# An effective criterion for multiple positive solutions to vertically parametrized polynomial systems

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## Vertically parametrized polynomial systems and positive solutions

Polynomial systems that arise in applications often have fixed support and their coefficients depend on a set of parameters via some function. An example is the class of *vertically parametrized systems* [13, 11, 14], which appear naturally, for example, in the study of chemical reaction networks [7], polynomial optimization [4], or geometric modelling [6]. These are systems defined by vectors of polynomials of the form

$$C\big(\kappa \circ x^M\big) \in \mathbb{R}[\kappa_1, \ldots, \kappa_m, x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$$

where $C, M \in \mathbb{R}^{n \times m}$ are matrices and $C$ has full rank, $x^M$ refers to the vector whose $i$-th entry is the monomial in variables $x_1, \ldots, x_n$ with exponents given by the $i$-th column of $M$, and $\kappa \circ x^M$ is component-wise multiplication with the vector of parameters $\kappa := (\kappa_1, \ldots, \kappa_m)$. To understand the structure of these systems, it is relevant to notice that each parameter is associated with a single monomial, that is, it only appears as a linear term of the coefficient of the same monomial. *Sparse (or freely parametrized) polynomial systems*, in which each monomial in each polynomial contributes with a different parameter, are a particular instance of vertically parametrized systems.

## Chemical reaction networks

The trajectories of the concentration of the species of a chemical reaction network in time is often modeled by a system of ordinary differential equations of the form

$$\frac{dx}{dt} = N\big(\kappa \circ x^M\big),$$

where, if $n$ is the number of species and $m$ the number of reactions, then $N \in \mathbb{Z}^{n \times m}$ is the stoichiometric matrix, $M \in \mathbb{N}^{n \times m}$ is given by the stoichiometry of the reactants, and $\kappa \in \mathbb{R}^m_{>0}$ are the reaction rate constants, treated often as parameters. The trajectories of the differential equations are contained in linear subspaces, called *stoichiometric compatibility classes*. Specifically, by letting $L \in \mathbb{R}^{d \times n}$ be a matrix of full rank $d$ and whose rows generate the kernel of $N^\top$, then the trajectories are confined to equations of the form $Lx - b = 0$ for some $b \in \mathbb{R}^d$. If $d \neq 0$, then $N$ does not have full rank, and we fix a matrix $C \in \mathbb{R}^{(n-d) \times m}$ a full rank matrix whose rows form a basis of the rowspan of $N$. The steady states of the system are, then, the solutions in $\mathbb{R}^n_{>0}$ of the polynomial system

$$C\big(\kappa \circ x^M\big) = 0\,, \qquad Lx - b = 0\,. \tag{1}$$

A longstanding problem in the theory of reaction networks has been to decide whether (1) admits more than two positive solutions for some choice of $\kappa \in \mathbb{R}^m_{>0}$ and $b \in \mathbb{R}^d$. This problem has been widely studied, e.g. [5, 16, 10, 18, 1, 17, 9]. Formally, we want to decide whether there exist distinct $x, y \in \mathbb{R}^n_{>0}$ and $\kappa \in \mathbb{R}^m_{>0}$ such that

$$C\big(\kappa \circ x^M\big) = 0, \qquad C\big(\kappa \circ y^M\big) = 0, \qquad L(x - y) = 0. \tag{2}$$

Our approach builds on the works in reaction network theory [16, 8, 5, 15], where the problem is transformed into the feasibility of a system of linear equalities and inequalities, which can be solved by using quantifier elimination techniques [2]. We extend these ideas to the general framework of vertically parametrized systems. While doing that, the ideas of the methods become more transparent.

