.02%    | 1.41% ±0.02%        |
| $P^{2D}_{\text{unif}}$ | 12      | 206% ±42.4%     | 66.9% ±3.26%        |
|                     | 24          | 91.3% ±14.3%    | 47.5% ±3.00%        |
|                     | 48          | 43.3% ±5.63%    | 30.1% ±2.29%        |
| $P^{2D}_{\text{nonunif}}$ | 12     | 113% ±20.8%     | 52.7% ±7.91%        |
|                     | 24          | 51.7% ±7.91%    | 33.8% ±3.08%        |
|                     | 48          | 24.7% ±3.40%    | 19.7% ±2.05%        |
| $P^{3D}_{\text{unif}}$ | 4       | 92.7% ±30.9%    | 48.3% ±7.25%        |
|                     | 8           | 38.8% ±9.09%    | 27.8% ±4.12%        |
|                     | 16          | 18.0% ±3.66%    | 15.2% ±2.36%        |
| $P^{3D}_{\text{nonunif}}$ | 4     | 77.8% ±22.6%    | 44.3% ±7.00%        |
|                     | 8           | 33.4% ±7.86%    | 25.1% ±4.04%        |
|                     | 16          | 15.7% ±3.20%    | 13.5% ±2.29%        |

Table 9.1

**Deterministic Value Function Comparison:** A performance comparison between the accuracy of the operator augmented estimator $\tilde{x}$ for the solution $x$ versus the naive estimator $\hat{x}$. The error is measured as a percentage with respect to the residual norm of the true solution. Since the error is calculated via Monte Carlo, we provide a 95% confidence interval in the ±2σ column.
### Isotropic Random Value Function Comparison

A performance comparison between the accuracy of the operator augmented estimator $\hat{x}$ for the solution $x$ versus the naive estimator $\bar{x}$. The value function is sampled from the prior $\mathcal{N}(0, I)$. The error is measured as a percentage with respect to the average residual norm of the true solutions from the prior. Since the error is calculated via Monte Carlo, we provide a 95% confidence interval in the $\pm 2\sigma$ column.

| Chain | Samples (N) | Naive Error $\pm 2\sigma$ | Augmented Error $\pm 2\sigma$ |
|-------|-------------|--------------------------|-------------------------------|
| $P^{(1D)}_{1/4,1/4}$ | 16 | 105% $\pm 25.4\%$ | 48.4% $\pm 6.16\%$ |
|       | 32 | 30.8% $\pm 2.95\%$ | 22.8% $\pm 1.70\%$ |
|       | 64 | 12.7% $\pm 1.00\%$ | 11.1% $\pm 0.77\%$ |
| $P^{(1D)}_{1/6,2/6}$ | 16 | 64.1% $\pm 16.0\%$ | 33.9% $\pm 5.52\%$ |
|       | 32 | 17.2% $\pm 1.77\%$ | 13.5% $\pm 1.14\%$ |
|       | 64 | 6.84% $\pm 0.52\%$ | 6.13% $\pm 0.41\%$ |
| $P^{(1D)}_{0,1/2}$ | 16 | 11.0% $\pm 3.30\%$ | 8.49% $\pm 2.40\%$ |
|       | 32 | 3.77% $\pm 0.33\%$ | 3.34% $\pm 0.26\%$ |
|       | 64 | 1.64% $\pm 0.11\%$ | 1.54% $\pm 0.10\%$ |
| $P^{(1D)}_{1/8,1/8,1/8}$ | 16 | 55.1% $\pm 2.62\%$ | 29.9% $\pm 0.59\%$ |
|       | 32 | 19.5% $\pm 0.44\%$ | 15.0% $\pm 0.24\%$ |
|       | 64 | 8.55% $\pm 0.15\%$ | 7.55% $\pm 0.12\%$ |
| $P^{(1D)}_{\text{complete}}$ | 16 | 6.21% $\pm 0.29\%$ | 5.81% $\pm 0.25\%$ |
|       | 32 | 2.98% $\pm 0.13\%$ | 2.89% $\pm 0.12\%$ |
|       | 64 | 1.46% $\pm 0.06\%$ | 1.43% $\pm 0.06\%$ |
| $P^{(2D)}_{\text{unif}}$ | 12 | 25.7% $\pm 7.51\%$ | 20.4% $\pm 4.89\%$ |
|       | 24 | 11.3% $\pm 2.93\%$ | 10.2% $\pm 2.38\%$ |
|       | 48 | 5.35% $\pm 1.31\%$ | 5.07% $\pm 1.19\%$ |
| $P^{(2D)}_{\text{nonunif}}$ | 12 | 20.2% $\pm 6.17\%$ | 16.7% $\pm 4.89\%$ |
|       | 24 | 8.96% $\pm 2.43\%$ | 8.20% $\pm 2.04\%$ |
|       | 48 | 4.26% $\pm 1.09\%$ | 4.07% $\pm 1.00\%$ |
| $P^{(3D)}_{\text{unif}}$ | 4 | 35.3% $\pm 35.0\%$ | 26.2% $\pm 20.8\%$ |
|       | 8 | 14.6% $\pm 11.8\%$ | 12.7% $\pm 9.11\%$ |
|       | 16 | 6.76% $\pm 5.03\%$ | 6.33% $\pm 4.43\%$ |
| $P^{(3D)}_{\text{nonunif}}$ | 4 | 33.4% $\pm 35.4\%$ | 25.1% $\pm 21.6\%$ |
|       | 8 | 13.9% $\pm 12.0\%$ | 1.22% $\pm 9.36\%$ |
|       | 16 | 6.43% $\pm 5.12\%$ | 6.03% $\pm 4.53\%$ |