Generalizations of data-driven balancing: what to sample for different balancing-based reduced models

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Abstract

The Quadrature-based Balanced Truncation (QuadBT) framework of [14] is a "non-intrusive" reformulation of balanced truncation; a classical projection-based model-order reduction technique for linear systems. QuadBT is non-intrusive in the sense that it builds approximate balanced reduced-order models entirely from system response data (e.g., transfer function measurements) without the need to reference an explicit state-space realization of the underlying full-order model. In this work, we generalize and extend QuadBT to other types of balanced truncation model reduction. Namely, we develop non-intrusive implementations for balanced stochastic truncation, positive-real balanced truncation, and bounded-real balanced truncation. We show that the data-driven construction of these balanced reduced-order models requires sampling certain spectral factors associated with the system of interest. Numerical examples are included in each case to validate our approach.

Key words: Balanced truncation, data-driven modeling, algebraic Riccati equations, spectral factors, numerical quadrature

1 Introduction

Model-order reduction (MoR) is the procedure by which one approximates a large-scale dynamical system with a surrogate reduced-order model (RoM). We refer the reader to, e.g. [1,2,4,5], for an overview of MoR of largescale dynamical systems. *Balanced truncation* (BT) MoR [19, 20] and its variants, e.g. [11, 15, 21], are considered among the "gold standards" for MoR of linear time-invariant (LTI) dynamical systems, which are the focus of this work. The allure of BT methods stems from the fact that they preserve certain desirable qualitative features (e.g., stability or passivity) of the full-order model (FoM), and satisfy tractable *a priori* bounds on either the relative or absolute \mathcal{H}_{∞} approximation error.

BT and its variants are "intrusive" by nature; that is, they require access to an explicit representation of the internal system dynamics (the state-space form) to compute the RoM from the full-order system matrices via projection. In this work, we are interested in *data-driven* approaches, which are "non-intrusive". In other words, data-driven methodologies construct surrogate RoMs *entirely* from input-output invariants (e.g., impulse response measurements or transfer function evaluations) without the need to reference a particular realization of the FoM. These data can be obtained either experimentally (e.g., by measuring the response of some physical system in laboratory setting) or synthetically (i.e., via numerical or "black box" simulation of the underlying model).

The recent contribution [14] introduces a data-driven reformulation of the classical BT: Quadrature-based balanced truncation (QuadBT). Other data-driven formulations of BT have been proposed throughout the years; see, e.g., [8,24,26,27]. Indeed, in [19], Moore had already motivated a time-domain data-driven BT. However, unlike QuadBT, these methods require state measurements as opposed to state-space invariant input-output data we focus on. In this work, we generalize the QuadBT framework of [14] to other types of balanced truncation. The variants studied here are balanced stochastic truncation (BST) [11,15], positive-real balanced truncation (PRBT) [11], and bounded-real balanced truncation (BRBT) [21]. The essential quantities to any type of balancing-based MoR are the system Gramians. The key

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insight we exploit in developing data-driven extensions of these BT-variants is that any BT-RoM is effectively determined by the *square-root factors* of the relevant Gramians. Beyond the choice of square-root factors, the algorithmic computation of any BT-RoM proceeds identically. By decomposing the relevant Gramians using appropriately chosen *quadrature-based* square-root factors, we show how to approximately realize the reduced-order quantities arising in different BT variants from various input-output invariant frequency-response data. These "data" required to mimic each type of balancing correspond to transfer function evaluations of certain *spectral factors* associated with the FoM.

The rest of this work is organized as follows: Section 2 outlines the key details of BT model reduction and the variants studied in this work. Section 3 presents a generalized derivation of QuadBT that shows how to reconstruct the key quantities present in any (square-root) balancing-based algorithm entirely from input-output data. This generalized framework is applicable to each variant of BT we study here. Section 4 derives datadriven implementations of BST, PRBT, and BRBT, and by applying the generalized framework of Section 3 answers the titular question: "What do you need to sample for different balancing-based reduced models?" We show that the computation of these data-driven RoMs requires sampling certain spectral factors associated with the underlying linear model. Several numerical experiments are included in Section 5 to illustrate the efficacy of the quadrature-based RoMs and validate our approach. Section 6 concludes the paper.

2 Balanced truncation model reduction

Throughout this work, we consider LTI dynamical systems given in state-space form as

$$\mathcal{G}: \begin{cases} \dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t). \end{cases}$$
(1)

The input and output are, respectively, given by $\mathbf{u}(t) \in \mathbb{R}^m$ and $\mathbf{y}(t) \in \mathbb{R}^p$; $\mathbf{x}(t) \in \mathbb{R}^n$ contains the state coordinates; $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, $\mathbf{C} \in \mathbb{R}^{p \times n}$, and $\mathbf{D} \in \mathbb{R}^{p \times m}$ are a state-space realization of \mathcal{G} . We assume the initial condition satisfies $\mathbf{x}(0) = \mathbf{0}$. For notation, we use $(\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D})$ to indicate a particular realization of \mathcal{G} . In this work, we assume that the eigenvalues of \mathbf{A} lie in the open left half-plane, i.e., \mathcal{G} is asymptotically stable. We also assume that the given realization is minimal, i.e., fully reachable and observable [1, Lemma 4.42]. The transfer function of \mathcal{G} , defined as

$$\mathbf{G}(s) := \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D} \in \mathbb{C}^{p \times m}, \qquad (2)$$

is a matrix-valued rational function analytic in the closed right half-plane; \mathbf{I}_n is the $n \times n$ identity matrix. The transfer function fully characterizes the input-output mapping of \mathcal{G} in the frequency domain and is state-space realization invariant. The \mathcal{H}_{∞} norm of \mathcal{G} is defined as $\|\mathcal{G}\|_{\mathcal{H}_{\infty}} := \sup_{\omega \in \mathbb{R}} \sigma_{\max} (\mathbf{G}(i\omega))$, where $\sigma_{\max}(\cdot)$ denotes the maximal singular value of (\cdot) and $i^2 = -1$. The *dual* to \mathcal{G} is the defined as the LTI system $(-\mathbf{A}^{\mathsf{T}}, -\mathbf{C}^{\mathsf{T}}, \mathbf{B}^{\mathsf{T}},$ \mathbf{D}^{T}) having the transfer function $\mathbf{G}(-s)^{\mathsf{T}}$.

Given a system \mathcal{G} as in (1), we seek a LTI-RoM \mathcal{G}_r

$$\mathcal{G}_r: \begin{cases} \dot{\mathbf{x}}_r(t) = \mathbf{A}_r \mathbf{x}_r(t) + \mathbf{B}_r \mathbf{u}(t) \\ \mathbf{y}_r(t) = \mathbf{C}_r \mathbf{x}_r(t) + \mathbf{D}_r \mathbf{u}(t), \end{cases}$$
(3)

having the reduced-order transfer function

$$\mathbf{G}_r(s) := \mathbf{C}_r(s\mathbf{I}_r - \mathbf{A}_r)^{-1}\mathbf{B}_r + \mathbf{D}_r \in \mathbb{C}^{p \times m},$$

where $\mathbf{x}_r(t) \in \mathbb{R}^r$, $\mathbf{y}_r(t) \in \mathbb{R}^p$, $\mathbf{A}_r \in \mathbb{R}^{r \times r}$, $\mathbf{B}_r \in \mathbb{R}^{r \times m}$, $\mathbf{C}_r \in \mathbb{R}^{p \times r}$, and $\mathbf{D}_r \in \mathbb{R}^{p \times m}$ for $r \ll n$. The objective of model reduction is that the surrogate \mathcal{G}_r accurately reproduces the input-output character of \mathcal{G} (i.e., $\mathbf{y}_r(t) \approx \mathbf{y}(t)$ for a variety of admissible inputs $\mathbf{u}(t)$) and preserves important qualitative features (e.g., stability and passivity) of \mathcal{G} . Projection-based model reduction algorithms, including BT methods. Given left and right model reduction subspaces spanned by $\mathbf{W}_r \in \mathbb{R}^{n \times r}$ and $\mathbf{V}_r \in \mathbb{R}^{n \times r}$ respectively, the order-r RoM ($\mathbf{A}_r, \mathbf{B}_r, \mathbf{C}_r, \mathbf{D}_r$) via *Petrov-Galerkin projection* is determined by

$$\mathbf{A}_r = \mathbf{W}_r^{\mathsf{T}} \mathbf{A} \mathbf{V}_r, \quad \mathbf{B}_r = \mathbf{W}_r^{\mathsf{T}} \mathbf{B}, \quad \mathbf{C}_r = \mathbf{C} \mathbf{V}_r.$$
(4)

In ProjMoR, it is common to choose $\mathbf{D}_r = \mathbf{D}$. ProjMoR methods differ in the way they choose \mathbf{V}_r ad \mathbf{W}_r ; see [1, 2,5] for more details on ProjMoR in general.

Balanced truncation (BT) and its variants are among the "gold standards" for ProjMoR of LTI dynamical systems. This is because BT-RoMs (i) preserve important systemtheoretic features of the FoM and (ii) satisfy tractable bounds on the \mathcal{H}_{∞} approximation error (which bounds the \mathcal{L}_2 output error $\mathbf{y} - \mathbf{y}_r$). The system Gramians are the key components of any balancing-based model reduction algorithm. In classical BT, the Gramians are the unique solutions to dual algebraic Lyapunov equations (ALEs). In many other variants of BT, the Gramians are the minimal stabilizing solutions of algebraic Riccati equations (AREs). Balancing is the simultaneous diagonalization of two such matrices. Once these two matrices are computed, one balances the FoM by an appropriate change of coordinate system in which the pertinent Gramians are diagonal and identical. Order reduction is then accomplished by effectively truncating the least important components of the state-space; these are precisely the states associated with the smallest magnitude singular values of the balanced Gramians.

Next, we recount the key details of the BT methods that are the focus of this work. All BT methods we consider fit under ProjMoR and the RoM is computed as in (4). Once the relevant system Gramians are computed (based on the variant of BT used) construction of \mathbf{V}_r and \mathbf{W}_r proceeds identically. In Sections 2.1–2.4, we specify what Gramians are diagonalized in each BT method. Then, Section 2.5 shows how to construct \mathbf{V}_r and \mathbf{W}_r given the Gramians of choice. For a more general treatise of BT model reduction, see [1, Ch. 7], [3, 10, 17].

Lyapunov balanced truncation 2.1

BT was independently introduced in the works [19, 20]. In its original setting (that we will refer to as Lyapunov balancing) the central quantities are the *observability* and reachability Gramians $\mathbf{Q} \in \mathbb{R}^{n \times n}$ and $\mathbf{P} \in \mathbb{R}^{n \times n}$ of \mathcal{G} . These Gramians are the unique solutions to dual ALEs:

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q} + \mathbf{Q}\mathbf{A} + \mathbf{C}^{\mathsf{T}}\mathbf{C} = \mathbf{0},\tag{5}$$

and
$$\mathbf{AP} + \mathbf{PA}^{\mathsf{T}} + \mathbf{BB}^{\mathsf{T}} = \mathbf{0}.$$
 (6)

The uniqueness of \mathbf{Q} and \mathbf{P} follows from the asymptotic stability of \mathcal{G} [1, Prop. 6.2].

The Gramians \mathbf{Q} and \mathbf{P} are symmetric positive definite (SPD) by minimality of \mathcal{G} , and in turn, there exist nonsingular matrices $\mathbf{L}, \mathbf{U} \in \mathbb{R}^{n \times n}$ such that $\mathbf{Q} = \mathbf{L} \mathbf{L}^{\mathsf{T}}$ and $\mathbf{P} = \mathbf{U}\mathbf{U}^{\mathsf{T}}$. The Hankel singular values of \mathcal{G} are the singular values of $\mathbf{L}^{\mathsf{T}}\mathbf{U}$, denoted $\sigma(\mathbf{L}^{\mathsf{T}}\mathbf{U})$. In this balanced basis the states that are weakly reachable are simultaneously weakly observable; these are precisely the states identified by the smallest magnitude Hankel singular values. One constructs the BT-RoM by effectively truncating those components of the state space. Lyapunov BT-RoMs retain the asymptotic stability of the FoM [22] and satisfy an *a priori* upper bound on the \mathcal{H}_{∞} approximation error $\|\mathcal{G} - \mathcal{G}_r\|_{\mathcal{H}_{\infty}}$ in terms of the neglected Hankel singular values [12].