## Positive critical points

As an example of the application of our method beyond chemical reaction networks, we can study the critical points of a hypersurface. Namely, let $f \in \mathbb{R}[x_1, \dots, x_n]$ be a polnomial with a prescribed signed support $(\mathcal{A}, \varepsilon)$ where $\mathcal{A} \subset \mathbb{Z}^n$ and $\varepsilon : \mathcal{A} \mapsto \{\pm\}$. In other words, we can write $f$ as

$$f = \sum_{a \in \mathcal{A}} \varepsilon(a) \kappa_a x^a.$$

In this context, we can ask whether there is a choice of the coefficients $(\kappa_a) \in \mathbb{R}^{\mathcal{A}}_{>0}$ such that $V(f)$ has multiple positive critical points? These critical points correspond to positive solutions of the system

$$f = x_1 \frac{d}{dx_1} f = \cdots = x_n \frac{d}{dx_n} f = 0, \tag{3}$$

which is vertically parametrized. Namely, if $M$ is a matrix whose columns correspond to the supports $\mathcal{A}$, then the system (3) is of the form

$$\overline{M}(\kappa \circ x^M) = 0 \quad \overline{M} = \begin{pmatrix} 1 \\ M \end{pmatrix}$$

The characterization that we provide in Theorem 1 below can be used to answer the question of multiple positive critical points of $V(f)$. We will provide several examples of signed supports in which there can only be a single positive critical point. The critical system (3) can also be related to the number of connected components of $V(f)$ in the positive orthant [3] and to the $\mathcal{A}$-discriminant [12].

## A characterization of multiple solutions

In order to state the main characterization of multiple positive solutions, we need to consider the signs of the vector space $\ker(L)$, or equivalently, the orthants $\mathbb{R}_{\mathcal{O}}$ that $\ker(L)$ intersects nontrivially. We consider also the signs of the vectors in the orthogonal complement of $\ker(C) \cap \mathbb{R}^m_{>0}$. If $C$ has rank $s := n - d$, we can assume that $C$ is in row reduced echelon form, that is,

$$C = \begin{pmatrix} \mathrm{id}_s & -P \end{pmatrix} \tag{4}$$

for some matrix $P \in \mathbb{R}^{s \times \ell}$. This allows us to formulate the main characterization of positive solutions in (2).

**Theorem 1** *Given two matrices $C, M \in \mathbb{R}^{n \times m}$ and $P \in \mathbb{R}^{s \times \ell}$ as in (4), the system*

$$C\big(\kappa \circ x^M\big) = 0, \qquad Lx - b = 0$$

*admits multiple positive solutions for some choice of $\kappa \in \mathbb{R}^m_{>0}$ and $b \in \mathbb{R}^d$, if and only if, there exist a nontrivial orthant $\mathbb{R}_{\mathcal{O}} \subseteq \mathbb{R}^n$ that intersects $\ker(L)$, $\mu \in \mathbb{R}^{\ell}_{>0}$, and $\rho \in \mathbb{R}^m_{>0}$ such that*

*1) $\rho \in M^{\top}(\mathbb{R}_{\mathcal{O}})$.*

*2) $\mu \in \mathbb{R}^{\ell}_{>0}$ is a solution to the system of linear equalities and inequalities,*

$$F_\rho \mu = 0\,, \qquad P\mu > 0 \tag{5}$$

*where $F_\rho \in \mathbb{R}^{s \times \ell}$ is defined as*

$$(F_\rho)_{ij} := P_{ij}(e^{\rho_i} - e^{\rho_{s+j}}) \quad i = 1, \dots, s \quad j = 1, \dots, \ell.$$

The system (5) is not linear in $\rho$ as the coefficients of $F_\rho$ are not linear. However, due to the strictly increasing nature of the exponential function, the signs of the matrix $F_\rho$ only depend on the signs of $\rho_i - \rho_{s+j}$, which are given by linear inequalities. Therefore, for each sign matrix $\mathcal{S} \in \{\pm 1, 0\}^{s\times \ell}$, we can determine the set of parameters $\rho$ for which the matrix $F_\rho$ attains this sign pattern, by imposing inequalities in $\rho$. If, for a given sign matrix $\mathcal{S}$ and orthant $\mathbb{R}_{\mathcal{O}}$, the set of $\rho$ satisfying this the conditions of Theorem 1 is not empty, then the set

$$\mathcal{C}_{\mathcal{S},\mathcal{O}} = \big\{(\rho,\delta) \in \mathbb{R}^m \times \mathbb{R}_{\mathcal{O}} \mid \rho = M^\top(\delta),\ \mathrm{sign}(F_\rho) = \mathcal{S}\big\}.$$

will be non-empty. As each of the conditions defining this set are linear equalities and inequalities, $\mathcal{C}_{\mathcal{S},\mathcal{O}}$ is a polyhedral cone.

