

# Metabolite mediated modeling of microbial community dynamics captures emergent behavior more effectively than species-species modeling: Model Parameters.

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## 1 Generalized Lotka-Volterra Model

The generalized Lotka-Volterra model is

$$\frac{d}{dt}x_i = r_i x_i \left( 1 - \frac{1}{K_i} x_i + \sum_{j \neq i} \alpha_{ij} x_j \right) \quad (1)$$

The  $\alpha_{ij}$  values fitted to growth data from Friedman et al. were

	Ea	Pa	Pch	Pci	Pf	Pp	Pv	Sm
Ea	1.0	-0.486	-0.632	0.001	-0.608	-0.999	-0.999	-0.58
Pa	1.829	1.0	-1.436	0.051	-0.641	-0.062	1.416	-0.336
Pch	0.892	0.39	1.0	0.167	-0.242	1.221	0.832	0.269
Pci	24.167	-4.832	-0.999	1.0	387583.497	-0.999	-0.114	18.68
Pf	0.006	-0.526	-1.48	-1.001	1.0	-0.256	-0.318	-0.103
Pp	-0.692	-0.999	-0.833	0.31	-0.448	1.0	0.556	1.567
Pv	-0.063	-0.901	-0.743	0.54	-0.083	-3.13	1.0	1.078
Sm	-2.375	-0.638	-0.574	0.017	-0.535	-1.947	-0.999	1.0

and the result of the computational search was

	Ea	Pa	Pch	Pci	Pf	Pp	Pv	Sm
Ea	1.0	-0.486	-0.632	-0.0548	-0.2485	-0.999	-0.999	-0.58
Pa	1.829	1.0	-1.436	-0.0357	-0.7197	-0.1022	1.416	-0.336
Pch	0.892	0.39	1.0	0.167	-0.242	1.221	0.832	0.269
Pci	24.0296	-5.0578	-0.999	1.0	387583.497	-0.999	-0.114	18.68
Pf	-0.066	-0.682	-1.48	-1.001	1.0	-0.256	-0.2578	-0.103
Pp	-0.692	-0.5257	-0.833	0.31	-0.448	1.0	0.556	1.567
Pv	-0.063	-0.901	-0.743	0.54	-0.3406	-3.13	1.0	1.0836
Sm	-2.375	-0.638	-0.574	0.017	-0.535	-1.947	-0.9384	1.0

## 2 Metabolite mediated model

Each species is modeled by

$$\frac{dx_i}{dt} = \kappa_{1i} x_i y_1 - d_1 x_i + \sum_{p \in \mathcal{P}} \kappa_p^i x_i y_p + \sum_{t \in \mathcal{T}} \psi_t^i x_i y_t \quad (2)$$

where  $\mathcal{P}$  is the set of all pairs and  $\mathcal{T}$  the set of all trios. If species  $i$  is not involved pair  $p$ , then  $k_p^i = 0$ , and similarly if  $i$  is not involved in trio  $t$ ,  $k_t^i = 0$ . Additionally, the trio (Pp,Sm,Pv) has a second trio metabolite. Note that some  $\kappa_p^k = 0$  for both members of  $p$ , and so  $y_p$  need not be included in the model (there is no cross talk in that pair). Similarly, some trios do not include cross talk, and so  $y_t$

The single metabolite assumed initially present is modeled

$$\frac{dy_1}{dt} = 1 - 0.49y_1 - \sum_{i \in sp} \kappa_{1i} x_i y_1 \quad (3)$$

The metabolites that allow cross talk between pairs are modeled

$$\frac{dy_p}{dt} = \kappa_{1s_1} x_{s_1} y_1 + \kappa_{1s_2} x_{s_2} y_1 - 0.49y_p - \kappa_p^{s_1} x_{s_1} y_p - \kappa_p^{s_2} x_{s_2} y_p \quad (4)$$

where  $p = (s_1, s_2)$ .

The metabolites that allow cross talk between trios are modeled

$$\begin{aligned} \frac{dy_t}{dt} = & \kappa_{s_1 s_2}^{s_1} x_{s_1} y_{s_1 s_2} + \kappa_{s_1 s_2}^{s_2} x_{s_2} y_{s_1 s_2} + \kappa_{s_1 s_3}^{s_1} x_{s_3} y_{s_1 s_3} + \kappa_{s_1 s_3}^{s_3} x_{s_3} y_{s_1 s_3} + \kappa_{s_2 s_3}^{s_2} x_{s_2} y_{s_2 s_3} + \kappa_{s_2 s_3}^{s_3} x_{s_3} y_{s_2 s_3} \\ & - 0.49y_t - \psi_t^{s_1} x_{s_1} y_t - \psi_t^{s_2} x_{s_2} y_t - \psi_t^{s_3} x_{s_3} y_t \end{aligned} \quad (5)$$

where  $t = (s_1, s_2, s_3)$ .

The values of  $\kappa_{1i}$  are:

	Ea	Pa	Pch	Pci	Pf	Pp	Pv	Sm
$k_{1i}$	1.36	1.613	2.0	1.1	1.468	1.9	1.559	1.2

and  $d_i$  are:

	Ea	Pa	Pch	Pci	Pf	Pp	Pv	Sm
$d_i$	1.866	1.708	1.1	1.8	1.59	1.0	1.802	1.9

The remaining  $\kappa_p^i$  are found in `pair_metabolites.csv`, and the  $\psi_t^i$  are found in `trio_metabolites.csv`, and below.