2.2Balanced stochastic truncation

Assume now that \mathcal{G} has two additional properties: (i) \mathcal{G} is square (that is, the input and output dimensions are the same, m = p, and (ii) the input feed-through term **D** is nonsingular. For an extension to non-square dynamical systems, see [6]. Balanced stochastic truncation (BST) [11,15] balances the reachability Gramian of \mathcal{G} against the *minimal stabilizing* solution of an ARE

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{W}} + \mathbf{Q}_{\mathcal{W}}\mathbf{A} + (\mathbf{C} - \mathbf{B}_{\mathcal{W}}^{\mathsf{T}}\mathbf{Q}_{\mathcal{W}})^{\mathsf{T}}(\mathbf{D}\mathbf{D}^{\mathsf{T}})^{-1}(\mathbf{C} - \mathbf{B}_{\mathcal{W}}^{\mathsf{T}}\mathbf{Q}_{\mathcal{W}}) = \mathbf{0},$$
(7)

where $\mathbf{B}_{\mathcal{W}} := (\mathbf{P}\mathbf{C}^{\mathsf{T}} + \mathbf{B}\mathbf{D}^{\mathsf{T}})$. Any solution $\mathbf{Q}_{\mathcal{W}} \in \mathbb{R}^{n \times n}$ to (7) is *not* unique; based on the assumptions on \mathcal{G} , there exist (unique) maximal and minimal solutions to (7)that obey the partial order $\mathbf{Q}_{\mathcal{W}}^{\min} \leq \mathbf{Q}_{\mathcal{W}} \leq \mathbf{Q}_{\mathcal{W}}^{\max}$ [28, Theorem 13.11]. A balanced stochastic realization is obtained by balancing $\mathbf{P} \in \mathbb{R}^{n \times n}$ against this minimal solution $\mathbf{Q}_{\mathcal{W}}^{\min} \in \mathbb{R}^{n \times n}$. For simplicity of notation, we take $\mathbf{Q}_{\mathcal{W}}$ to denote the minimal solution of (7) moving forward. A system \mathcal{G} is said to be *minimum phase* if the poles and the zeros of its transfer function lie in the open left half-plane; BST-RoMs preserve this minimum-phase property of the FoM. Moreover, BST-RoMs satisfy an upper bound on the *relative* \mathcal{H}_{∞} error, i.e., $\|\mathcal{G}^{-1}(\mathcal{G} - \mathcal{G})\|$ \mathcal{G}_r) $\|_{\mathcal{H}_{\infty}}$. The error bound is due to [16].

2.3Positive-real balanced truncation

Again suppose that \mathcal{G} is square. A closely related method to that of BST is positive-real balanced truncation (PRBT), also introduced in [15]. PRBT is primarily utilized for the model reduction of passive linear systems. Passive systems are ubiquitous in applications of physics and engineering; electrical circuits are one such example. Passive systems also have port-Hamiltonian structure, an important focus of recent work in the modeling community [18].

For $s \in \mathbb{C}$ that is not an eigenvalue of either **A** or $-\mathbf{A}$, the *Popov function* of \mathcal{G} is defined as

$$\Phi(s) := \mathbf{G}(s) + \mathbf{G}(-s)^{\mathsf{T}}.$$
(8)

An asymptotically stable and square system \mathcal{G} is said to be *positive-real* if its transfer function satisfies

$$\Phi(i\omega) = \mathbf{G}(i\omega) + \mathbf{G}(-i\omega)^{\mathsf{T}} \ge 0, \quad \omega \in \mathbb{R}.$$
(9)

 \mathcal{G} is strictly positive-real if the inequality (9) is strict. (For simplicity, we consider only strictly positive-real systems in this work, and take positive-realness to mean strict positive-realness moving forward.) Any positivereal system is necessarily passive; see [1, Theorem 5.30]. Equivalently, \mathcal{G} is strictly positive real if and only if there exists a SPD matrix $\mathbf{Q}_{\mathcal{M}} \in \mathbb{R}^{n \times n}$ that satisfies the ARE

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{M}} + \mathbf{Q}_{\mathcal{M}}\mathbf{A} + (\mathbf{C} - \mathbf{B}^{\mathsf{T}}\mathbf{Q}_{\mathcal{M}})^{\mathsf{T}}(\mathbf{D} + \mathbf{D}^{\mathsf{T}})^{-1}(\mathbf{C} - \mathbf{B}^{\mathsf{T}}\mathbf{Q}_{\mathcal{M}}) = \mathbf{0}, \quad (10)$$

see, e.g., [28, Corollary 13.27]. The dual ARE to (10) is

$$\mathbf{A} \mathbf{P}_{\mathcal{N}} + \mathbf{P}_{\mathcal{N}} \mathbf{A}^{\mathsf{T}} + \\ (\mathbf{B} - \mathbf{P}_{\mathcal{N}} \mathbf{C}^{\mathsf{T}}) (\mathbf{D} + \mathbf{D}^{\mathsf{T}})^{-1} (\mathbf{B} - \mathbf{P}_{\mathcal{N}} \mathbf{C}^{\mathsf{T}})^{\mathsf{T}} = \mathbf{0},$$
 (11)

for SPD $\mathbf{P}_{\mathcal{N}} \in \mathbb{R}^{n \times n}$. ($\mathbf{D} + \mathbf{D}^{\mathsf{T}}$ is nonsingular by the positive-real assumption.) We refer to (10) and (11) as the positive-real AREs (PR-AREs). As in the BST set-

. . .

ting, any SPD solution to each of the PR-AREs (10) and (11) lies between two extremal solutions; $\mathbf{Q}_{\mathcal{M}}^{\min} \leq \mathbf{Q}_{\mathcal{M}} \leq \mathbf{Q}_{\mathcal{M}}^{\max}$ and $\mathbf{P}_{\mathcal{N}}^{\min} \leq \mathbf{P}_{\mathcal{N}} \leq \mathbf{P}_{\mathcal{N}}^{\max}$. A positive-real balanced realization is obtained by balancing the minimal solutions $\mathbf{Q}_{\mathcal{M}}^{\min}$ and $\mathbf{P}_{\mathcal{N}}^{\min}$ to (10) and (11). We take $\mathbf{Q}_{\mathcal{M}}$ and $\mathbf{P}_{\mathcal{N}}$ to denote the minimal solutions to the PR-AREs moving forward. PRBT-RoMs are guaranteed to maintain the asymptotic stability and passivity of the FoM. Additionally, there exists a relative type of bound on the \mathcal{H}_{∞} reduction error; see [17, Lemma 3].

2.4 Bounded-real balanced truncation

The last variant studied here is bounded-real balanced truncation (BRBT) [21]. An important class of systems is those having transfer functions which are bounded along the imaginary axis; such systems are used in parameterizing all stabilizing controllers of a system such that the closed-loop system satisfies a particular \mathcal{H}_{∞} constraint [13]. These systems are called bounded-real. Formally, an asymptotically system \mathcal{G} is called boundedreal if its transfer function $\mathbf{G}(s)$ satisfies

$$\gamma^2 \mathbf{I}_m - \mathbf{G}(-i\omega)^{\mathsf{T}} \mathbf{G}(i\omega) \ge 0, \quad \omega \in \mathbb{R}, \qquad (12)$$

where $\gamma := \|\mathcal{G}\|_{\mathcal{H}_{\infty}}$. Condition (12) can be alternatively posed as $\|\mathcal{G}\|_{\mathcal{H}_{\infty}} \leq \gamma$. Since it is always possible to normalize $\mathbf{G}(s)$ so that $\|\mathcal{G}\|_{\mathcal{H}_{\infty}} \leq 1$, without loss of generality we assume that $\gamma = 1$ in this work. (A system is *strictly* bounded-real if the inequality (12) is strict; for simplicity, we assume strict bounded-realness, and take bounded-realness to mean strict bounded-realness.) According to the Bounded-real Lemma [28, Corollary 13.24], \mathcal{G} is strictly bounded-real if and only if there exists a SPD matrix $\mathbf{Q}_{\mathcal{J}} \in \mathbb{R}^{n \times n}$ that satisfies the ARE

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{J}} + \mathbf{Q}_{\mathcal{J}}\mathbf{A} + \mathbf{C}^{\mathsf{T}}\mathbf{C} + (\mathbf{B}^{\mathsf{T}}\mathbf{Q}_{\mathcal{J}} + \mathbf{D}^{\mathsf{T}}\mathbf{C})^{\mathsf{T}} \times (\mathbf{I}_{m} - \mathbf{D}^{\mathsf{T}}\mathbf{D})^{-1} (\mathbf{B}^{\mathsf{T}}\mathbf{Q}_{\mathcal{J}} + \mathbf{D}^{\mathsf{T}}\mathbf{C}) = \mathbf{0}.$$
 (13)

The dual ARE to (13) has a SPD solution $\mathbf{P}_{\mathcal{K}} \in \mathbb{R}^{n \times n}$

$$\mathbf{AP}_{\mathcal{K}} + \mathbf{P}_{\mathcal{K}}\mathbf{A}^{\top} + \mathbf{BB}^{\top} + (\mathbf{P}_{\mathcal{K}}\mathbf{C}^{\top} + \mathbf{BD}^{\top}) \times (\mathbf{I}_{p} - \mathbf{DD}^{\top})^{-1} (\mathbf{P}_{\mathcal{K}}\mathbf{C}^{\top} + \mathbf{BD}^{\top})^{\top} = \mathbf{0}.$$
(14)

(The nonsingularity of $\mathbf{I}_m - \mathbf{D}^{\mathsf{T}}\mathbf{D}$ and $\mathbf{I}_p - \mathbf{D}\mathbf{D}^{\mathsf{T}}$ is guaranteed by the strictly bounded-real assumption on \mathcal{G} and its dual, respectively.) We refer to (13) and (14) as the *bounded-real AREs* (BR-AREs). Any SPD solutions to (13) and (14) lie between some extremal solutions; $\mathbf{Q}_{\mathcal{J}}^{\min} \leq \mathbf{Q}_{\mathcal{S}} \leq \mathbf{Q}_{\mathcal{J}}^{\max}$ and $\mathbf{P}_{\mathcal{K}}^{\min} \leq \mathbf{P}_{\mathcal{Z}} \leq \mathbf{P}_{\mathcal{K}}^{\max}$. A bounded-real balanced realization is obtained by balancing $\mathbf{Q}_{\mathcal{J}}^{\min}$ and $\mathbf{P}_{\mathcal{K}}^{\min}$; we take $\mathbf{Q}_{\mathcal{J}}$ and $\mathbf{P}_{\mathcal{K}}$ to denote the minimal solutions to the BR-AREs moving forward. BRBT-RoMs preserve the asymptotic stability and bounded-realness of the FoM, as well as satisfy an *a priori* error bound on the absolute \mathcal{H}_{∞} error [21].

2.5 The square-root algorithm for BT-MoR

Let $\mathbf{P}_{\mathcal{X}} \in \mathbb{R}^{n \times n}$ and $\mathbf{Q}_{\mathcal{Y}} \in \mathbb{R}^{n \times n}$ denote the "relevant" pair of system Gramians (that is, relevant to the type of balancing being considered). In other words, we treat these matrices as agnostic with respect to any of the balancing-based variants studied in this work. For example, in the Lyapunov setting, we would have $\mathbf{P}_{\mathcal{X}} = \mathbf{P}$ and $\mathbf{Q}_{\mathcal{Y}} = \mathbf{Q}$ that solve (6) and (5). In BST, instead we would have $\mathbf{Q}_{\mathcal{Y}} = \mathbf{Q}_{\mathcal{W}}$, the minimal solution to (7).

In a numerical setting, one never computes the fullbalancing transformation since this transformation is notoriously ill-conditioned, see, e.g., [1, Sec. 7.3]. Indeed, one does not even need $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$, but only their square-root factors $\mathbf{U}_{\mathcal{X}} \in \mathbb{R}^{n \times n}$ and $\mathbf{L}_{\mathcal{Y}} \in \mathbb{R}^{n \times n}$:

$$\mathbf{P}_{\mathcal{X}} = \mathbf{U}_{\mathcal{X}}\mathbf{U}_{\mathcal{X}}^{\mathsf{T}}, \quad \mathbf{Q}_{\mathcal{Y}} = \mathbf{L}_{\mathcal{Y}}\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}.$$
 (15)

The factors $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ can be obtained directly without forming $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$ explicitly; see, e.g., the surveys [7,25]. In a practical setting, balancing and truncation are achieved simultaneously by **ProjMoR**. The left and right projection subspaces are obtained from the singular-value decomposition (SVD) of $\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}}$. This approach is known as the *square-root algorithm* for BT [1, Ch 7.4]; its key details are presented in Algorithm 1. This approach is numerically well-conditioned and lends itself to a low-rank implementation by replacing the $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ with approximate *low-rank* factors $\widetilde{\mathbf{U}}_{\mathcal{X}}$ and $\widetilde{\mathbf{L}}_{\mathcal{Y}}$.

Once the SVD of $\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}}$ is computed as in (16), the model reduction bases \mathbf{W}_r and \mathbf{V}_r are *completely* determined, and constructed according to (17). Finally, a RoM is computed via ProjMoR as in (18). We re-emphasize that the square-root implementation of Algorithm 1 can be applied for *any variant of BT* (i.e., using any pair of Gramians) and in particular those discussed in this work. The key algorithmic difference is the pair of square-root factors $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ (15) derived from the appropriate Gramians $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$. Otherwise, steps (2)-(4) remain exactly the same.

3 A generalized framework for QuadBT

Algorithm 1 is "intrusive" insofar as it demands an explicit internal realization $(\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D})$ of \mathcal{G} in order to compute the BT-RoM. By contrast, the recent work [14] derives a novel "non-intrusive" or *data-driven* reformulation of BT; *quadrature-based balanced truncation* (QuadBT). "Data" for our purposes refers to input-output frequency-response data (e.g., particular transfer function measurements) sampled along $i\mathbb{R}$. As the name suggests, this is accomplished by (implicitly) replacing the exact square-root factors used in Algorithm 1 with approximate *quadrature-based* factors derived from integral representations of \mathbf{P} and \mathbf{Q} .