Thus, if all the polyhedral cones $\mathcal{C}_{\mathcal{S},\mathcal{O}}$ are empty, Theorem A implies that there cannot be multiple positive solutions. However, if we want to derive the existence of multiple solutions of the system, we must assume additional hypotheses on the sparsity of the matrix $P$. Namely, we consider the bipartite graph $G_P$ induced by the rows and columns of $P$ such that there is one edge for each nonzero entry. If $G_P$ is a forest, we say that $P$ *induces a forest.*

Note that we can make an exhaustive list (which we omit in this abstract) of sign matrices $\mathcal{S}$ which can never lead to solutions of (5). For instance, sign matrices that have rows with all nonzero entries of a fixed sign can never lead to solutions of $F_\rho \mu = 0$. We say the cone $\mathcal{C}_{\mathcal{S},\mathcal{O}}$ is *non-segregated* if it corresponds to sign matrices that do not belong to this list.

**Theorem 2** *Assume that $P$ induces a forest. There exists a matrix of signs $\mathcal{S} \in \{\pm 1, 0\}^{s\times \ell}$ and a nontrivial orthant $\mathbb{R}_{\mathcal{O}}$ that intersects $S$ such that the cone $\mathcal{C}_{\mathcal{S},\mathcal{O}}$ is non-empty and non-segregated, if and only if, the system*

$$C\big(\kappa \circ x^M\big) = 0\,, \qquad Lx - b = 0$$

*admits multiple positive solutions for some choice of $\kappa \in \mathbb{R}^m_{>0}$ and $b \in \mathbb{R}^d$.*

**Example 3** *Consider the vertically parametrized system with equations*

$$\begin{aligned}\kappa_2 x_3 + \kappa_3 x_3 - \kappa_4 x_1 x_2 = \kappa_2 x_3 - \kappa_4 x_1 x_2 + \kappa_6 x_4 x_5 = \kappa_1 x_3 x_4 - \kappa_5 x_5 - \kappa_6 x_4 x_5 \\ = x_4 - x_2 - x_3 - b_1 = x_5 - x_1 - x_2 - b_2 = 0.\end{aligned}$$

*This system is vertically parametrized for matrices $C, M \in \mathbb{R}^{n\times m}$ as follows*

$$C = \begin{pmatrix} 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 & -1 \end{pmatrix} \quad M = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

*The row reduced echelon form of $C$ is*

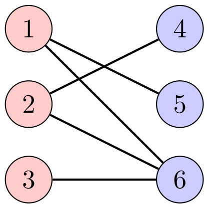
$$\begin{pmatrix}\mathrm{id} & -P\end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & -1 & -1 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{pmatrix}.$$

*The stoichiometry subspace is given by:*

$$S = \{x \in \mathbb{R}^5 \quad x_4 - x_2 - x_3 = x_5 - x_1 - x_2 = 0\}.$$

*By looking at the sparsity of the matrix $P$, the graph $G_P$ that we are considering has nodes in the set $\{1,\ldots,6\}$ and the edge structure of the figure below. In this case, there are no non-empty non-segregated cones $\mathcal{C}_{\mathcal{S},\mathcal{O}}$, deducing that the vertically parametrized system does not admit multiple positive solutions.*

The assumption that $P$ induces a forest requires this matrix to be sparse. This is usually the case of the systems coming from chemical reaction network theory, except for the fact that there are often proportional columns of the matrix $P$. Theorem 1 and Theorem 2 can be adapted to this case after simplifying the matrix $P$.

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