Structured storage functions for cascaded systems

Thomas P. Prescott^{1,2}

Antonis Papachristodoulou¹

Abstract—Dissipativity analysis is an important tool for the analysis of the dynamic response of systems of Ordinary Differential Equations to structural and parametric perturbations. In order to certify dissipativity, semi-definite programming is commonly used for the computation of storage functions of polynomial systems, but is currently not a practical solution for large-scale systems. This paper formulates the computation of a class of structured storage functions that exploit the structure of systems that can be decomposed into cascades. Structured storage functions allow the decomposition of the semi-definite programs used to prove dissipativity, thereby reducing the computational cost of SOS programming and making its application to large-scale systems more practical. Thus structured storage functions deliver additional speed and flexibility to the dissipativity approach to parametric and structural sensitivity analysis.

I. Introduction

In the analysis and control of complex systems there is a trade-off between the accuracy and tractability of the models used, since accurate models tend to be complicated and difficult to analyse. Model decomposition [1], [3], [9], [10], [11], [16], [17], [23] is an approach which seeks to exploit the structure of a system to decompose a particular problem by splitting analysis or design tasks across subsystems. Various ways to exploit system structure in the analysis of large-scale systems have been investigated [2], [4], [18], [20], [21], [22]. In this paper we will demonstrate how, by identifying cascade structures, we can decompose the construction of storage functions using semi-definite programming, with applications to a dynamic parameter sensitivity analysis of a nonlinear system.

There are many different types of sensitivity analyses which are very often application-specific [19], [24]. In the context of biochemical reaction networks, for example, different versions of control analysis [5], [6], [8] quantify the steady-state response to parameter changes. Here we assume that, while the transient dynamics respond to a parameter perturbation, the steady state is independent of the perturbed parameters, and therefore does not respond. Our measure of the parameter sensitivity is the \mathcal{L}_2 norm of the difference in output trajectories between the nominal and perturbed model.

Consider an autonomous upstream system whose output u forms the input to a downstream system with output y. The problem is to understand how a parameter perturbation upstream changes the trajectory of y. Our approach is to

search for storage functions [7] which bound the output of an error system. As discussed in [15], the computational cost of a semi-definite programming approach to this problem quickly explodes with the increase in system dimension. We will show how to slow this very rapid increase by limiting the search for storage functions to a particular class of *structured* storage functions that reflect the cascade structure of the system.

This paper is structured as follows. In the rest of this section we briefly review the use of SOSTOOLS in constructing storage functions, and introduce an example cascade system which will illustrate our structured formulation. Section II develops the application of the SOS technique to structured parameter sensitivity analysis. In Section III we apply these methods to the example system, before discussing the implications for model reduction techniques in Section IV.

A. SOS programming and dissipativity

This paper focuses on the proof of dissipativity of various dynamical systems with respect to given supply rates. Dissipativity can be certified by the construction of a storage function. For polynomial (and rational polynomial) systems of ODEs, storage functions can be calculated using semi-definite programming, which is enabled by a relaxation of positivity constraints into SOS constraints, as follows.

Suppose we have a system with dynamics

$$\dot{x} = f(x, u) \tag{1}$$

with y = y(x), for state $x \in \mathbb{R}^n$, input $u \in \mathbb{R}^p$ and output $y \in \mathbb{R}^m$. For a given *supply rate* s(u, y), the system's dissipativity is defined as follows.

Definition 1: The system (1) is dissipative with respect to s(u,y) if there exists a function V(x) of the state that is positive semi-definite, such that

$$\frac{\mathrm{d}V}{\mathrm{d}t} + s(u, y) \le 0 \tag{2}$$

along the trajectory of x(t). Then V is a storage function.

SOSTOOLS [12] is a MATLAB toolbox that implements an SOS programming technique for constructing polynomial storage functions V. We have used this software in previous work [15] to satisfy a dissipation inequality bounding the \mathcal{L}_2 error in the output incurred from model order reduction.

Definition 2: A polynomial function $\phi: \mathbb{R}^n \to \mathbb{R}$ is SOS, denoted $\phi \in \Sigma$, if there exist polynomial functions $p_1, \ldots, p_k: \mathbb{R}^n \to \mathbb{R}$ such that $\phi = \sum_{i=1}^k p_i^2$.

Clearly $\phi \in \Sigma$ implies that ϕ is a positive semi-definite polynomial; the converse, however, is not true [14]. Nevertheless, the stronger condition is useful because it can

^{*} The authors gratefully acknowledge support from EPSRC under projects EP/J012041/1, EP/I031944/1, and EP/J010537/1.

Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK

² Life Sciences Interface Doctoral Training Centre, University of Oxford, Parks Road, Oxford, OX1 3QU, UK

be formulated as a semi-definite feasibility problem by the following lemma, proved in [14]:

Lemma 3: The polynomial function $\phi \in \Sigma$ if and only if it is of even degree $deg(\phi) = 2d$ and there exists a positive semi-definite matrix $Q \succeq 0$ such that $\phi(x)$ can be written

$$\phi(x) = Z(x)^T Q Z(x),$$

where Z(x) is a vector of monomials in the components of x, of degrees at most d.

SOS programming exploits this result to implement the search for a storage function V as a semi-definite feasibility problem. Suppose $x \in \mathcal{D} \subset \mathbb{R}^n$, where the domain \mathcal{D} is defined by a set of k polynomial inequalities

$$\mathcal{D} = \{ x \in \mathbb{R}^n \mid g_i(x) \le 0 \text{ for } i = 1, \dots, k \}.$$
 (3)

The following lemma is adapted from [13], and formulates the search for a storage function as a SOS program.

Lemma 4: Assume that the dynamics f(x, u) and h(x), and the supply rate s(u, y), are polynomial functions. If there exists a polynomial function V(x) and k polynomial functions $\sigma_i(x)$ such that

$$V(x) \in \Sigma$$
, (4)

$$\forall i = 1, \dots, k, \quad \sigma_i(x) \in \Sigma, \quad (5)$$

$$-\left(\dot{V}(x) + s(u,y)\right) + \sum_{i=1}^{k} \sigma_i(x)g_i(x) \in \Sigma, \quad (6)$$

then V is a storage function certifying dissipativity, locally to \mathcal{D} , with respect to the supply s.

Note that if $\mathcal{D} = \mathbb{R}^n$ then we simply assume k = 0 in the conditions (4)–(6).

B. Small example system

We will introduce the structured storage function method in the context of the following small example system, taken from the theory of biochemical reaction networks. Consider the system

$$X_1 \stackrel{\alpha}{\to} X_2$$
 (7a)

$$X_1 \stackrel{\alpha}{\to} X_2 \tag{7a}$$

$$X_2 + X_3 \stackrel{\beta}{\to} X_4 \tag{7b}$$

of 4 reactants X_i taking part in 2 reactions. Assume that the initial concentrations $x_i(0)$ of species X_i form the vector $x(0) = [a, b, c, 0]^T$. This network has a cascade structure, where reaction (7a) is upstream of reaction (7b). This is reflected by the dynamics

$$\dot{u} = -\alpha u, \tag{8a}$$

$$\dot{\xi} = -\beta(a+b-k+\xi-u)(c-k+\xi),$$
 (8b)

where $k = \min(a+b, c)$, and with initial conditions u(0) = aand $\xi(0) = k$. The vector x of concentrations x_i of species X_i is recovered through the linear relationship

$$x = [u, a+b-k+\xi-u, c-k+\xi, k-\xi]^T$$
. (9)

The system is a clearly a cascade, as (8a) is an autonomous system forming the input into (8b). Note also that as $t \to \infty$ both u and ξ tend to 0.

II. PARAMETER SENSITIVITY

Suppose the reaction network (7) is perturbed by changing the value of α from α_1 to α_2 . The steady state of this reaction network remains constant, but the transient dynamics will be perturbed. In general, suppose we have a system of ODEs with dynamics $\dot{x} = f(x; \pi)$ for parameter vector π , with measured output y = y(x). Consider the nominal parameter value π_1 and the perturbed parameter value π_2 . We denote the dynamics of each case by $\dot{x}_i = f(x_i; \pi_i)$ and output $y_i =$ $y(x_i)$ for i=1,2. The effect of the perturbation can then be measured by a norm of the output difference $||y_1 - y_2||$, which we take as

$$||y_1 - y_2||_2^2 = \int_0^\infty |y_1 - y_2|^2 dt,$$

based on the Euclidean norm of \mathbb{R}^m . We assume that the steady states of the systems are equal, so that this measure is finite.

We shall discuss two methods of estimating $||y_1 - y_2||$. The first [15] uses SOS programming to calculate a single storage function, which we will term the *direct method*. However, large-scale systems often render this impractical. Thus this paper introduces a second method that exploits cascade structures to decompose the construction of a storage function. We first deal with the upstream perturbation and then characterise how that propagates to the downstream subsystem. This strategy can achieve significant computational savings. In the process of introducing structured storage functions, we will also demonstrate that the storage functions used to estimate incremental gain [18] are a class of structured storage functions.