Algorithm 1 Square-root Balanced Truncation

Input: System matrices $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, $\mathbf{C} \in \mathbb{R}^{p \times n}$, and order $1 \le r < n$ so that $\sigma_r > \sigma_{r+1}$.

Output: BT-RoM given by $\mathbf{A}_r \in \mathbb{R}^{r \times r}$, $\mathbf{B}_r \in \mathbb{R}^{r \times m}$, $\mathbf{C}_r \in \mathbb{R}^{p \times r}$.

- (1) Obtain square-root factors $\mathbf{U}_{\mathcal{X}}, \mathbf{L}_{\mathcal{Y}} \in \mathbb{R}^{n \times n}$ of the relevant system Gramians $\mathbf{P}_{\mathcal{X}}, \mathbf{Q}_{\mathcal{Y}} \in \mathbb{R}^{n \times n}$.
- (2) Compute the SVD of $\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}}$:

$$\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}} = \begin{bmatrix} \mathbf{Z}_1 \ \mathbf{Z}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{\Sigma}_1 \\ \boldsymbol{\Sigma}_2 \end{bmatrix} \begin{bmatrix} \mathbf{Y}_1^{\mathsf{T}} \\ \mathbf{Y}_2^{\mathsf{T}} \end{bmatrix}, \quad (16)$$

where $\Sigma_1 \in \mathbb{R}^{r \times r}$, $\Sigma_2 \in \mathbb{R}^{(n-r) \times (n-r)}$, $\mathbf{Z}_1, \mathbf{Y}_1 \in \mathbb{R}^{n \times r}$ and $\mathbf{Z}_2, \mathbf{Y}_2 \in \mathbb{R}^{n \times (n-r)}$.

(3) Build Petrov-Galerkin model reduction matrices:

$$\mathbf{W}_r = \mathbf{L}_{\mathcal{Y}}^{\mathsf{T}} \mathbf{Z}_1 \boldsymbol{\Sigma}_1^{-1/2}, \ \mathbf{V}_r = \mathbf{U}_{\mathcal{X}} \mathbf{Y}_1 \boldsymbol{\Sigma}_1^{-1/2}, \ (17)$$

where $\mathbf{W}_r^{\mathsf{T}} \mathbf{V}_r = \mathbf{I}_r$ by construction.

(4) Compute the BT-RoM via projection:

$$\mathbf{A}_{r} = \mathbf{W}_{r}^{\top} \mathbf{A} \mathbf{V}_{r} = \boldsymbol{\Sigma}_{1}^{-1/2} \mathbf{Z}_{1}^{\top} \left(\mathbf{L}_{\mathcal{Y}}^{\top} \mathbf{A} \mathbf{U}_{\mathcal{X}} \right) \mathbf{Y}_{1} \boldsymbol{\Sigma}_{1}^{-1/2}, \mathbf{B}_{r} = \mathbf{W}_{r}^{\top} \mathbf{B} = \boldsymbol{\Sigma}_{1}^{-1/2} \mathbf{Z}_{1}^{\top} \left(\mathbf{L}_{\mathcal{Y}}^{\top} \mathbf{B} \right),$$
(18)
$$\mathbf{C}_{r} = \mathbf{C} \mathbf{V}_{r} = (\mathbf{C} \mathbf{U}_{\mathcal{X}}) \mathbf{Y}_{1} \boldsymbol{\Sigma}_{1}^{-1/2}.$$

QuadBT [14] is restricted to the Lyapunov setting. As our first main contribution, we present a generalized framework for quadrature-based balancing that yields non-intrusive implementations of the BT-variants studied here. This generalized presentation contains QuadBT as a special case; see Remark 3.1. The key insight we exploit is that once the square-root factors of the relevant Gramians are specified, any (intrusive) BT-MoR proceeds identically according to Algorithm 1. The same can be said for a non-intrusive implementation; one only needs that the relevant Gramians elicit exploitable integral representations. Akin to Algorithm 1, this paves a way for deriving data-driven implementations of BST, PRBT, and BRBT by replacing $L_{\mathcal{Y}}$ and $U_{\mathcal{X}}$ with appropriately chosen quadrature-based factors.

3.1 Theoretical formulation for Generalized QuadBT

Let $\mathbf{Q}_{\mathcal{Y}} \in \mathbb{R}^{n \times n}$ and $\mathbf{P}_{\mathcal{X}} \in \mathbb{R}^{n \times n}$ denote an arbitrary pair of Gramians that are agnostic to any particular type of balancing. The only key assumption that we make is that the matrices $\mathbf{Q}_{\mathcal{Y}}$ and $\mathbf{P}_{\mathcal{X}}$ are the SPD solutions to a pair of Lyapunov equations:

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{Y}} + \mathbf{Q}_{\mathcal{Y}}\mathbf{A} + \mathbf{C}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{C}_{\mathcal{Y}} = \mathbf{0}, \qquad (19)$$

and
$$\mathbf{AP}_{\mathcal{X}} + \mathbf{P}_{\mathcal{X}}\mathbf{A}^{\mathsf{T}} + \mathbf{B}_{\mathcal{X}}\mathbf{B}_{\mathcal{X}}^{\mathsf{T}} = \mathbf{0}.$$
 (20)

Equations (19) and (20) yield an alternative perspective on the agnostic Gramians. We view $\mathbf{Q}_{\mathcal{Y}}$ as the observability Gramian of linear system \mathcal{Y} of the form (1) determined by the quadruple $(\mathbf{A}, \mathbf{B}_{\mathcal{Y}}, \mathbf{C}_{\mathcal{Y}}, \mathbf{D}_{\mathcal{Y}})$. Likewise, we view $\mathbf{P}_{\mathcal{X}}$ as the reachability Gramian of a linear system \mathcal{X} determined by the quadruple $(\mathbf{A}, \mathbf{B}_{\mathcal{X}}, \mathbf{C}_{\mathcal{X}}, \mathbf{D}_{\mathcal{X}})$. We let m_y, p_y , and m_x, p_x denote the input, output dimensions of \mathcal{Y} and \mathcal{X} , respectively. We allow for the system matrices, e.g., $\mathbf{C}_{\mathcal{Y}}$ and $\mathbf{B}_{\mathcal{X}}$, to possibly depend upon $\mathbf{Q}_{\mathcal{Y}}, \mathbf{P}_{\mathcal{X}}$ so that the AREs studied in this work can be re-written in the form of (19) and (20). Exact formulations of these systems (and the corresponding statespace quadruples) will be revealed in Section 4 for the different variants of BT studied here.

Consider the square-root factors $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ of $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$. Recall from (17) in Algorithm 1 that the BT-ProjMoR bases are defined as

$$\mathbf{W}_r = \mathbf{L}_{\mathcal{Y}} \mathbf{Z}_1 \boldsymbol{\Sigma}_1^{-1/2}$$
 and $BV_r = \mathbf{U}_{\mathcal{X}} \mathbf{Y}_1 \boldsymbol{\Sigma}_1^{-1/2}$

Since \mathbf{Z}_1 , \mathbf{Y}_1 , and $\mathbf{\Sigma}_1$ are extracted from the SVD of $\mathbf{L}_{\mathcal{Y}}^{\top}\mathbf{U}_{\mathcal{X}}$, the BT-RoM (18) is in essence entirely determined by the following key quantities:

$$\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}}, \quad \mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{A}\mathbf{U}_{\mathcal{X}}, \quad \mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{B}, \text{ and } \mathbf{C}\mathbf{U}_{\mathcal{X}}.$$
 (21)

We derive approximations to the matrices in (21) that are constructed entirely from different state-invariant input-output data. This will be accomplished by replacing $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ with certain quadrature-based squareroot factors derived from (implicit) numerical quadrature rules used to approximate $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$. These numerical quadratures are indeed *never constructed* but form the basis of the analysis. First, we introduce two definitions to aid our exposition.

Definition 3.1 Let $\mathbf{M} \in \mathbb{C}^{(pK) \times (mJ)}$. Then for $1 \leq j \leq J$ and $1 \leq k \leq K$, the matrix $\mathbf{M}_{k,j} \in \mathbb{C}^{p \times m}$ denotes the (k, j)th block of \mathbf{M} . When J = 1 or K = 1, we use \mathbf{M}_i to denote the *i*th $p \times m$ -sized row or column block of \mathbf{M} , respectively. In the SISO case of m = p = 1, $\mathbf{M}_{k,j} = \mathbf{M}(k, j)$ is a scalar quantity.

Definition 3.2 For a proper rational function

$$\mathbf{G}(s) = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D} \in \mathbb{C}^{p \times m}$$

as in (2), we denote the strictly proper part of $\mathbf{G}(s)$ by $\mathbf{G}_{\infty}(s)$, defined as

$$\mathbf{G}_{\infty}(s) = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} = \mathbf{G}(s) - \lim_{s \to \infty} \mathbf{G}(s). \quad (22)$$

The linear systems \mathcal{X} and \mathcal{Y} are asymptotically stable because they share the same **A** matrix as the underlying model \mathcal{G} . Consequently, the solutions to (20) and (19) are unique [1, Prop. 6.2] and admit the integral formulae

$$\mathbf{P}_{\mathcal{X}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} (i\zeta \mathbf{I}_n - \mathbf{A})^{-1} \mathbf{B}_{\mathcal{X}} \times$$
(23)
$$\mathbf{B}_{\mathcal{X}}^{\mathsf{T}} (-i\zeta \mathbf{I}_n - \mathbf{A}^{\mathsf{T}})^{-1} d\zeta,$$

and
$$\mathbf{Q}_{\mathcal{Y}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} (-i\omega \mathbf{I}_n - \mathbf{A}^{\mathsf{T}})^{-1} \mathbf{C}_{\mathcal{Y}}^{\mathsf{T}} \times (24)$$

 $\mathbf{C}_{\mathcal{Y}} (i\omega \mathbf{I}_n - \mathbf{A})^{-1} d\omega.$

Consider a numerical quadrature rule determined by the weights ρ_j and nodes ζ_j for $j = 1, 2, \ldots, J$. By applying this rule to the integral form of $\mathbf{P}_{\mathcal{X}}$ in (23), i.e.

$$\mathbf{P}_{\mathcal{X}} pprox \sum_{j=1}^{J} \rho_{j}^{2} (i \zeta_{j} \mathbf{I}_{n} - \mathbf{A}) \mathbf{B}_{\mathcal{X}} \mathbf{B}_{\mathcal{X}}^{\mathsf{T}} (-i \zeta_{j} \mathbf{I}_{n} - \mathbf{A}^{\mathsf{T}})^{-1},$$

one obtains the approximate quadrature-based squareroot factorization $\mathbf{P}_{\mathcal{X}} \approx \widetilde{\mathbf{U}}_{\mathcal{X}} \widetilde{\mathbf{U}}_{\mathcal{X}}^*$ of $\mathbf{P}_{\mathcal{X}}$. The quadraturebased factor $\widetilde{\mathbf{U}}_{\mathcal{X}} \in \mathbb{C}^{n \times (m_x J)}$ is defined (according to Definition 3.1) by

$$(\widetilde{\mathbf{U}}_{\mathcal{X}})_j = \rho_j \left(i \zeta_j \mathbf{I}_n - \mathbf{A} \right)^{-1} \mathbf{B}_{\mathcal{X}} \in \mathbb{C}^{n \times m_x},$$
 (25)

for all $j = 1, \ldots, J$. A similar quadrature-based factorization can be obtained for $\mathbf{Q}_{\mathcal{Y}}$ in (24). Consider weights ϕ_k and nodes ω_k for all $k = 1, 2, \ldots, K$. Then, $\mathbf{Q}_{\mathcal{Y}} \approx \widetilde{\mathbf{L}}_{\mathcal{Y}} \widetilde{\mathbf{L}}_{\mathcal{Y}}^*$ where $\widetilde{\mathbf{L}}_{\mathcal{Y}}^* \in \mathbb{C}^{(p_y K) \times n}$ is defined by

$$(\widetilde{\mathbf{L}}_{\mathcal{Y}}^*)_k = \phi_k \mathbf{C}_{\mathcal{Y}} (i\omega_k \mathbf{I}_n - \mathbf{A})^{-1} \in \mathbb{C}^{p_y \times n},$$
 (26)

for all k = 1, ..., K, respectively. These factors can be used in lieu of of $\mathbf{U}_{\mathcal{X}}$ and $\mathbf{L}_{\mathcal{Y}}$ in Algorithm 1. Then, the quadrature-based quantities

$$\widetilde{\mathbf{L}}_{\mathcal{Y}}^* \widetilde{\mathbf{U}}_{\mathcal{X}}, \quad \widetilde{\mathbf{L}}_{\mathcal{Y}}^* \mathbf{A} \widetilde{\mathbf{U}}_{\mathcal{X}}, \quad \widetilde{\mathbf{L}}_{\mathcal{Y}}^* \mathbf{B}, \text{ and } \mathbf{C} \widetilde{\mathbf{U}}_{\mathcal{X}},$$
 (27)

replace those in (21) and completely specify the approximate BT-RoM. We refer to this framework as *generalized quadrature-based balanced truncation* (GenQuadBT). However, there are two major questions left to make GenQuadBT a fully data-driven approach:

- Q1. Can the modified/generalized quantities be computed non-intrusively using transfer function data?
- Q2. If so, what do you need to sample for different *data-driven* balancing-based reduced models?