$p$	Sp1	Sp2	$\kappa_p^{Sp1}$	$\kappa_p^{Sp2}$
Ea & Pa	Ea	Pa	1.885	0
Ea & Pch	Ea	Pch	2.531	0
Ea & Pci	Ea	Pci	0	1.887
Ea & Pf	Ea	Pf	1.837	0
Ea & Pp	Ea	Pp	2.55	0
Ea & Pv	Ea	Pv	1.678	0
Ea & Sm	Ea	Sm	0	0
Pa & Pch	Pa	Pch	0	0
Pa & Pci	Pa	Pci	0	0
Pa & Pf	Pa	Pf	0	1.075
Pa & Pp	Pa	Pp	2.158	0
Pa & Pv	Pa	Pv	0	1.315
Pa & Sm	Pa	Sm	0	2.308
Pch & Pci	Pch	Pci	0	0
Pch & Pf	Pch	Pf	0	0
Pch & Pp	Pch	Pp	1.064	0
Pch & Pv	Pch	Pv	0	2.294
Pch & Sm	Pch	Sm	0	2.697
Pci & Pf	Pci	Pf	2.296	0
Pci & Pp	Pci	Pp	0	0
Pci & Pv	Pci	Pv	0	0
Pci & Sm	Pci	Sm	1.26	0
Pf & Pp	Pf	Pp	2.102	0
Pf & Pv	Pf	Pv	0	1.241
Pf & Sm	Pf	Sm	0	2.278
Pp & Pv	Pp	Pv	0	0
Pp & Sm	Pp	Sm	0	0
Pv & Sm	Pv	Sm	0	2.182

$t$	Sp1	Sp2	Sp3	$\psi_t^{Sp1}$	$\psi_t^{Sp2}$	$\psi_t^{Sp3}$
Ea & Pa & Sm	Ea	Pa	Sm	0	0	-10
Ea & Pch & Pa	Ea	Pch	Pa	0	0	0
Ea & Pch & Sm	Ea	Pch	Sm	0	0	-10
Ea & Pf & Sm	Ea	Pf	Sm	0	0	-10
Pa & Ea & Pci	Pa	Ea	Pci	0	0	-10
Pa & Pf & Pci	Pa	Pf	Pci	0	0	-10
Pa & Sm & Pci	Pa	Sm	Pci	0	0	-10
Pch & Ea & Pci	Pch	Ea	Pci	0	0	0
Pch & Ea & Pf	Pch	Ea	Pf	0	0	0
Pch & Pp & Pf	Pch	Pp	Pf	0	0	0
Pch & Sm & Pci	Pch	Sm	Pci	0	0	0
Pp & Ea & Pv	Pp	Ea	Pv	0	0	0
Pp & Pa & Pv	Pp	Pa	Pv	0	0	0
Pp & Pa & Sm	Pp	Pa	Sm	0	0	-10
Pp & Pch & Pa	Pp	Pch	Pa	0	0	0
Pp & Pf & Pci	Pp	Pf	Pci	0	0	-10
Pp & Pf & Pv	Pp	Pf	Pv	0	0	0
Pp & Pf & Sm	Pp	Pf	Sm	0	0	-10
Pv & Pch & Pa	Pv	Pch	Pa	0	0	0
Pv & Pf & Pci	Pv	Pf	Pci	0	0	0
Pv & Sm & Pci	Pv	Sm	Pci	0	0	-10
Sm & Pch & Pa	Sm	Pch	Pa	0	0	0
Ea & Pci & Sm	Ea	Pci	Sm	0	0	10
Pch & Pv & Pf	Pch	Pv	Pf	0	0	10
Pch & Sm & Pf	Pch	Sm	Pf	0	0	10
Pp & Ea & Pci	Pp	Ea	Pci	0	0	10
Pp & Pch & Pv	Pp	Pch	Pv	-10	0	0
Pp & Pch & Sm	Pp	Pch	Sm	0	0	-10
Pf & Pa & Sm	Pf	Pa	Sm	0	0	0
Pf & Pci & Ea	Pf	Pci	Ea	0	0	0
Pf & Pp & Ea	Pf	Pp	Ea	0	0	0
Pf & Pv & Ea	Pf	Pv	Ea	0	0	0
Pf & Sm & Pci	Pf	Sm	Pci	0	0	0
Pp & Pa & Ea	Pp	Pa	Ea	0	0	0
Pv & Pa & Ea	Pv	Pa	Ea	0	0	0
Pv & Pch & Ea	Pv	Pch	Ea	0	0	0
Pf & Pa & Ea	Pf	Pa	Ea	-10	0	0
Pf & Pa & Pp	Pf	Pa	Pp	-10	0	0
Pf & Pa & Pv	Pf	Pa	Pv	-10	0	0
Pf & Sm & Pv	Pf	Sm	Pv	-10	0	0
Pp & Pch & Ea	Pp	Pch	Ea	-10	0	0
Sm & Pa & Pv	Sm	Pa	Pv	-10	0	0
Sm & Pv & Pch	Sm	Pv	Pch	-10	0	0
Pci & Pp & Pa	Pci	Pp	Pa	0	0	0
Pci & Pp & Pch	Pci	Pp	Pch	0	0	0
Pci & Pv & Pa	Pci	Pv	Pa	0	0	0
Pci & Pv & Pch	Pci	Pv	Pch	0	0	0
Sm & Pp & Ea	Sm	Pp	Ea	0	0	0
Pch & Pf & Pci	Pch	Pf	Pci	0	0	0
Pf & Pch & Pa	Pf	Pch	Pa	0	0	0
Pp & Sm & Pci	Pp	Sm	Pci	0	0	0
Pp & Sm & Pv	Pp	Sm	Pv	0	0	0
Pci & Pch & Pa	Pci	Pch	Pa	0	0	0
Pv & Pp & Pci	Pv	Pp	Pci	0	0	0