A. Direct method

Consider the following auxiliary system of autonomous **ODEs**

$$\dot{x}_i = f(x_i; \pi_i), \tag{10a}$$

$$y_e = y_1 - y_2 = y(x_1) - y(x_2),$$
 (10b)

with initial conditions $x_i(0)$. The following theorem, proved in [15], relates a storage function for the dissipativity of this system to an upper bound on the dynamic response to the parameter perturbation.

Theorem 5: Let $V(x_1, x_2)$ be a storage function certifying the dissipativity of (10) in \mathcal{D} with respect to storage function $s = |y_1 - y_2|^2$. Then

$$||y_1 - y_2||_2^2 \le V|_{t=0} \tag{11}$$

holds.

Proof: By definition V satisfies (2). Integrating this inequality proves (11): see [15] for details.

We can now utilise SOS programming by applying Lemma 4 to construct an appropriate storage function through the following optimisation problem, where g_i define the state space \mathcal{D} in (3).

Lemma 6: Define decision variables $V(x_1,x_2)\in \Sigma$ and $\sigma_i(x_1,x_2)\in \Sigma$. Minimise $V|_{t=0}=V(x_1(0),x_2(0))$ subject to the SOS constraint

$$-\left(\dot{V} + |y_1 - y_2|^2\right) + \sum_{i=1}^k \sigma_i g_i \in \Sigma.$$
 (12)

Then (11) holds.

Proof: The function V satisfies the conditions of Lemma 4 with supply rate $s = |y_1 - y_2|^2$, and is therefore a storage function certifying the dissipativity of (10) with respect to s. By Theorem 5, the error bound holds.

Note that, since we assume given initial conditions, we can impose the objective $\min(V|_{t=0})$ to ensure that the resulting bound (11) is as tight as possible.

For example, consider (10) for f given by (8). This consists of four differential equations

$$\dot{u}_i = -\alpha_i u_i \tag{13a}$$

$$\dot{\xi}_i = -\beta(a+b-k+\xi_i-u_i)(c-k+\xi_i)$$
 (13b)

for i=1,2, with initial conditions $u_i(0)=a$ and $\xi_i(0)=k=\min(a+b,c)$. Suppose we are interested in the sensitivity of the trajectory of X_4 . According to (9), this sensitivity is measured by $\|(k-\xi_1)-(k-\xi_2)\|_2=\|\xi_1-\xi_2\|_2$.

By Lemma 6, we seek a storage function $V(u_1,\xi_2,u_2,\xi_2)\in \Sigma$ to satisfy (12) for $y_i=\xi_i$, from which we can conclude the bound $\|\xi_1-\xi_2\|^2\leq V(a,k,a,k)$ on the sensitivity. This bound is optimised for given initial conditions by imposing the objective function $\min(V(a,k,a,k))$.

B. Structured storage functions

We call the SOS method described above the direct method for estimating the perturbation response. However, a common problem with its implementation is the impractically large computational cost in large-dimensional state space. We will now demonstrate how to exploit cascade structures to reduce the cost of the resulting SOS problem.

Recall the dynamical system $\dot{x}=f(x;\pi)$ with parameter vector π , state $x(t)\in\mathcal{D}\subset\mathbb{R}^n$ and output $y(t)=h(x(t))\in\mathbb{R}^m$. Now suppose that the system is a cascade, whereby a decomposition $x^T=[u^T,\xi^T]$ and $\pi^T=[\pi_u^T,\pi_\xi^T]$ exists such that

$$\dot{u} = f_u(u; \pi_u), \quad z = z(u; \pi_u),$$
 (14a)

$$\dot{\xi} = f_{\xi}(\xi, z; \pi_{\xi}), \quad y = y(\xi; \pi_{\xi})$$
 (14b)

We interpret u and ξ as the states of the upstream and downstream systems respectively, with the downstream system driven by input z and with output y.

The task of this section is to measure the effect on y of perturbing the upstream parameters π_u . As with the auxiliary system in (10b), we can write two instances of (14) indexed by i=1,2 to correspond to two parameter vectors $(\pi_u)_i$. Recall that the direct method in Theorem 5 seeks a storage function $V(u_1,\xi_1,u_2,\xi_2)$ such that $\dot{V}+|y_1-y_2|^2\leq 0$ for all t. However, an intuitive way to exploit the cascade structure (14) to calculate a *structured storage function* V is to first

identify the effect on z, and then determine how that passes downstream to y.