Our first main result answers Q1.

Theorem 3.1 Define the transfer functions:

$$\mathbf{G}_{\sigma,\mathbf{A}}(s) = \mathbf{C}_{\mathcal{Y}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{X}} \in \mathbb{C}^{p_y \times m_x}, \qquad (28)$$

$$\mathbf{G}_{\mathbf{B}}(s) = \mathbf{C}_{\mathcal{Y}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} \in \mathbb{C}^{p_y \times m}, \qquad (29)$$

$$\mathbf{G}_{\mathbf{C}}(s) = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{X}} \in \mathbb{C}^{p \times m_x}.$$
 (30)

Let $\widetilde{\mathbf{U}}_{\mathcal{X}}$ and $\widetilde{\mathbf{L}}_{\mathcal{Y}}$ be defined as in (25) and (26) respectively. Define the matrices

$$\widetilde{\mathbb{L}} := \widetilde{\mathbf{L}}_{\mathcal{Y}}^{*} \widetilde{\mathbf{U}}_{\mathcal{X}} \in \mathbb{C}^{(p_{y}K) \times (m_{x}J)},
\widetilde{\mathbb{M}} := \widetilde{\mathbf{L}}_{\mathcal{Y}}^{*} \mathbf{A} \widetilde{\mathbf{U}}_{\mathcal{X}} \in \mathbb{C}^{(p_{y}K) \times (m_{x}J)},
\widetilde{\mathbb{H}} := \widetilde{\mathbf{L}}_{\mathcal{Y}}^{*} \mathbf{B} \in \mathbb{C}^{(p_{y}K) \times m},
\widetilde{\mathbb{G}} := \mathbf{C} \widetilde{\mathbf{U}}_{\mathcal{X}} \in \mathbb{C}^{p \times (m_{x}J)}.$$
(31)

Then, the (k, j)th blocks of $\widetilde{\mathbb{L}}$ and $\widetilde{\mathbb{M}}$ are given by

$$\widetilde{\mathbb{L}}_{k,j} = -\phi_k \rho_j \frac{\mathbf{G}_{\sigma,\mathbf{A}}(i\omega_k) - \mathbf{G}_{\sigma,\mathbf{A}}(i\zeta_j)}{i\omega_k - i\zeta_j}, \qquad (32)$$

$$\widetilde{\mathbb{M}}_{k,j} = -\phi_k \rho_j \frac{i\omega_k \mathbf{G}_{\sigma,\mathbf{A}}(i\omega_k) - i\zeta_j \mathbf{G}_{\sigma,\mathbf{A}}(i\zeta_j)}{i\omega_k - i\zeta_j}, \quad (33)$$

and the kth and jth blocks of $\widetilde{\mathbb{H}}$ and $\widetilde{\mathbb{G}}$ are given by

$$\widetilde{\mathbb{H}}_{k} = \rho_{k} \mathbf{G}_{\mathbf{B}}(\boldsymbol{i}\omega_{k}) \quad and \quad \widetilde{\mathbb{G}}_{j} = \phi_{j} \mathbf{G}_{\mathbf{C}}(\boldsymbol{i}\zeta_{j}), \qquad (34)$$

for each $1 \leq k \leq K$ and $1 \leq j \leq J$.

Proof 3.1 Let \mathbf{e}_i be the *i*th canonical unit vector, *i.e.*, its *i*th entry is 1, and all other entries are 0. Additionally, for any positive integers i and ℓ define the matrix:

$$\mathbf{E}_{i,\ell} = \begin{bmatrix} \mathbf{e}_{(i-1)\ell+1} \ \mathbf{e}_{(i-1)\ell+2} \ \cdots \ \mathbf{e}_{i\ell} \end{bmatrix} \in \mathbb{R}^{n \times \ell}.$$

The result exploits two resolvent identities. For $s, z \in \mathbb{C}$ that are not in the spectrum of \mathbf{A} , we have

$$(s\mathbf{I}_n - \mathbf{A})^{-1}(z\mathbf{I}_n - \mathbf{A})^{-1} = \frac{(z\mathbf{I}_n - \mathbf{A})^{-1} - (s\mathbf{I}_n - \mathbf{A})^{-1}}{s - z}.$$
(35)

Using the definitions of $\widetilde{\mathbb{L}}$ in (31), $\widetilde{\mathbf{L}}_{\mathcal{Y}}$ in (26), $\widetilde{\mathbf{U}}_{\mathcal{X}}$ in (25) and the resolvent identity (35), it follows that

$$\begin{split} \widetilde{\mathbf{L}}_{k,j} &= \mathbf{E}_{k,py}^{\top} \widetilde{\mathbf{L}} \mathbf{E}_{j,m_{x}} = \left(\mathbf{E}_{k,p_{y}}^{\top} \widetilde{\mathbf{L}}_{\mathcal{Y}}^{*} \right) \left(\widetilde{\mathbf{U}}_{\mathcal{X}} \mathbf{E}_{j,m_{x}} \right) \\ &= \phi_{k} \rho_{j} \mathbf{C}_{\mathcal{Y}} (i \omega_{k} \mathbf{I}_{n} - \mathbf{A})^{-1} (i \zeta_{j} \mathbf{I}_{n} - \mathbf{A})^{-1} \mathbf{B}_{\mathcal{X}} \\ &= \phi_{k} \rho_{j} \mathbf{C}_{\mathcal{Y}} \left(\frac{(i \zeta_{j} \mathbf{I}_{n} - \mathbf{A})^{-1} - (i \omega_{k} \mathbf{I}_{n} - \mathbf{A})^{-1}}{i \omega_{k} - i \zeta_{j}} \right) \mathbf{B}_{\mathcal{X}} \\ &= -\phi_{k} \rho_{j} \frac{\mathbf{G}_{\sigma, \mathbf{A}} (i \omega_{k}) - \mathbf{G}_{\sigma, \mathbf{A}} (i \zeta_{j})}{i \omega_{k} - i \zeta_{j}}, \end{split}$$

where the last line follows from the definition of $\mathbf{G}_{\sigma,\mathbf{A}}(s)$.

This proves (32). For arbitrary $s, z \in \mathbb{C}$ that are not in the spectrum of \mathbf{A} , the second resolvent identity states

$$z (z \mathbf{I}_{n} - \mathbf{A})^{-1} - s (s\mathbf{I}_{n} - \mathbf{A})^{-1}$$

= $-(z - s) (z\mathbf{I}_{n} - \mathbf{A})^{-1} \mathbf{A} (s\mathbf{I}_{n} - \mathbf{A})^{-1}.$ (36)

To prove (33), we use (36) and the definitions of $\widetilde{\mathbb{M}}$ in (31), $\widetilde{\mathbb{U}}_{\mathcal{X}}$ in (25), and $\widetilde{\mathbb{L}}_{\mathcal{Y}}$ in (26) to obtain

$$\begin{split} \widetilde{\mathbb{M}}_{k,j} &= \mathbf{E}_{k,p_y}^{\top} \widetilde{\mathbb{M}} \mathbf{E}_{j,m_x} = \left(\mathbf{E}_{k,p_y}^{\top} \widetilde{\mathbf{L}}_{\mathcal{Y}}^{*} \right) \mathbf{A} \left(\widetilde{\mathbf{U}}_{\mathcal{X}} \mathbf{E}_{j,m_x} \right) \\ &= \phi_k \rho_j \mathbf{C}_{\mathcal{Y}} \left(i \omega_k \mathbf{I}_n - \mathbf{A} \right)^{-1} \mathbf{A} (i i \zeta_j \mathbf{I}_n - \mathbf{A})^{-1} \mathbf{B}_{\mathcal{X}} \\ &= \phi_k \rho_j \mathbf{C}_{\mathcal{Y}} \left(\frac{i \zeta_j (i \zeta_j (\mathbf{I}_n - \mathbf{A})^{-1} - i \omega_k (i \omega_k \mathbf{I}_n - \mathbf{A})^{-1}}{i \omega_k - i \zeta_j} \right) \mathbf{B}_{\mathcal{X}} \\ &= -\phi_k \rho_j \frac{i \omega_k \mathbf{G}_{\sigma, \mathbf{A}} (i \omega_k) - i \zeta_j \mathbf{G}_{\sigma, \mathbf{A}} (i \zeta_j)}{i \omega_k - i \zeta_j}. \end{split}$$

The final claims (34) for $\widetilde{\mathbb{H}}$ and $\widetilde{\mathbb{G}}$ follow directly from the definitions of $\widetilde{\mathbb{H}}$, $\widetilde{\mathbf{L}}_{\mathcal{Y}}$, and $\widetilde{\mathbb{G}}$, $\widetilde{\mathbf{U}}_{\mathcal{X}}$. Observe that:

$$\widetilde{\mathbb{H}}_{k} = \mathbf{E}_{k,p_{y}}^{\top} \widetilde{\mathbb{H}} = \phi_{k} \mathbf{C}_{\mathcal{Y}} \left(i \omega_{k} \mathbf{I}_{n} - \mathbf{A} \right)^{-1} \mathbf{B} = \phi_{k} \mathbf{G}_{\mathbf{B}} (i \omega_{k}),$$

and for $\widetilde{\mathbb{G}}$:

$$\widetilde{\mathbb{G}}_{j} = \widetilde{\mathbb{G}} \mathbf{E}_{j,m_{x}} = \rho_{j} \mathbf{C} \left(i \zeta_{j} \mathbf{I}_{n} - \mathbf{A} \right)^{-1} \mathbf{B}_{\mathcal{X}} = \rho_{j} \mathbf{G}_{\mathbf{C}} (i \zeta_{j}),$$

thus completing the proof.

This result provides the key ingredients for GenQuadBT that we present in Algorithm 2. The choice of notation $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ for the transfer functions in (28)-(30) is intentional; the underscored quantities in each transfer function correspond to the quantities in the data-driven RoM that require samples of that transfer function. Put differently, Theorem 3.1 (and the associated notation) can be interpreted as follows: (i) The construction of $\widetilde{\mathbb{L}}$ (and hence its SVD) and the reducedorder $\widetilde{\mathbf{A}}_r$ in steps (2) and (3) of Algorithm 2 require samples of $\mathbf{G}_{\sigma,\mathbf{A}}(s)$; (ii) Construction of the reduced-order $\widetilde{\mathbf{B}}_r$ in step (3) of Algorithm 2 requires samples of $\mathbf{G}_{\mathbf{B}}(s)$; (iii) Construction of the reduced-order $\widetilde{\mathbf{C}}_r$ in step (3) of Algorithm 2 requires samples of $\mathbf{G}_{\mathbf{C}}(s)$.

3.2 Algorithmic formulation for Generalized QuadBT

Having established its theoretical formulation, an algorithmic formulation for GenQuadBT is presented in Algorithm 2 next. In principle, it only requires the left and right quadrature weights/nodes used implicitly in approximating $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$, and samples of the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$ and $\mathbf{G}_{\mathbf{C}}(s)$ given in (28)–(30) (or at least, the ability to evaluate them).

Some remarks are in order. We emphasize that at no

Algorithm 2 Generalized-QuadBT (GenQuadBT)

Input: Mappings $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, $\mathbf{G}_{\mathbf{C}}(s)$, and:

- "Left" weights/nodes $\{\rho_j, \zeta_j\}_{j=1}^J$,
- "Right" weights/nodes $\{\phi_k, \omega_k\}_{k=1}^K$,

and reduction order $1 \le r \le n$.

Output: GenQuadBT-RoM determined by the statespace matrices $\widetilde{\mathbf{A}}_r \in \mathbb{R}^{r \times r}$, $\widetilde{\mathbf{B}}_r \in \mathbb{R}^{r \times m}$, $\widetilde{\mathbf{C}}_r \in \mathbb{R}^{p \times r}$. (1) Obtain samples $\{\mathbf{G}_{\sigma,\mathbf{A}}(i\zeta_j)\}_{j=1}^J, \{\mathbf{G}_{\mathbf{C}}(i\zeta_j)\}_{j=1}^J, \{\mathbf{G}_{\mathbf{C}}(i\zeta_j)\}$

- (1) Obtain samples $\{\mathbf{G}_{\sigma,\mathbf{A}}(i\zeta_j)\}_{j=1}^{J}, \{\mathbf{G}_{\mathbf{C}}(i\zeta_j)\}_{j=1}^{J}, \{\mathbf{G}_{\sigma,\mathbf{A}}(i\omega_k)\}_{k=1}^{K}, \text{ and } \{\mathbf{G}_{\mathbf{B}}(i\omega_k)\}_{k=1}^{K}.$ Construct matrices $(\widetilde{\mathbb{L}}, \widetilde{\mathbb{M}}, \widetilde{\mathbb{H}}, \widetilde{\mathbb{G}})$ according to Theorem 3.1.
- (2) Compute the SVD of \mathbb{L} :

$$\widetilde{\mathbb{L}} = \begin{bmatrix} \widetilde{\mathbf{Z}}_1 \ \widetilde{\mathbf{Z}}_2 \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{\Sigma}}_1 \\ & \widetilde{\mathbf{\Sigma}}_2 \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{Y}}_1^* \\ & \widetilde{\mathbf{Y}}_2^* \end{bmatrix} \in \mathbb{C}^{(p_y K) \times (m_x J)},$$

where $\widetilde{\Sigma}_1 \in \mathbb{R}^{r \times r}$, $\widetilde{\Sigma}_2 \in \mathbb{R}^{(p_y K - r) \times (m_x J - r)}$, $\widetilde{\mathbf{Z}}_1, \widetilde{\mathbf{Y}}_1$ and $\widetilde{\mathbf{Z}}_2, \widetilde{\mathbf{Y}}_2$ are partitioned conformally. (3) Compute the GenQuadBT-RoM:

$$\begin{split} \widetilde{\mathbf{A}}_{r} &= \widetilde{\boldsymbol{\Sigma}}_{1}^{-1/2} \widetilde{\mathbf{Z}}_{1}^{*} \left(\widetilde{\mathbb{M}} \right) \widetilde{\mathbf{Y}}_{1} \widetilde{\boldsymbol{\Sigma}}_{1}^{-1/2} \\ \widetilde{\mathbf{B}}_{r} &= \widetilde{\boldsymbol{\Sigma}}_{1}^{-1/2} \widetilde{\mathbf{Z}}_{1}^{*} \left(\widetilde{\mathbb{H}} \right), \\ \widetilde{\mathbf{C}}_{r} &= \left(\widetilde{\mathbb{G}} \right) \widetilde{\mathbf{Y}}_{1} \widetilde{\boldsymbol{\Sigma}}_{1}^{-1/2}. \end{split}$$

point do we explicitly compute the quadrature-based approximations of the Gramians $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$. These are leveraged *implicitly* to derive the quadrature-base square-root factors in (25) and (26) and realize the approximate **BT-RoM** solely from input-output data. The key deviation from the work of [14] is that the transfer function evaluations required in this generalized setting are not necessarily those of $\mathbf{G}(s)$ (the transfer function of the linear model being approximated). Rather, Algorithm 2 requires samples of $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ as in (28)-(30) Nonetheless, Algorithm 2 avoids any explicit reference to "internal" quantities (e.g., a statespace realization of \mathcal{G} , or any other linear model).

Remark 3.1 Theorem 3.1 and Algorithm 2 contain QuadBT of [14] as a special case. Indeed, the proof uses similar tools as in [14]. In the Lyapunov setting, we simply have that $\mathbf{Q}_{\mathcal{Y}} = \mathbf{Q}$ and $\mathbf{P}_{\mathcal{X}} = \mathbf{P}$, and so the generalized equations (19) and (20) are the dual ALEs (5) and (6) corresponding to \mathcal{G} . Then, $\mathbf{B}_{\mathcal{X}} = \mathbf{B}$, $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}$, and the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ all equal $\mathbf{G}_{\infty}(s)$; this is precisely the aggregate result of [14, Prop. 3.1, Prop. 3.3].

What remains to be seen is what the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ correspond to for different variants of BT. We investigate exactly this question next

for the case of BST, PRBT, and BRBT. Using this generalized framework, we answer Q2: what does one need to sample for different *data-driven* balancing-based reduced models? Unlike in the Lyapunov setting, the tobe-sampled "data" will not necessarily be the measurements of $\mathbf{G}(s)$, the transfer function of the FoM \mathcal{G} . We ultimately show that in the aforementioned contexts, the general quantities in (28)-(30) can be interpreted in terms of certain *spectral factorizations* associated with the AREs that the relevant Gramians are solutions to.

4 What to sample for **BT**-variants

In this section, we derive data-driven implementations of BST, PRBT, and BRBT. This is accomplished by applying the generalized framework of Section 3 to the aforementioned variants. *Spectral factorizations* will provide the main tool for interpreting Theorem 3.1 as it applies to the data-driven extensions of BST, PRBT, and BRBT (and in particular, determining what the transfer functions in equations (28)-(30) correspond to). Indeed, the Gramians relevant to each variant will be interpreted as either the observability or reachability Gramian of some spectral factor. Our treatise of spectral factorizations follows [28, Chapter 13.4]; we refer the reader here for a more detailed study.

We sequentially present the data-driven derivations of BST, PRBT, and BRBT. The particular organizational structure of this section is as follows: (i) For each variant, we introduce the relevant spectral factorizations associated with the appropriate AREs. (ii) We interpret the result of Theorem 3.1 in the context of each variant and show that the transfer functions (28)-(30) can be written in terms of the aforementioned spectral factors.

4.1 BST from data: QuadBST

Recall the assumptions of Subsection 2.2; namely that \mathcal{G} is square (m = p) and \mathbf{D} is nonsingular. Again let $\mathbf{Q}_{\mathcal{W}} \in \mathbb{R}^{n \times n}$ denote the minimal stabilizing solution to the BST-ARE (7). By [28, Corollary 13.28], there exists $\mathbf{W}(s) \in \mathbb{C}^{m \times m}$ such that $\mathbf{W}(s)$ is a left spectral factor of $\mathbf{G}(s)\mathbf{G}(-s)^{\mathsf{T}}$, meaning $\mathbf{G}(s)\mathbf{G}(-s)^{\mathsf{T}} = \mathbf{W}(-s)^{\mathsf{T}}\mathbf{W}(s)$. Further, define

$$\mathbf{B}_{\mathcal{W}} := \mathbf{P}\mathbf{C}^{\mathsf{T}} + \mathbf{B}\mathbf{D}^{\mathsf{T}} \in \mathbb{R}^{n \times m},$$

and
$$\mathbf{C}_{\mathcal{W}} := \mathbf{D}^{-1} \left(\mathbf{C} - \mathbf{B}_{\mathcal{W}}\mathbf{Q}_{\mathcal{W}}\right) \in \mathbb{R}^{m \times n},$$
 (37)

where **P** is the reachability Gramian of \mathcal{G} . Then **W**(*s*) is the rational transfer function of an asymptotically stable and minimal linear system \mathcal{W} defined by the state-space quadruple (**A**, **B**_{\mathcal{W}}, **C**_{\mathcal{W}}, **D**^{\top}), i.e.

$$\mathbf{W}(s) = \mathbf{C}_{\mathcal{W}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{W}} + \mathbf{D}^{\mathsf{T}}.$$
 (38)

Such a spectral factor is said to be *minimal phase*, as the matrix $\mathbf{Q}_{\mathcal{W}}$ used in its construction is the minimal stabilizing solution to the corresponding ARE (7). (Although in general, we note that the solution (7) need not be extremal for the construction of \mathcal{W} .) Note that any given realization of \mathcal{W} can be computed from a state-space realization of \mathcal{G} and the corresponding Gramian $\mathbf{Q}_{\mathcal{W}}$.

With this, we now describe explicitly how the generalized framework of Section 3 can be applied in this instance. Recall that we require the relevant Gramians $\mathbf{Q}_{\mathcal{Y}}$ and $\mathbf{P}_{\mathcal{X}}$ be given as solutions to the observability and reachability Lyapunov equations (19) and (20) of some linear systems \mathcal{Y} and \mathcal{X} (so that, in turn, they elicit exploitable integral representations (24) and (23)). By definition of $\mathbf{C}_{\mathcal{W}}$ in (37), the ARE (7) can be re-written in the generalized form of (19):

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{W}} + \mathbf{Q}_{\mathcal{W}}\mathbf{A} + \mathbf{C}_{\mathcal{W}}^{\mathsf{T}}\mathbf{C}_{\mathcal{W}} = \mathbf{0}, \qquad (39)$$

which is the observability Lyapunov equation of \mathcal{W} , the system associated with the minimal phase factor $\mathbf{W}(s)$. Thus for BST, the relevant observability Gramian $\mathbf{Q}_{\mathcal{Y}} =$ $\mathbf{Q}_{\mathcal{W}}$ is the observability Gramian of $\mathcal{Y} = \mathcal{W}$ determined by $(\mathbf{A}, \mathbf{B}_{\mathcal{Y}}, \mathbf{C}_{\mathcal{Y}}, \mathbf{D}_{\mathcal{Y}}) = (\mathbf{A}, \mathbf{B}_{\mathcal{W}}, \mathbf{C}_{\mathcal{W}}, \mathbf{D}^{-1})$. By the asymptotic stability of \mathcal{W} , the solution to (39) is unique, and so $\mathbf{Q}_{\mathcal{W}}$ has the integral representation

$$\mathbf{Q}_{\mathcal{W}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} (-i\omega \mathbf{I}_n - \mathbf{A}^{\mathsf{T}})^{-1} (\mathbf{C} - \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} \mathbf{Q}_{\mathcal{W}})^{\mathsf{T}} \mathbf{D}^{-\mathsf{T}} \times \mathbf{D}^{-1} (\mathbf{C} - \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} \mathbf{Q}_{\mathcal{W}}) (i\omega \mathbf{I}_n - \mathbf{A})^{-1} d\omega.$$

(Note that this agrees with (24) for $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}_{\mathcal{W}}$.) The relevant reachability Gramian in BST is $\mathbf{P}_{\mathcal{X}} = \mathbf{P}$, that of the linear system $\mathcal{X} = \mathcal{G}$ with $(\mathbf{A}, \mathbf{B}_{\mathcal{X}}, \mathbf{C}_{\mathcal{X}}, \mathbf{D}_{\mathcal{X}}) = (\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D})$. Thus \mathbf{P} and $\mathbf{Q}_{\mathcal{W}}$ can be decomposed into quadrature-based square-root factors (25) and (26) with $\mathbf{B}_{\mathcal{X}} = \mathbf{B}$ and $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}_{\mathcal{W}}$. Particularly, (26) becomes

$$(\widetilde{\mathbf{L}}_{\mathcal{W}}^*)_k = \phi_k \mathbf{D}^{-1} (\mathbf{C} - \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} \mathbf{Q}_{\mathcal{W}}) (i \omega_k \mathbf{I}_n - \mathbf{A})^{-1},$$

for k = 1, ..., K. Theorem 3.1 (and Algorithm 2) can then be applied to realize a *data-driven* implementation of BST, that we call *Quadrature-based BST* (QuadBST). The question remains: what do the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s), \mathbf{G}_{\mathbf{B}}(s), \text{ and } \mathbf{G}_{\mathbf{C}}(s) \text{ in } (28)-(30)$ correspond to in the context of QuadBST? We answer this with Theorem 4.1, that shows how to interpret these transfer functions in terms of $\mathbf{G}(s)$ and the spectral factor $\mathbf{W}(s)$.

In the following we use $[\cdot]_+$ to denote the *purely stable* part of a rational transfer function. Additionally, when the notation (**A**, **B**, **C**, **D**) does not fit in a single line (as in (42)), we represent the corresponding system by

$$\left(\begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{C} & \mathbf{D} \end{array}\right).$$

Theorem 4.1 Let $\mathbf{Q}_{\mathcal{W}} \in \mathbb{R}^{n \times n}$ be the observability Gramian of the system \mathcal{W} corresponding to the minimal phase spectral factor as in (38) and $\mathbf{P} \in \mathbb{R}^{n \times n}$ be the reachability Gramian of \mathcal{G} as in (1). Then, in the setting of BST, the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ defined as in (28)-(30) of Theorem 3.1 (and Algorithm 2) are

$$\mathbf{G}_{\mathbf{C}}(s) = \mathbf{G}_{\infty}(s), and \tag{40}$$

$$\mathbf{G}_{\sigma,\mathbf{A}}(s) = \mathbf{G}_{\mathbf{B}}(s) = \left[\left(\mathbf{W}(-s)^{\mathsf{T}} \right)^{-1} \mathbf{G}_{\infty}(s) \right]_{+}.$$
 (41)

Proof 4.1 Here, $\mathbf{B}_{\mathcal{X}} = \mathbf{B}$, and $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}_{\mathcal{W}}$ in (37). So by definition of $\mathbf{G}_{\mathbf{C}}(s)$ in (30)

$$\mathbf{G}_{\mathbf{C}}(s) = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{X}} = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} = \mathbf{G}_{\infty}(s),$$

proving (40). To prove (41), first note that

$$\mathbf{G}_{\sigma,\mathbf{A}}(s) = \mathbf{G}_{\mathbf{B}}(s) = \mathbf{C}_{\mathcal{W}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B},$$

by (28), (29). Thus, (41) amounts to proving

$$\mathbf{C}_{\mathcal{W}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} = \left[\left(\mathbf{W}(-s)^{\mathsf{T}}\right)^{-1}\mathbf{G}_{\infty}(s) \right]_{+}.$$