Theorem 7: Suppose that (14a) satisfies

$$\dot{V}_u(u_1, u_2) + s_u(z_1, z_2) \le 0 \tag{15a}$$

for a particular supply rate s_u . Define the positive semi-definite function

$$V(u_1, \xi_1, u_2, \xi_2) = V_0(\xi_1, \xi_2) + V_u(u_1, u_2)V_1(\xi_1, \xi_2)$$
 (15b)

for positive semi-definite functions V_0 and V_1 . Then if the inequality

$$\dot{V}_0 + V_u \dot{V}_1 - s_u V_1 + |y_1 - y_2|^2 \le 0 \tag{15c}$$

holds, V is called a structured storage function, and the sensitivity of y can be bounded above by

$$||y_1 - y_2||^2 \le V|_{t=0}. (16)$$

Proof: Consider the derivative $\dot{V}=\dot{V}_0+V_u\dot{V}_1+\dot{V}_uV_1$. By (15a) this is bounded above such that $\dot{V}\leq\dot{V}_0+V_u\dot{V}_1-s_uV_1$. Thus (15c) implies that $\dot{V}+|y_1-y_2|^2\leq 0$. Therefore V satisfies (2) and $V(x_1,x_2)$ is a storage function for the supply rate $|y_1-y_2|$. By Theorem 5 the bound (16) follows.

As in Section II-A, we can use Lemma 4 to construct polynomial functions V_0 and V_1 that satisfy (15) as follows:

Lemma 8: Assume that the upstream system satisfies (15a) for a particular polynomial supply rate s_u and storage function V_u . Now extend the downstream state space (ξ_1,ξ_2) with a new dummy variable $v_u(t)$. Define decision variables $V_j(\xi_1,\xi_2)\in \Sigma$ for j=0,1, to construct $\bar{V}(\xi_1,\xi_2,v_u)=V_0+v_u^2V_1$. Define also slack variables $\sigma_i\in \Sigma$ for $i=1,\ldots,k$ with arguments (ξ_1,ξ_2,v_i) . Minimise $V|_{t=0}$ subject to the SOS constraint

$$-\left(\dot{V}_0 + v_u \dot{V}_1 - s_u V_1 + |y_1 - y_2|^2\right) + \sum_{i=1}^k \sigma_i g_i \in \Sigma. \tag{17}$$

Then the effect of the perturbation can be bounded such that (16) holds for V with the substitution for the dummy variable $v_u = V_u$.

Proof: Finding feasible V_j and σ_i for (17) implies that for $\xi_i \in \mathcal{D}$ and v_u such that $\dot{v}_u + s_u \leq 0$ we have $\dot{\bar{V}} + |y_1 - y_2|^2 \leq 0$. Substituting $v_u = V_u$ into \bar{V} means that the resulting $V = \bar{V}(\xi_1, \xi_2, V_u)$ satisfies all of (15), and thus (16) follows by Theorem 7.

Note that if $V_1 = \gamma^2$ is a constant, a structured storage function is simply a linear combination of the upstream storage function V_0 . Many decomposed approaches to dissipativity analysis questions consider linear combinations of subsystem storage functions [11], [18]. However, the key distinction between these methods and the function V in (15b) is that $V_1(\xi_1, \xi_2) \in \Sigma$ is not necessarily a constant, but is allowed to be a general SOS polynomial of a specified degree. We will show in Section III-A that this can allow for less conservative upper

bounds on sensitivity than those deduced from taking linear combinations.

We now consider the computational savings of structured storage functions. Suppose that the states u and ξ have dimension N_u and N_ξ respectively, so that the full state x has dimension $N=N_u+N_\xi$. Using the direct method as described by Lemma 6 results in a single SOS program of 2N variables. The structured approach instead gives two SOS programs, where the upstream program is of dimension $2N_u$. Suppose that the input z from the upstream to downstream system is a vector in a space of dimension $N_z \leq N_u$. The downstream program is in $2N_\xi+1+2N_z$ variables, where the extra 1 comes from the dummy variable v_u . Thus we reduce the number of variables from the large SOS program if the inequality $N_z < N_u$ is strict. As will be seen in the results of Section III, smaller N_z compared to N_u results in significant computational saving.

C. Adapting structured storage functions

To improve the bound (16) further, we may be able to 'import' even more information from the upstream system by adapting (15b) to use additional upstream storage functions.

Corollary 9: Suppose the upstream system satisfies the R storage inequalities

$$s_i(z_1, z_2) + \dot{V}_{u,i}(u_1, u_2) \le 0$$

for $j = 1, \dots, R$. Define the positive semi-definite function

$$V(u_1, \xi_1, u_2, \xi_2) = V_0(\xi_1, \xi_2) + \sum_{i=1}^{R} V_j(\xi_1, \xi_2) V_{u,j}(u_1, u_2)$$

for positive semi-definite functions V_j , j = 0, 1, ..., R. If the inequality

$$|y_1 - y_2|^2 + \dot{V}_0 + \sum_{j=1}^R \left(\dot{V}_j V_{u,j} - s_j V_j\right) \le 0$$

holds, then the system is dissipative with respect to the supply rate $|y_1-y_2|^2$ with structured storage function V, so that

$$||y_1 - y_2||^2 \le V|_{t=0}$$
.

Proof: This result can be deduced by the repeated application of Theorem 7. \blacksquare

The equivalent SOS constraint to (17) is given by

$$|y_1 - y_2|^2 + \dot{V}_0 + \sum_{j=1}^R \left(\dot{V}_j v_{u,j} - s_j V_j \right) + \sum_{i=1}^k \sigma_i g_i \in \Sigma$$
 (18)

for a state space with R additional variables $v_{u,j}$.

III. NUMERICAL RESULTS

The following two examples illustrate the construction of structured storage functions. First, recall the dynamics (13) of the system in Section I-B. We will show the importance of the additional flexibility that structured storage functions bring to quantifying parameter sensitivity.

A. Low dimensional cascade

Fix the reaction rates $\alpha_1=1,\ \alpha_2=1.1$ and $\beta=1$ in (13). We can estimate the sensitivity $\|\xi_1-\xi_2\|_2$ of X_4 both directly, and with structured storage functions, using the SOS programs described by Lemmas 6 and 8. We will observe in this example that we can find structured storage functions when incremental gain methods fail, considering three instances of the parameters p=(a,b,c) in turn: $p_1=(1,0,2),\ p_2=(1,2,1),$ and $p_3=(1,1,1,5).$

First substitute $(a, b, c) = p_1$ into (13), with initial conditions $(u_i(0), \xi_i(0)) = (1, 1)$. We can apply Lemma 6 to these dynamics, where \mathcal{D} is such that $\xi_i \in [0, 1]$. In this instance, (12) results in the SOS constraint

$$-|\xi_1 - \xi_2|^2 - \dot{V} + \sigma_1(\xi_1 - 1)\xi_1 + \sigma_2(\xi_2 - 1)\xi_2 \in \Sigma.$$
 (19)

By optimising V(1,1,1,1), the SOS program returns an upper bound of $\|\xi_1 - \xi_2\|_2^2 \le V(1,1,1,1) = 0.00164$. A simulation of the two systems shows that this estimate agrees with a sensitivity of $\|\xi_1 - \xi_2\|_2^2 \approx 0.0016$. Similar results hold for (a,b,c) equal to p_2 and p_3 , with tight estimates of 1.57×10^{-5} and 3.54×10^{-4} respectively.

We now decompose the search for V by applying Lemma 8 to exploit the cascade structure of (13). For all p_m , we can use Lemma 6 on (13a) to easily calculate a degree two storage function V_u for the upstream dynamics (13a) that returns $\|u_1-u_2\|^2 \leq 0.00217$ as a bound on the upstream perturbation. The aim is now to observe how this sensitivity propagates downstream for each p_m .

For each $(a,b,c)=p_m$, m=1,2,3, we seek a structured storage function V of the form (15b) to prove the dissipativity of the downstream system, locally to the state space where $\xi_i \in [0,k], \ u_i \in [0,a],$ and where $x_2=a+b-k+\xi_i-u_i$ is positive. For $(a,b,c)=p_1$, we first seek V such that $V_1=\gamma^2$ is a non-negative constant, meaning that $V=V_0+\gamma^2V_u$ is a linear combination of downstream and upstream storage functions. Implementing the SOS program with constraint (17), and seeking to minimise the upper bound $V_0(1,1)+\gamma^2V_u(1,1)$, we find an upper bound of $\|\xi_1-\xi_2\|_2^2 \leq 0.0022$ using a fourth-order storage function $V_0(\xi_1,\xi_2)$, where the resulting value of γ^2 is 1.0002.

Next, seeking a similarly structured storage function $V=V_0+\gamma^2V_u$ in the case where $(a,b,c)=p_2$ results in an upper bound of $\|\xi_1-\xi_2\|^2\leq 1.69\times 10^{-4}$, with $\gamma^2=0.0762$. However, if we now allow V_1 to vary over degree-2 SOS polynomials, this bound can be improved to $\|\xi_1-\xi_2\|^2\leq 1.361\times 10^{-4}$. Thus, the flexibility of allowing non-constant V_1 in (15b) improves error bounds past those which can be constructed by linear combinations of upstream and downstream storage functions.