Using the state-space of \mathcal{W} in (38) and of \mathcal{G} in (1), the state-space of the cascaded system with transfer function $(\mathbf{W}(-s)^{\mathsf{T}})^{-1} \mathbf{G}_{\infty}(s)$ can be realized by

$$\begin{pmatrix} -\mathbf{A}^{\mathsf{T}} + \mathbf{C}_{\mathcal{W}}^{\mathsf{T}} \mathbf{D}^{-1} \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} & \mathbf{C}_{\mathcal{W}}^{\mathsf{T}} \mathbf{D}^{-1} \mathbf{C} & \mathbf{0}_{n \times m} \\ \mathbf{0}_{n} & \mathbf{A} & \mathbf{B} \\ \hline \mathbf{D}^{-1} \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} & \mathbf{D}^{-1} \mathbf{C} & \mathbf{0}_{m} \end{pmatrix}, \quad (42)$$

where $\mathbf{0}_n \in \mathbb{R}^{n \times n}$ and $\mathbf{0}_{n \times m} \in \mathbb{R}^{n \times m}$ denote the matrices with all zero entries. The ARE (7) can be rearranged to be written as

$$(-\mathbf{A}^{\scriptscriptstyle \top} + \mathbf{C}_{\mathcal{W}}^{\scriptscriptstyle \top} \mathbf{D}^{-1} \mathbf{B}_{\mathcal{W}}^{\scriptscriptstyle \top})(-\mathbf{Q}_{\mathcal{W}}) + \mathbf{A} \mathbf{Q}_{\mathcal{W}} + \mathbf{C}_{\mathcal{W}}^{\scriptscriptstyle \top} \mathbf{D}^{-1} \mathbf{C} = \mathbf{0}.$$

 $Using \ this \ reformulation, \ the \ state-space \ transformation$

$$\mathbf{T} = \begin{vmatrix} \mathbf{I}_n & -\mathbf{Q}_{\mathcal{W}} \\ \mathbf{0}_n & \mathbf{I}_n \end{vmatrix} \in \mathbb{R}^{2n \times 2n} \text{ decouples the cascaded}$$

system realization (42). In other words, the transformed state-space is given by

$$\begin{pmatrix} -\mathbf{A}^{\mathsf{T}} + \mathbf{C}_{\mathcal{W}}^{\mathsf{T}} \mathbf{D}^{-1} \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} & \mathbf{0}_{n} & \mathbf{Q}_{\mathcal{W}} \mathbf{B} \\ \hline \mathbf{0}_{n} & \mathbf{A} & \mathbf{B} \\ \hline \mathbf{D}^{-1} \mathbf{B}_{\mathcal{W}}^{\mathsf{T}} & \mathbf{C}_{\mathcal{W}} & \mathbf{0}_{m} \end{pmatrix}.$$
(43)

Note that the (1,1) block of the cascaded system is purely antistable (e.g., the poles lie in the open right half-plane) and the (2,2) block is purely stable. Since $(\mathbf{W}(-s)^{\mathsf{T}})^{-1} \mathbf{G}_{\infty}(s)$ is the transfer function of (43), it can be written as

$$\left(\mathbf{W}(-s)^{\mathsf{T}}\right)^{-1}\mathbf{G}_{\infty}(s) = \star + \underbrace{\mathbf{C}_{\mathcal{W}}(s\mathbf{I}_{n}-\mathbf{A})^{-1}\mathbf{B}}_{=\mathbf{G}_{\sigma,\mathbf{A}}(s)=\mathbf{G}_{\mathbf{B}}(s)},$$

where the unspecified \star corresponds to the anti-stable part of $(\mathbf{W}(-s)^{\top})^{-1} \mathbf{G}(s)$. Thus, both $\mathbf{G}_{\sigma,\mathbf{A}}(s)$ and $\mathbf{G}_{\mathbf{B}}(s)$ are equivalent to $\left[(\mathbf{W}(-s)^{\top})^{-1} \mathbf{G}_{\infty}(s) \right]_{+}$, as claimed in (41).

In conjunction, Theorems 3.1 and 4.1 realize QuadBST as a fully-fledged data-driven and non-intrusive implementation of BST. Algorithm 2 yields QuadBST when the transfer functions $\mathbf{G}_{\mathbf{C}}(s)$ and $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$ to be sampled are chosen as in (40) and (41), respectively.

4.2 PRBT from data: QuadPRBT

Recall the assumptions of Subsection 2.3; namely that \mathcal{G} is square and strictly positive real. Define $\mathbf{R} := \mathbf{D} + \mathbf{D}^{\mathsf{T}} \in \mathbb{R}^{n \times n}$; \mathbf{R} is SPD by the strict positive realness of \mathcal{G} . Let $\mathbf{Q}_{\mathcal{M}}, \mathbf{P}_{\mathcal{N}} \in \mathbb{R}^{n \times n}$ be the minimal stabilizing solutions to the PR-AREs (10) and (11), respectively. By [28, Corollary 13.27], the Popov function $\Phi(s)$ in (8) has a minimum phase left spectral factor $\mathbf{M}(s) \in \mathbb{C}^{m \times m}$

$$\Phi(s) = \mathbf{G}(s) + \mathbf{G}(-s)^{\mathsf{T}} = \mathbf{M}(-s)^{\mathsf{T}}\mathbf{M}(s).$$

The rational function $\mathbf{M}(s)$ is the transfer function of the asymptotically stable and minimal linear system \mathcal{M} determined by the state-space quadruple $(\mathbf{A}, \mathbf{B}, \mathbf{C}_{\mathcal{M}}, \mathbf{R}^{1/2})$, where

$$\mathbf{C}_{\mathcal{M}} := \mathbf{R}^{-1/2} (\mathbf{C} - \mathbf{B}^{\mathsf{T}} \mathbf{Q}_{\mathcal{M}}), \qquad (44)$$

and
$$\mathbf{M}(s) := \mathbf{C}_{\mathcal{M}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} + \mathbf{R}^{1/2}.$$
 (45)

Applying [28, Corollary 13.27] to the dual of \mathcal{G} , one obtains a right minimal phase spectral factor $\mathbf{N}(s)$ of $\Phi(s)$

$$\Phi(s) = \mathbf{G}(s) + \mathbf{G}(-s)^{\mathsf{T}} = \mathbf{N}(s)\mathbf{N}(-s)^{\mathsf{T}}.$$

The rational function $\mathbf{N}(s)$ is the transfer function of the asymptotically stable and minimal linear system \mathcal{N} determined by the quadruple $(\mathbf{A}, \mathbf{B}_{\mathcal{N}}, \mathbf{C}, \mathbf{R}^{1/2})$, where

$$\mathbf{B}_{\mathcal{N}} := (\mathbf{B} - \mathbf{P}_{\mathcal{N}} \mathbf{C}^{\mathsf{T}}) \mathbf{R}^{-1/2}, \qquad (46)$$

and
$$\mathbf{N}(s) := \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{N}} + \mathbf{R}^{1/2}.$$
 (47)

By definitions of $\mathbf{C}_{\mathcal{M}}$ and $\mathbf{B}_{\mathcal{N}}$ in (44) and (46), the dual PR-AREs (10) and (11) can be cast in the generalized

forms of (19) and (20):

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{M}} + \mathbf{Q}_{\mathcal{M}}\mathbf{A} + \mathbf{C}_{\mathcal{M}}^{\mathsf{T}}\mathbf{C}_{\mathcal{M}} = \mathbf{0}, \qquad (48)$$

and
$$\mathbf{A}\mathbf{P}_{\mathcal{N}} + \mathbf{P}_{\mathcal{N}}\mathbf{A}^{\mathsf{T}} + \mathbf{B}_{\mathcal{N}}\mathbf{B}_{\mathcal{N}}^{\mathsf{T}} = \mathbf{0}.$$
 (49)

Equation (48) is the observability Lyapunov equation of the linear system $\mathcal{Y} = \mathcal{M}$ that is associated with the spectral factor (45) and defined by $(\mathbf{A}, \mathbf{B}_{\mathcal{Y}}, \mathbf{C}_{\mathcal{Y}}, \mathbf{D}_{\mathcal{Y}}) =$ $(\mathbf{A}, \mathbf{B}, \mathbf{C}_{\mathcal{M}}, \mathbf{R}^{1/2}); \mathbf{Q}_{\mathcal{Y}} = \mathbf{Q}_{\mathcal{M}}$ is thus the observability Gramian of \mathcal{M} . Similarly, (49) is the reachability Lyapunov equation of the linear system $\mathcal{X} = \mathcal{N}$ that is associated with the spectral factor (47) and defined by $(\mathbf{A}, \mathbf{B}_{\mathcal{X}}, \mathbf{C}_{\mathcal{X}}, \mathbf{D}_{\mathcal{X}}) = (\mathbf{A}, \mathbf{B}_{\mathcal{N}}, \mathbf{C}, \mathbf{R}^{1/2}); \mathbf{P}_{\mathcal{X}} = \mathbf{P}_{\mathcal{N}}$ is the reachability Gramian of \mathcal{N} . By the asymptotic stability of \mathcal{N} and \mathcal{M} , Gramians $\mathbf{P}_{\mathcal{N}}$ and $\mathbf{Q}_{\mathcal{M}}$ have integral representations (23) and (24), and can be decomposed into the quadrature-based square-root factors (25) and (26) with $\mathbf{B}_{\mathcal{X}} = \mathbf{B}_{\mathcal{N}}$ and $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}_{\mathcal{M}}$. Thus, Theorem 3.1 (and Algorithm 2) can be applied to derive a data-driven implementation of PRBT; Quadrature-based PRBT (QuadPRBT). Similar to QuadBST, the necessary data $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ can be understood in terms of the spectral factors $\mathbf{M}(s)$ and $\mathbf{N}(s)$ of the Popov function associated with $\mathbf{G}(s)$.

Theorem 4.2 Let $\mathbf{Q}_{\mathcal{M}} \in \mathbb{R}^{n \times n}$ and $\mathbf{P}_{\mathcal{N}} \in \mathbb{R}^{n \times n}$ be the observability Gramian and reachability Gramian of the systems \mathcal{M} and \mathcal{N} corresponding to the minimal phase spectral factors (45) and (47), respectively. Then, in the setting of PRBT, the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ defined in (28)-(30) of Theorem 3.1 (and Algorithm 2) are given by:

$$\mathbf{G}_{\sigma,\mathbf{A}}(s) = \left[\left(\mathbf{M}(-s)^{\mathsf{T}} \right)^{-1} \mathbf{N}_{\infty}(s) \right]_{+}, \qquad (50)$$

$$\mathbf{G}_{\mathbf{B}}(s) = \mathbf{M}_{\infty}(s), \quad \mathbf{G}_{\mathbf{C}}(s) = \mathbf{N}_{\infty}(s).$$
(51)

Proof 4.2 Here, $\mathbf{B}_{\mathbf{X}} = \mathbf{B}_{\mathcal{N}}$, and $\mathbf{C}_{\mathcal{Y}} = \mathbf{C}_{\mathcal{M}}$ as in (46) and (44). So, from (29) and (30)

$$\begin{aligned} \mathbf{G}_{\mathbf{B}}(s) &= \mathbf{C}_{\mathcal{M}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} = \mathbf{M}_{\infty}(s), \\ \mathbf{G}_{\mathbf{C}}(s) &= \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{N}} = \mathbf{N}_{\infty}(s), \end{aligned}$$

thus proving (51). The claim in (50) follows nearly identically from the argument of Theorem 4.1, by replacing $\mathbf{W}(s)$ with $\mathbf{M}(s)$ and $\mathbf{G}_{\infty}(s)$ with $\mathbf{N}_{\infty}(s)$, as well as the associated state-space realizations.

Theorem 4.2 shows how to interpret the transfer functions in Theorem 3.1 in the context of PRBT, yielding a non-intrusive data-driven reformulation of the variant. Algorithm 2 yields QuadPRBT when the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$ and $\mathbf{G}_{\mathbf{B}}(s)$, $\mathbf{G}_{\mathbf{C}}(s)$ to be sampled are chosen as in (50) and (51), respectively.