Finally consider $(a,b,c)=p_3$. There is no feasible V_0 and V_1 (constant or polynomial) that satisfies (15c) for the given $s_u=(u_1-u_2)^2$. We can overcome this problem by first constructing \hat{V}_u satisfying (15a) with $\hat{s}_u=(u_1+u_2)^2$. Substituting \hat{s}_u into (17) now results in a feasible SOS problem. This gives an upper bound $\|\xi_1-\xi_2\|^2 \leq 0.1999$ when searching over $\deg V_0=4$ and $\deg V_1=2$. Clearly

this bound is very conservative compared to the direct error bound of 3.54×10^{-4} found above. Alternatively, we can apply Corollary 9 to collect together the information from $s_u = (u_1 - u_2)^2$ and $\hat{s}_u = (u_1 + u_2)^2$. We define a structured storage function $V = V_0 + V_u V_1 + \hat{V}_u V_2$ for SOS polynomials V_0 , V_1 , and V_2 . Minimising $V|_{t=0}$ subject to (18) with $\deg V_0 = 4$ and $\deg V_1 = \deg V_2 = 2$ results in a much improved upper bound of $\|\xi_1 - \xi_2\|^2 \leq 0.001$.

This example is an extremely simple system that illustrates how we can use the flexibility of structured storage functions to improve the analysis of how sensitivity propagates through systems past seeking linear combinations of the storage functions. However, the simplicity of this example is also its weakness: the state space dimension is so small that there is no computational saving in this method, since $N_\xi = N_u = N_z = 1$. However, the next example demonstrates of the capacity of structured storage functions for significant computational savings over the direct method.

B. High dimensional cascade

Now suppose that the value of α in (7a) is a time-varying quantity, proportional to the concentration of a certain enzyme E, which takes part in the biomolecular network

$$\begin{array}{ccc} P_i & \stackrel{\mu_i}{\longrightarrow} & E_i, & i=1,2, \\ E_1 + E_2 & \stackrel{k_{on}}{\rightleftharpoons} & E, \end{array}$$

such that E is formed from the binding of the two proteins E_i , each of which activated from P_i at rate μ_i . Assume that the initial concentrations of P_i are given by π_i , with E_i and E initially at 0 concentration. This layer is then modelled in $N_u=3$ variables as

$$\dot{u}_1 = -\mu_1 u_1,$$
 (20a)

$$\dot{u}_2 = -\mu_2 u_2, \tag{20b}$$

$$\dot{u}_3 = k_{on}(\pi_1 - \eta - u_1 - u_3)(\pi_2 - \eta - u_2 - u_3) - k_{off}(u_3 + \eta), \tag{20c}$$

with initial conditions $u_i(0) = \pi_i$, i = 1, 2, and $u_3(0) = -\eta$. Here η is the unique solution $0 < \eta < \min(\pi_1, \pi_2)$ to

$$0 = k_{on}(\pi_1 - \eta)(\pi_2 - \eta) - k_{off}\eta.$$

The downstream dynamics of (7) can now be written in $N_{\xi}=2$ variables as

$$\dot{\xi}_1 = -\alpha(u_3 + \eta)\xi_1, (20d)$$

$$\dot{\xi}_2 = -\beta(a + b - k + \xi_2 - \xi_1)(c - k + \xi_2), (20e)$$

where $\xi_1(0) = a$ and $\xi_2(0) = k$. The steady state of $x^T = [u^T, \xi^T]$ is 0, and there is a single input $N_z = 1$.

Suppose that we perturb $\mu_1=1$ to $\tilde{\mu}_1=2$, for example, where tilde now must denote the perturbed system. We estimate the effect on the trajectory of X_4 by the norm $E=\|\xi_2-\tilde{\xi}_2\|^2$. We estimate a benchmark value of $E\approx 0.0106$ by simulating the two systems, with the other parameters fixed at choices $[a,b,c,\pi_1,\pi_2]=[1,0,2,1,2]$ and $\mu_2=k_{on}=k_{off}=\alpha=\beta=1$. Using the direct method of Section II-A, the resulting SOS program is in 10 variables, and

requires 16 SOS multipliers σ_i to constrain the certification of dissipativity to the state space where each concentration is non-negative. Assuming $\deg(V) = \deg(\sigma_i) = 2$, the resulting SOS program is of dimension 6,392 and takes 23.4 s to return an upper bound of $E \leq 0.5412$. Increasing the degree of V to 4 gives a much tighter bound of $E \leq 0.0108$, at the cost of a 82,337-dimension problem that takes 4742 s = 1 h 19 m to complete.