4.3 BRBT from data: QuadBRBT

Suppose \mathcal{G} is strictly bounded-real. Define the matrices $\mathbf{R}_{\mathcal{J}} := \mathbf{I}_m - \mathbf{D}^{\mathsf{T}} \mathbf{D} \in \mathbb{R}^{m \times m}$ and $\mathbf{R}_{\mathcal{K}} := \mathbf{I}_p - \mathbf{D} \mathbf{D}^{\mathsf{T}} \in \mathbb{R}^{p \times p}$. Both $\mathbf{R}_{\mathcal{J}}$ and $\mathbf{R}_{\mathcal{K}}$ are SPD by the strict boundedrealness of \mathcal{G} and its dual. Let $\mathbf{Q}_{\mathcal{J}}, \mathbf{P}_{\mathcal{K}} \in \mathbb{R}^{n \times n}$ be the minimal stabilizing solutions to the BR-AREs (13) and (14), respectively. By [28, Corollary 13.21], there exists $\mathbf{J}(s) \in \mathbb{C}^{m \times m}$ such that $\mathbf{J}(s)$ is a minimal phase left spectral factor of $\mathbf{I}_m - \mathbf{G}(-s)^{\mathsf{T}}\mathbf{G}(s)$, i.e.

$$\mathbf{I}_m - \mathbf{G}(-s)^{\mathsf{T}}\mathbf{G}(s) = \mathbf{J}(-s)^{\mathsf{T}}\mathbf{J}(s).$$

The (rational) function $\mathbf{J}(s)$ is the transfer function of the asymptotically stable and minimal system \mathcal{J} determined by the quadruple $(\mathbf{A}, \mathbf{B}, \mathbf{C}_{\mathcal{J}}, \mathbf{R}_{\mathcal{J}}^{1/2})$, where

$$\mathbf{C}_{\mathcal{J}} := -\mathbf{R}_{\mathcal{I}}^{-1/2} (\mathbf{B}^{\mathsf{T}} \mathbf{Q}_{\mathcal{J}} + \mathbf{D}^{\mathsf{T}} \mathbf{C}), \qquad (52)$$

and
$$\mathbf{J}(s) := \mathbf{C}_{\mathcal{J}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} + \mathbf{R}_{\mathcal{J}}^{1/2}.$$
 (53)

Similarly, the dual result [28, Corollary 13.22] states there exists a minimal phase right spectral factor $\mathbf{K}(s) \in \mathbb{C}^{p \times p}$ of $\mathbf{I}_p - \mathbf{G}(s)\mathbf{G}(-s)^{\mathsf{T}}$, i.e.,

$$\mathbf{I}_p - \mathbf{G}(s)\mathbf{G}(-s)^{\mathsf{T}} = \mathbf{K}(s)\mathbf{K}(-s)^{\mathsf{T}}.$$

Similarly, $\mathbf{K}(s)$ is the transfer function of the asymptotically stable and minimal system \mathcal{K} determined by the quadruple $(\mathbf{A}, \mathbf{B}_{\mathcal{K}}, \mathbf{C}, \mathbf{R}_{\mathcal{K}}^{1/2})$, where

$$\mathbf{B}_{\mathcal{K}} := -\left(\mathbf{P}_{\mathcal{K}}\mathbf{C}^{\mathsf{T}} + \mathbf{B}\mathbf{D}^{\mathsf{T}}\right)\mathbf{R}_{\mathcal{K}}^{-1/2},\tag{54}$$

and
$$\mathbf{K}(s) := \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B}_{\mathcal{K}} + \mathbf{R}_{\mathcal{K}}^{1/2}.$$
 (55)

The dual BR-AREs (13) and (14) can now be interpreted as the relevant Lyapunov equations (19) and (20) of some related linear systems; although, these are *not* specifically \mathcal{J} and \mathcal{K} corresponding to the aforementioned factors as in the previous instances. Define the matrices:

$$\widehat{\mathbf{B}}_{\mathcal{K}} := \begin{bmatrix} \mathbf{B} \ \mathbf{B}_{\mathcal{K}} \end{bmatrix} \in \mathbb{R}^{n \times 2m}, \quad \widehat{\mathbf{R}}_{\mathcal{K}} := \begin{bmatrix} \mathbf{D} \ \mathbf{R}_{\mathcal{K}}^{1/2} \end{bmatrix} \in \mathbb{R}^{p \times 2m}$$

$$\widehat{\mathbf{C}}_{\mathcal{J}} := \begin{bmatrix} \mathbf{C} \\ \mathbf{C}_{\mathcal{J}} \end{bmatrix} \in \mathbb{R}^{2p \times n}, \qquad \widehat{\mathbf{R}}_{\mathcal{J}} := \begin{bmatrix} \mathbf{D} \\ \mathbf{R}_{\mathcal{J}}^{1/2} \end{bmatrix} \in \mathbb{R}^{2p \times m}.$$
(56)

Then, (13) and (14) can be written as

$$\mathbf{A}^{\mathsf{T}}\mathbf{Q}_{\mathcal{J}} + \mathbf{A}\mathbf{Q}_{\mathcal{J}} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}}\widehat{\mathbf{C}}_{\mathcal{J}} = \mathbf{0}, \qquad (57)$$

and
$$\mathbf{A}\mathbf{P}_{\mathcal{K}} + \mathbf{A}^{\mathsf{T}}\mathbf{P}_{\mathcal{K}} + \mathbf{B}_{\mathcal{K}}\mathbf{B}_{\mathcal{K}}^{\mathsf{T}} = \mathbf{0},$$
 (58)

respectively. So, we consider (57) to be the *observ-ability Lyapunov equation* of the asymptotically stable

linear system $\mathcal{Y} = \widehat{\mathcal{J}}$ defined by $(\mathbf{A}, \mathbf{B}_{\mathcal{Y}}, \mathbf{C}_{\mathcal{Y}}, \mathbf{D}_{\mathcal{Y}}) = (\mathbf{A}, \mathbf{B}, \widehat{\mathbf{C}}_{\mathcal{J}}, \widehat{\mathbf{R}}_{\mathcal{J}}); \mathbf{Q}_{\mathcal{Y}} = \mathbf{Q}_{\mathcal{J}}$ is the *observability Gramian* of $\widehat{\mathcal{J}}$. The transfer function $\widehat{\mathbf{J}}(s) \in \mathbb{C}^{2p \times m}$ of $\widehat{\mathcal{J}}$ is

$$\widehat{\mathbf{J}}(s) := \widehat{\mathbf{C}}_{\mathcal{J}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} + \widehat{\mathbf{R}}_{\mathcal{J}} = \begin{bmatrix} \mathbf{G}(s) \\ \mathbf{J}(s) \end{bmatrix}.$$
(59)

(Note that the choice for $\mathbf{D}_{\mathcal{Y}}$ as $\widehat{\mathbf{R}}_{\mathcal{J}}$ is so that $\widehat{\mathbf{J}}(s)$ can be interpreted in terms of $\mathbf{G}(s)$ and the spectral factor $\mathbf{J}(s)$.) Similarly (58) is the *reachability Lyapunov equation* of the asymptotically stable linear system $\mathcal{X} = \widehat{\mathcal{K}}$ defined by $(\mathbf{A}, \mathbf{B}_{\mathcal{X}}, \mathbf{C}_{\mathcal{X}}, \mathbf{D}_{\mathcal{X}}) = (\mathbf{A}, \widehat{\mathbf{B}}_{\mathcal{K}}, \mathbf{C}, \widehat{\mathbf{R}}_{\mathcal{K}}); \mathbf{P}_{\mathcal{X}} =$ $\mathbf{P}_{\mathcal{K}}$ is the *reachability Gramian* of $\widehat{\mathcal{K}}$. The transfer function $\widehat{\mathbf{K}}(s) \in \mathbb{C}^{p \times 2m}$ of $\widehat{\mathcal{K}}$ is

$$\widehat{\mathbf{K}}(s) := \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\widehat{\mathbf{B}}_{\mathcal{K}} + \widehat{\mathbf{R}}_{\mathcal{K}} = \left[\mathbf{G}(s) \ \mathbf{K}(s)\right].$$
(60)

This fits the generalized framework of Section 3. By the asymptotic stability of $\hat{\mathcal{K}}$ and $\hat{\mathcal{J}}$, the relevant Gramians $\mathbf{P}_{\mathcal{K}}$ and $\mathbf{Q}_{\mathcal{J}}$ admit integral formulae (23) and (24) along with the analogous quadrature-based square-root factors (25) and (26) where $\mathbf{B}_{\mathcal{X}} = \hat{\mathbf{B}}_{\mathcal{K}}$ and $\mathbf{C}_{\mathcal{Y}} = \hat{\mathbf{C}}_{\mathcal{J}}$. Once more, this sets the stage for the application of Theorem 3.1; we refer to the resulting non-intrusive variant of BRBT as quadrature-based BRBT (QuadBRBT). The necessary data $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ can be understood in terms of $\mathbf{J}(s)$, $\hat{\mathbf{J}}(s)$, $\mathbf{K}(s)$, and $\hat{\mathbf{K}}(s)$.

Theorem 4.3 Let $\mathbf{Q}_{\mathcal{J}} \in \mathbb{R}^{n \times n}$ and $\mathbf{P}_{\mathcal{K}} \in \mathbb{R}^{n \times n}$ be the observability Gramian and reachability Gramian of the linear systems $\widehat{\mathcal{J}}$ and $\widehat{\mathcal{K}}$ defined in (59) and (60), respectively. Then the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, $\mathbf{G}_{\mathbf{B}}(s)$, and $\mathbf{G}_{\mathbf{C}}(s)$ given in equations (28)-(30) of Theorem 3.1 (and Algorithm 2) are given by:

$$\mathbf{G}_{\sigma,\mathbf{A}}(s) = \begin{bmatrix} \mathbf{I}_{p} & \mathbf{0}_{p \times m} \\ \mathbf{G}_{\infty}(-s)^{\mathsf{T}} & \mathbf{J}_{\infty}(-s)^{\mathsf{T}} \end{bmatrix}^{-1} \times \\ \begin{bmatrix} \mathbf{G}_{\infty}(s) & \mathbf{K}_{\infty}(s) \\ -\mathbf{D}^{\mathsf{T}}\mathbf{G}_{\infty}(s) & -\mathbf{D}^{\mathsf{T}}\mathbf{K}_{\infty}(s) \end{bmatrix} \end{bmatrix}_{+}^{+},$$

$$\mathbf{G}_{\mathbf{B}}(s) = \widehat{\mathbf{J}}_{\infty}(s), \quad \mathbf{G}_{\mathbf{C}}(s) = \widehat{\mathbf{K}}_{\infty}(s).$$
(61)
(62)

Proof 4.3 Here, $\mathbf{B}_{\mathcal{X}} = \widehat{\mathbf{B}}_{\mathcal{K}}$ and $\mathbf{C}_{\mathcal{Y}} = \widehat{\mathbf{C}}_{\mathcal{J}}$ as in (56). So, from (29) and (30) we have that

$$\mathbf{G}_{\mathbf{B}}(s) = \widehat{\mathbf{C}}_{\mathcal{J}}(s\mathbf{I}_n - \mathbf{A})^{-1}\mathbf{B} = \widehat{\mathbf{J}}_{\infty}(s),$$

$$\mathbf{G}_{\mathbf{C}}(s) = \mathbf{C}(s\mathbf{I}_n - \mathbf{A})^{-1}\widehat{\mathbf{B}}_{\mathcal{K}} = \widehat{\mathbf{K}}_{\infty}(s),$$

proving (62). Next, define the matrices $\widehat{\mathbf{B}} \in \mathbb{R}^{n \times (p+m)}$,

$$\widehat{\mathbf{C}} \in \mathbb{R}^{(p+m) \times n}$$
, and $\widehat{\mathbf{R}} \in \mathbb{R}^{(p+m) \times (p+m)}$ by

$$\widehat{\mathbf{B}} := \begin{bmatrix} \mathbf{0}_{n imes p} \ \mathbf{B} \end{bmatrix}, \ \widehat{\mathbf{C}} := \begin{bmatrix} \mathbf{C} \\ -\mathbf{D}^{\mathsf{T}} \mathbf{C} \end{bmatrix}, \ \widehat{\mathbf{R}} := \begin{bmatrix} \mathbf{I}_p \\ \mathbf{R}_{\mathcal{J}}^{1/2} \end{bmatrix}.$$

It is straightforward to verify that the linear systems corresponding to the transfer functions

$$\begin{bmatrix} \mathbf{I}_p & \mathbf{0}_{p \times m} \\ \mathbf{G}_{\infty}(-s)^{\mathsf{T}} & \mathbf{J}_{\infty}(-s)^{\mathsf{T}} \end{bmatrix}^{-1}, \begin{bmatrix} \mathbf{G}_{\infty}(s) & \mathbf{K}_{\infty}(s) \\ -\mathbf{D}^{\mathsf{T}}\mathbf{G}_{\infty}(s) & -\mathbf{D}^{\mathsf{T}}\mathbf{K}_{\infty}(s) \end{bmatrix},$$

have realizations given by $(-\mathbf{A}^{\mathsf{T}} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}} \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{B}}^{\mathsf{T}}, -\widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}} \mathbf{R}^{-1}, \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{B}}^{\mathsf{T}}, \widehat{\mathbf{R}}^{-1})$ and $(\mathbf{A}, \widehat{\mathbf{B}}_{\mathcal{K}}, \widehat{\mathbf{C}}, \mathbf{0}_{p+m})$, respectively, where $\widehat{\mathbf{C}}_{\mathcal{J}}$ and $\widehat{\mathbf{B}}_{\mathcal{K}}$ are defined as in (56). The resulting cascaded system on the right-hand side of the claimed equality in (61) then has a realization:

$$\begin{pmatrix} -\mathbf{A}^{\scriptscriptstyle \top} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\scriptscriptstyle \top} \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{B}}^{\scriptscriptstyle \top} & \widehat{\mathbf{C}}_{\mathcal{J}}^{\scriptscriptstyle \top} \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{C}} & \mathbf{0}_{n \times (p+m)} \\ \\ \hline \mathbf{0}_n & \mathbf{A} & \widehat{\mathbf{B}}_{\mathcal{K}} \\ \hline & \widehat{\mathbf{R}}^{-1} \mathbf{B}^{\scriptscriptstyle \top} & \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{C}} & \mathbf{0}_{p+m} \\ \end{pmatrix}.$$