This relatively large optimisation can now be decomposed into the search for a structured storage function according to Lemma 8. The upstream analysis requires a SOS program of $2N_u=6$ variables. Constructing V_u of degree 4 that satisfies (15a) with $s_u=(u_3-\tilde{u}_3)^2$ and minimising $V_u|_{t=0}$ takes a dimension 7303 SOS program 43 s to complete. According to Lemma 8, the downstream program has $2N_\xi+2N_z+1=7$ variables. However, with this choice of s_u , fixing any reasonable value of $\deg(V_0)$, $\deg(V_1)$ and $\deg(\sigma_i)$ results in an infeasible SOS program.

The search for a structured storage function can again be extended using Corollary 9, where we set $V_{u,1} = V_u$ and $s_1 = s_u$ as defined above. We now construct a second function $V_{u,2}$ for the upstream supply rate $s_2 = (u_3 + \tilde{u}_3)^2$, again in 43 s. The downstream SOS program is now in $2N_\xi + 2N_z + 2 = 8$ variables. Seeking $\deg(V_0) = \deg(V_1) = \deg(V_2) = 4$, the downstream program, of dimension 26, 105, completes in 221 s. The cost of this significant speed-up, compared to the direct approach, is that the final error bound of $E \leq 0.0845$ is more conservative than the previous bound $E \leq 0.0108$.

An important benefit of the structured storage function can be seen if we consider a new perturbation $\tilde{\mu}_1=2.5$, with simulated error $E\approx 0.0152$. To bound this error using the direct method, with $\deg(V)=4$, would take over one hour. However, we can re-use elements of the structured storage function to further speed analysis. We can determine new functions $V_{u,j}$ for the upstream system, optimised to the new perturbation, in 86 s (or half of this time if the two upstream programs are run in parallel). However, we do not need to repeat the downstream analysis: the previously calculated functions V_0 and V_1 are both still feasible for (15), although they are no longer optimal. Hence, we can quickly construct an upper bound of $E\leq 0.0969$ in around one minute, rather than over one hour.

IV. DISCUSSION

It is clear from the results of Section III that the direct method in Theorem 5 returns upper bounds on the parameter sensitivity which very closely match the simulated sensitivity. By reducing the space of storage functions we can search over, the structured approach of Theorem 7 is comparatively conservative. This conservatism is the price of reducing computational cost. The other computational benefit of this decomposition, shown in Section III-B, is a consequence of decoupling the calculations. Once we have computed V_0 and V_1 to satisfy the test (15c), these SOS polynomials remain valid for any $V_u \in \Sigma$ satisfying (15a). Hence the downstream SOS program does not need to be re-run to find

a valid (although suboptimal) bound on the sensitivity of the downstream system to a different upstream perturbation, further reducing the computational cost.

Both examples also showed that $s_u = (u_1 - u_2)^2$ may fail to achieve a feasible structured storage function, and is therefore not always necessarily the best choice of s_u . More research is needed to determine how to choose the upstream supply rates to provide the optimal upper bound (16) with the lowest computational cost.

Recall that the technique for sensitivity analysis is adapted from a technique originally applied to bounding error in model order reduction [15]. The structured analysis in this paper can therefore be extended to decompose the problem of error estimation for model order reduction into the order reduction of subsystems. Rather than perturbing an upstream layer's parameters, suppose its order is reduced. Finding the resulting error in the downstream output can be decomposed in a similar way to parameter sensitivity by using Theorem 7. In this paper and in [15] we consider storage functions in autonomous systems. However, the introduction of a structured storage function approach should allow the more general application of this method to bound perturbations in systems with external inputs. Further work will need to be carried out to also generalise this approach to non-cascade interconnection structures.

V. CONCLUSIONS

We have introduced the concept of structured storage functions to decompose the dissipativity analysis of nonlinear cascade systems (applied to dynamic parameter sensitivity analysis). Assuming that the size of the output of the upstream system is small relative to the state dimension, this can significantly reduce the computational burden of the required SOS optimisation problems. Moreover, structured storage functions allow for greater flexibility and less conservative error bounds than approaches that seek linear combinations of subsystem storage functions. This framework will have further applications for model order reduction and sensitivity analysis of more complicated, non-cascade, non-autonomous systems.