After some manipulations, the ARE (13) can be rearranged to be written as

$$(-\mathbf{A}^{\mathsf{T}} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}} \ \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{B}}^{\mathsf{T}})(-\mathbf{Q}_{\mathcal{J}}) + \mathbf{A}\mathbf{Q}_{\mathcal{J}} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}} \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{C}} = \mathbf{0}.$$

Using this reformulation of (13), the state-space transformation $\mathbf{T} = \begin{bmatrix} \mathbf{I}_n & -\mathbf{Q}_{\mathcal{J}} \\ \mathbf{0}_n & \mathbf{I}_n \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$ decouples the cascaded system realization above. In other words, the

the cascaded system realization above. In other words, the transformed state-space is given by

$$\begin{pmatrix} -\mathbf{A}^{\mathsf{T}} + \widehat{\mathbf{C}}_{\mathcal{J}}^{\mathsf{T}} \widehat{\mathbf{R}}^{-1} \widehat{\mathbf{B}}^{\mathsf{T}} & \mathbf{0}_{n} & \mathbf{Q}_{\mathcal{J}} \widehat{\mathbf{B}}_{\mathcal{K}} \\ \\ \hline \mathbf{0}_{n} & \mathbf{A} & \widehat{\mathbf{B}}_{\mathcal{K}} \\ \hline \widehat{\mathbf{R}}^{-1} \mathbf{B}^{\mathsf{T}} & \widehat{\mathbf{C}}_{\mathcal{J}} & \mathbf{0}_{p+m} \end{pmatrix}.$$
 (63)

Evidently, the stable part of this system has the transfer function $\widehat{\mathbf{C}}_{\mathcal{J}}(s\mathbf{I}_n - \mathbf{A})^{-1}\widehat{\mathbf{B}}_{\mathcal{K}}$. Recalling that $\mathbf{B}_{\mathcal{X}} = \widehat{\mathbf{B}}_{\mathcal{K}}$, $\mathbf{C}_{\mathcal{Y}} = \widehat{\mathbf{C}}_{\mathcal{J}}$, this is precisely $\mathbf{G}_{\sigma,\mathbf{A}}(s)$ according to (28).

Theorem 4.3 shows how to interpret the transfer functions in Theorem 3.1 in the context of BRBT, yielding a non-intrusive data-driven reformulation of the variant. Algorithm 2 yields QuadBRBT when the transfer functions $\mathbf{G}_{\sigma,\mathbf{A}}(s)$, and $\mathbf{G}_{\mathbf{B}}(s)$, $\mathbf{G}_{\mathbf{C}}(s)$ to be sampled are chosen as in (61) and (62), respectively.

5 Numerical Examples

In this section we provide a proof of concept for our data-driven BT-RoMs. For each of the variants studied (BST, PRBT, BRBT) we compare the performance of our approach (i.e., data-driven RoMs computed via QuadBST, QuadPRBT, and QuadBRBT following the layout of Algorithm 2) against their respective intrusive counterparts via Algorithm 1. These experiments were performed on a MacBook Pro equipped with 8 gigabytes of RAM and a 2.3 GHz Dual-Core Intel Core i5 processor running macOS Ventura version 13.6.1. The experiments were run using MATLAB version 23.2.0.2428915 (R2023b) Update 4. All MATLAB code and data for reproducing the subsequent experiments are available publicly at [23].

We briefly outline our experimental set-up. The system we study is an order n = 400 single-input single-output RLC circuit model \mathcal{G} presented in [17]; the choice of physical parameters parameters are R = C = L = 0.1, and $\overline{R} = 1$. The system is both passive and square by construction, and contains a non-trivial and nonsingular input feedthrough term **D**. In the case of Quad-BRBT, we additionally normalize the circuit model so that $\|\mathcal{G}\|_{\mathcal{H}_{\infty}} = 0.5$, and \mathcal{G} satisfies the bounded-real assumption (12). The intrusive BST, PRBT, and BRBT-RoMs that we benchmark against our data-driven RoMs were computed using the MATLAB toolbox MORLAB [9]. For the data-driven GenQuadBT-RoMs, the necessary data given in Theorems 4.1-4.3 are obtained numerically by explicitly sampling the relevant transfer functions. The GenQuadBT-RoMs are then computed according to Algorithm 2. In generating these data, the built-in MAT-LAB routine 'icare' was used in computing the minimal solutions to the appropriate AREs. To (implicitly) approximate the *relevant* Gramians $\mathbf{P}_{\mathcal{X}}$ and $\mathbf{Q}_{\mathcal{Y}}$ we employ the Trapezoidal rule using N = 40, 80, 160 quadrature nodes. These are chosen as logarithmically-spaced points in the interval $i[10^{-1}, 10^4] \subset i\mathbb{R}$, closed under complex conjugation.

Figures 1, 2, and 3 compare the performance of QuadBST, QuadPRBT, and QuadBRBT, respectively, to their classical intrusive formulation. In each figure, the top plot depicts the *true* singular values of $\sigma(\mathbf{L}_{\mathcal{Y}}^{\mathsf{T}}\mathbf{U}_{\mathcal{X}})$ against the data-driven $\sigma(\widetilde{\mathbf{L}}_{\mathcal{Y}}^{*}\widetilde{\mathbf{U}}_{\mathcal{X}})$, and the bottom plot depicts the relative \mathcal{H}_{∞} error $\|\mathcal{G} - \mathcal{G}_{r}\|_{\mathcal{H}_{\infty}}/\|\mathcal{G}\|_{\mathcal{H}_{\infty}}$ induced by the intrusive and data-driven RoMs. As illustrated by the figures, for each BT-variant the data-driven singular values capture the true (dominant) ones accurately. And similarly the data-driven GenQuadBT-RoMs approach the approximation quality of their intrusive counterpart as the number of nodes N increases. Therefore, using only the relevant input-output data without having access to a state-space form, we are able to match the performance of the intrusive BT-RoMs.

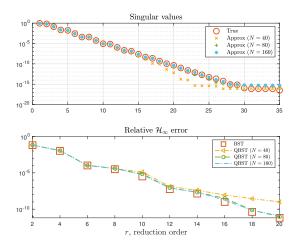


Figure 1. The true singular values compared against the approximate quadrature-based ones using N quadrature nodes (top) and the relative \mathcal{H}_{∞} approximation error for BST and QuadBST-RoMs for orders $r = 2, 4, \ldots, 20$ (bottom).

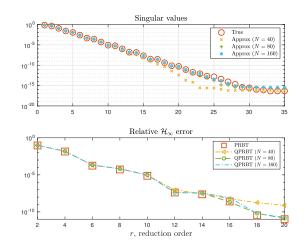


Figure 2. The true singular values compared against the approximate quadrature-based ones using N quadrature nodes (top) and the relative \mathcal{H}_{∞} approximation error for PRBT and QuadPRBT-RoMs for orders $r = 2, 4, \ldots, 20$ (bottom).

6 Conclusion

We have developed data-driven implementations for some important extensions of BT; namely BST, PRBT, and BRBT. These formulations are entirely non-intrusive and require only system-response data, i.e., the measurements of certain transfer functions. Moreover, these data-driven BT-RoMs require sampling certain *spectral factorizations* associated with the underlying model. The numerical examples illustrate the accuracy of the data-driven RoMs. In this work, we focused on the theoretical formulation of the data-driven BT variants. How to obtain the required samples of the relevant spectral factors in an experimental or "real-world" setting is still an open question and an ongoing work.

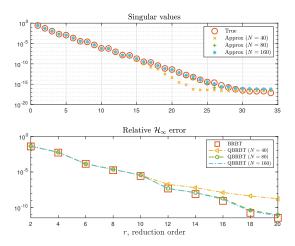


Figure 3. The true singular values compared against the approximate quadrature-based ones using N quadrature nodes (top) and the relative \mathcal{H}_{∞} approximation error for BRBT and QuadBRBT-RoMs for orders $r = 2, 4, \ldots, 20$ (bottom).

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References

- A. C. Antoulas. Approximation of large-scale dynamical systems. SIAM, 2005.
- [2] A. C. Antoulas, C. A. Beattie, and S. Güğercin. Interpolatory methods for model reduction. SIAM, 2020.
- [3] P. Benner and T. Breiten. Model order reduction based on system balancing. In *Model reduction and approximation:* theory and algorithms, chapter 6, pages 261–295. SIAM, 2017.
- [4] P. Benner, S. Grivet-Talocia, A. Quarteroni, G. Rozza, W. Schilders, and L. M. Silveira, editors. Model Order Reduction: Volume 1: System- and Data-Driven Methods and Algorithms. De Gruyter, Berlin, Boston, 2021.
- [5] P. Benner, M. Ohlberger, A. Cohen, and K. Willcox, editors. *Model Reduction and Approximation: Theory and Algorithms.* Computational Science & Engineering. SIAM, Philadelphia, PA, 2017.
- [6] P. Benner, E. S. Quintana-Ortí, and G. Quintana-Ortí. Efficient numerical algorithms for balanced stochastic truncation. *International Journal of Applied Mathematics* and Computer Science, 11(5):1123–1150, 2001.
- [7] P. Benner and J. Saak. Efficient balancing-based MOR for large-scale second-order systems. *Mathematical and Computer Modelling of Dynamical Systems*, 17(2):123–143, 2011.
- [8] P. Benner and A. Schneider. Balanced truncation model order reduction for LTI systems with many inputs or outputs. In *Proceedings of the 19th International Symposium* on Mathematical Theory of Networks and Systems-MTNS, volume 5, 2010.
- [9] P. Benner and S. W. R. Werner. MORLAB—the model order reduction LABoratory. *Model Reduction of Complex Dynamical Systems*, pages 393–415, 2021.

- [10] T. Breiten and T. Stykel. Balancing-related model reduction methods. System-and Data-Driven Methods and Algorithms, 1:15–56, 2021.
- [11] U. Desai and D. Pal. A transformation approach to stochastic model reduction. *IEEE Transactions on Automatic Control*, 29(12):1097–1100, 1984.
- [12] D. F. Enns. Model reduction with balanced realizations: An error bound and a frequency weighted generalization. In *The* 23rd IEEE Conference on Decision and Control, pages 127– 132. IEEE, 1984.
- [13] K. Glover and J. C. Doyle. State-space formulae for all stabilizing controllers that satisfy an H_∞-norm bound and relations to relations to risk sensitivity. Systems and Control Letters, 11(3):167–172, 1988.
- [14] I. V. Gosea, S. Gugercin, and C. Beattie. Data-driven balancing of linear dynamical systems. SIAM Journal on Scientific Computing, 44(1):A554–A582, 2022.
- [15] M. Green. Balanced stochastic realizations. *Linear Algebra* and its Applications, 98:211–247, 1988.
- [16] M. Green. A relative error bound for balanced stochastic truncation. *IEEE Transactions on Automatic Control*, 33(10):961–965, 1988.
- [17] S. Gugercin and A. C. Antoulas. A survey of model reduction by balanced truncation and some new results. *International Journal of Control*, 77(8):748–766, 2004.
- [18] V. Mehrmann and B. Unger. Control of port-Hamiltonian differential-algebraic systems and applications. Acta Numerica, 32:395–515, 2023.
- [19] B. Moore. Principal component analysis in linear systems: Controllability, observability, and model reduction. *IEEE Transactions on Automatic Control*, 26(1):17–32, 1981.
- [20] C. Mullis and R. A. Roberts. Synthesis of minimum roundoff noise fixed point digital filters. *IEEE Trans. Circuits Syst.*, 23(9):551–562, 1976.
- [21] P. C. Opdenacker and E. A. Jonckheere. A contraction mapping preserving balanced reduction scheme and its infinity norm error bounds. *IEEE Transactions on Circuits* and Systems, 35(2):184–189, 1988.
- [22] L. Pernebo and L. Silverman. Model reduction via balanced state space representations. *IEEE Transactions on Automatic Control*, 27(2):382–387, 1982.
- [23] S. Reiter. Code, data, and results for numerical experiments in "Generalizations of data-driven balancing: what to sample for different balancing-based reduced models" (version 1.0), December 2023. doi:10.5281/zenodo.10403185.
- [24] C. W. Rowley. Model reduction for fluids, using balanced proper orthogonal decomposition. Int. J. Bifurcat. Chaos, 15(3):997—1013, 2005.
- [25] V. Simoncini. Computational methods for linear matrix equations. SIAM Review, 58(3):377–441, 2016.
- [26] J. R. Singler and B. A. Batten. A proper orthogonal decomposition approach to approximate balanced truncation of infinite dimensional linear systems. *Intern. J. Computer Mathematics*, 86(2):355–371, 2009.
- [27] K. Willcox and J. Peraire. Balanced model reduction via the proper orthogonal decomposition. AIAA Journal, 40(11):2323–2330, 2002.
- [28] K. Zhou, J. C. Doyle, and K. Glover. Robust and optimal control. Prentice-Hall, 1996. ISBN: 978-0-13-456567-5.