REFERENCES

- J. Anderson and A. Papachristodoulou. A decomposition technique for nonlinear dynamical system analysis. *IEEE Transactions on Automatic* Control, 57(6):1516–1521, 2012.
- [2] D. Angeli. A Lyapunov approach to incremental stability properties. IEEE Transactions on Automatic Control, 47(3):410–421, 2002.
- [3] L. Bakule. Decentralized control: An overview. Annual Reviews in Control, 32:87–98, 2008.

- [4] B. Besselink, N. van de Wouw, and H. Nijmeijer. Model reduction for nonlinear systems with incremental gain or passivity properties. *Automatica*, 49:861–872, 2013.
- [5] F. J. Bruggeman, J. L. Snoep, and H. V. Westerhoff. Control, responses and modularity of cellular regulatory networks: a control analysis perspective. *IET Systems Biology*, 2(6):397–410, 2008.
- [6] D. A. Fell. Metabolic control analysis: a survey of its theoretical and experimental development. *Biochemical Journal*, 286:313–330, 1992.
- [7] W. M. Haddad and V. Chellaboina. Nonlinear Dynamical Systems and Control: A Lyapunov-Based Approach. Princeton University Press, 2008
- [8] B. N. Kholodenko, A. Kiyatkin, F. J. Bruggeman, E. Sontag, and H. V. Westerhoff. Untangling the wires: A strategy to trace functional interactions in signaling and gene networks. *PNAS*, 99(20):12841– 12846, 2002.
- [9] M. Lang, S. Summers, and J. Stelling. Cutting the wires: Modularization of cellular networks for experimental design. *Biophysical Journal*, 106:321–331, 2014.
- [10] C. Meissen, L. Lessard, M. Arcak, and A. Packard. Performance certification of interconnected nonlinear systems using admm. In Proceedings of the IEEE Conference on Decision and Control (CDC), 2014.
- [11] C. Meissen, L. Lessard, and A. Packard. Performance certification of interconnected systems using decomposition techniques. In *Proceedings of the American Control Conference*, 2014.
- [12] A. Papachristodoulou, J. Anderson, G. Valmorbida, S. Prajna, P. Seiler, and P. A. Parrilo. SOSTOOLS: Sum of squares optimization toolbox for MATLAB. http://arxiv.org/abs/1310.4716, 2013. Available from http://www.eng.ox.ac.uk/control/sostools.
- [13] A. Papachristodoulou and S. Prajna. On the construction of Lyapunov functions using the Sum of Squares decomposition. In *Proceedings of* the 41st IEEE Conference on Decision and Control (CDC), 2002.
- [14] P. A. Parrilo. Structured Semidefinite Programs and Semialgebraic Geometry Methods in Robustness and Optimization. PhD thesis, Caltech, Pasadena, CA, 2000.
- [15] T. P. Prescott and A. Papachristodoulou. Guaranteed error bounds for structured complexity reduction of biochemical networks. *Journal of Theoretical Biology*, 302:172–182, 2012.
- [16] T. P. Prescott and A. Papachristodoulou. Layered decomposition for the model order reduction of timescale separated biochemical reaction networks. *Journal of Theoretical Biology*, 356:113–122, 2014.
- [17] T. P. Prescott and A. Papachristodoulou. Signal propagation across layered biochemical networks. In *Proceedings of the American Control Conference (ACC)*, pages 3399–3404, 2014.
- [18] B. G. Romanchuk and M. R. James. Characterization of the L_p incremental gain for nonlinear systems. In *Proceedings of the 35th Conference on Decision and Control (CDC)*, 1996.
- [19] A. Saltelli, S. Tarantola, and F. Campolongo. Sensitivity analysis as an ingredient of modeling. *Statistical Science*, 15:377–395, 2000.
- [20] H. Sandberg and R. M. Murray. Model reduction of interconnected linear systems. *Optimal Control Applications and Methods*, 30:225– 245, 2009.
- [21] P. Trnka, C. Sturk, H. Sandberg, V. Havlena, and J. Řehoř. Structured model order reduction of parallel models in feedback. *IEEE Transactions on Automatic Control*, 21(3):739–752, 2013.
- [22] A. Vandendorpe and P. van Dooren. Model reduction of interconnected systems. In *Model Order Reduction: Theory, Research Aspects and Applications*. Springer, 2008.
- [23] A. I. Zečević and D. D. Šiljak. Control of Complex Systems: Structural Constraints and Uncertainty. Springer, 2010.
- [24] Z. Zi. Sensitivity analysis approaches applied to systems biology models. *IET Systems Biology*, 5(6):336–346, 2011.