Elementary vectors for microbial communities

Stefan Müller
Faculty of Mathematics, University of Vienna

universität
wien

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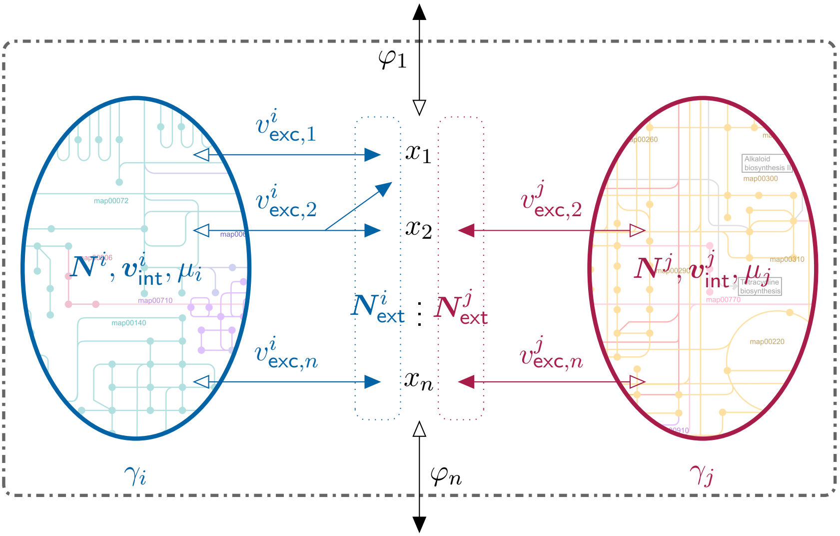
Joint work

Jürgen Zanghellini

Biochemical Network Analysis
Department of Analytical Chemistry
University of Vienna

S. Müller, M. Predl, J. Zanghellini
Elementary compositions of microbial communities
on arXiv/bioRxiv by end of February . . .

Microbial community



species i species j

Q&A

Question

Given

– a set of microbial species (their metabolic models),

– a medium, and

– a growth rate:

What are the "minimal" communities?
And their interactions?

Q&A

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– a set of microbial species (their metabolic models),

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– a growth rate:

What are the “minimal” communities?
And their interactions?

Answer

We define:

elementary compositions & exchange fluxes (eCXs)

↙ ↘

elementary compositions (eCOs) *elementary exchange fluxes (eXFs)*

Metabolic networks

Stoichiometry:

$$\mathsf{A} + \mathsf{B} + \mathcal{E} \rightleftharpoons \mathsf{C} + \mathcal{E}$$

metabolites A, B, C and enzyme $\mathcal{E}$

Kinetics:

$$v_{\mathcal{E}} = c_{\mathcal{E}} \cdot \kappa_{\mathcal{E}}(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}}; p)$$

(total) enzyme conc. $c_{\mathcal{E}} \geq 0$

metabolite conc. $x_{\mathsf{A}}(t), x_{\mathsf{B}}(t), x_{\mathsf{C}}(t) \geq 0$

external metabolite conc., rate constants, etc. $p \geq 0$

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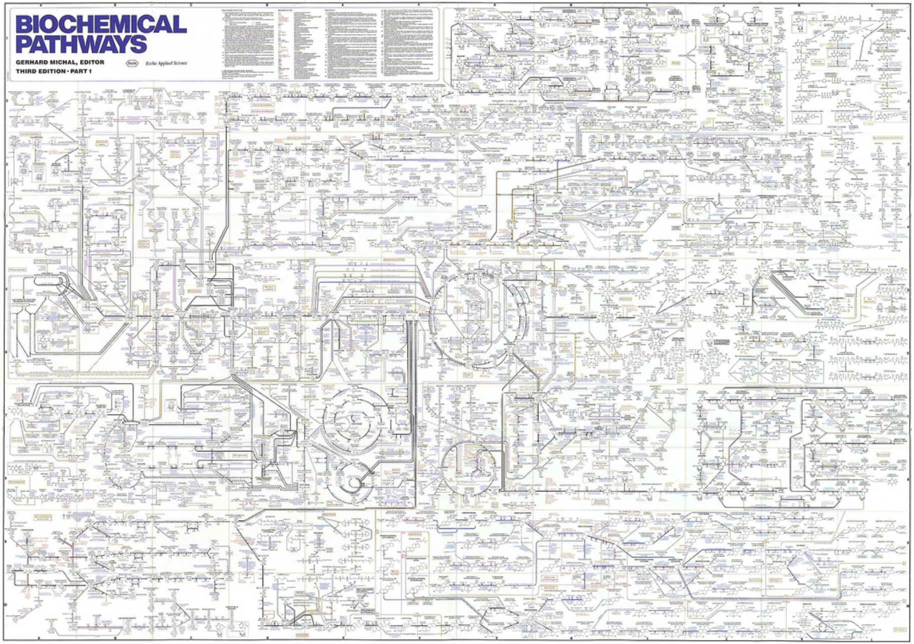
Network dynamics:

$$\frac{\mathsf{d}}{\mathsf{d}t}\begin{pmatrix} x_{\mathsf{A}} \\ x_{\mathsf{B}} \\ x_{\mathsf{C}} \\ x_{\mathsf{D}} \\ \vdots \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ 1 \\ 0 \\ \vdots \end{pmatrix} v_{\mathcal{E}} + \cdots, \qquad \frac{\mathsf{d}x}{\mathsf{d}t} = Nv = N(c \circ \kappa(x,p))$$

stoichiometric matrix N, rate vector v

componentwise product $\circ$

Genome-scale metabolic models



Stoichiometric models

Based on $N \in \mathbb{R}^{1500 \times 2000}$, no kinetics

Flux vector v (vector of steady-state net reaction rates):

$$\frac{dx}{dt} = Nv = 0$$

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Linear methods:

- flux balance analysis (FBA):
  flux polyhedron

$$P = \{v \mid Nv = 0,\ v^{\mathrm{lb}} \leq v \leq v^{\mathrm{ub}}\}$$

$$\max_{v \in P} a^T v$$

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- elementary flux mode (EFM) analysis:
  flux cone

$$C = \{v \mid Nv = 0,\ v_i \geq 0 \text{ for } i \in \mathcal{R}_{\rightarrow}\}$$

  flux mode: $f \in C$
  EFM: $e \in C$ with minimal support

Elementary vectors in metabolic pathway analysis

- Elementary flux modes (EFMs) — flux cone
  Elementary flux vectors (EFVs) — flux polyhedron (FBA)
- Elementary conversion modes (ECMs) — exchange fluxes
- Elementary growth modes (EGMs) — next-generation models
  resource balance analysis (RBA)
- eCXs — microbial communities
  eCOs, eXFs

Elementary vectors

Linear subspace S:
elementary vector (EV): $e \in S$ with minimal support

Theorem (Rockafellar 1969)

Every $f \in S$ is a finite, conformal sum of EVs:

$$f = \sum_e e \quad \textit{with} \quad \operatorname{sign}(e) \leq \operatorname{sign}(f)$$

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Conformal refinement of Minkowski's theorem
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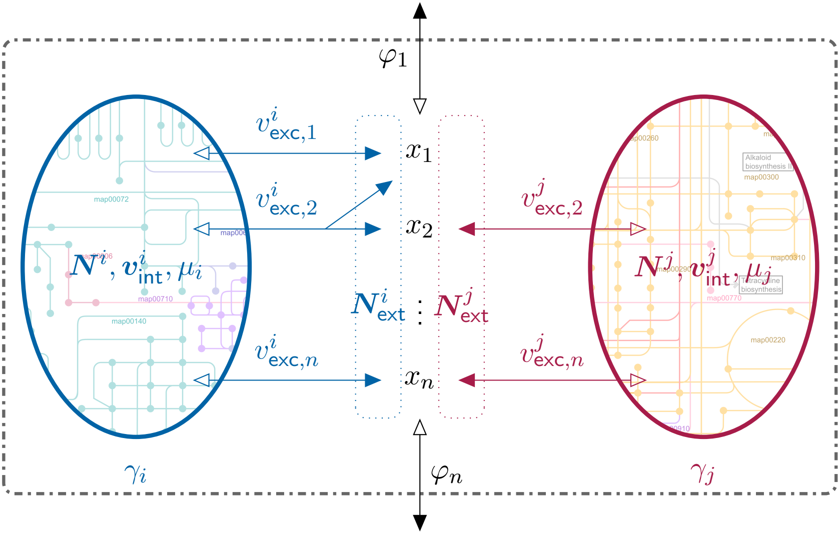
Generalization (Müller, Regensburger 2016)

linear subspace $S \to$ general polyhedral cone (e.g. flux cone C),
polyhedron (e.g. flux polyhedron P)

elementary vector: conformally non-decomposable

Microbial community



Single species: From ‘next-generation’ metabolic models ...

$$N_{\textsf{nxt-gen}} = \begin{array}{c} \\ \textsf{SMet} \\ \textsf{SMac} \end{array} \begin{array}{c} \begin{array}{cc} \textsf{RMet} & \textsf{RSyn} \end{array} \\ \left(\begin{array}{cc} N & S \\ 0 & I \end{array} \right) \end{array}$$

Growth dynamics:

$$\frac{\mathsf{d}x}{\mathsf{d}t} = N_{\textsf{nxt-gen}}\, v - \mu\, x$$

for $x = \frac{X}{M}$

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mass $M = \omega \cdot X$
vector of molar masses ω

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$\Longrightarrow$

$$\mu = \omega \cdot N_{\text{nxt-gen}}\, v$$

... to 'standard' models

Steady state:

$$0 = \begin{pmatrix} N & S \\ 0 & I \end{pmatrix} \begin{pmatrix} v_{\mathsf{Met}} \\ v_{\mathsf{Syn}} \end{pmatrix} - \mu \begin{pmatrix} x_{\mathsf{Met}} \\ x_{\mathsf{Mac}} \end{pmatrix}$$

$\implies$

$$0 = N v_{\mathsf{Met}} - \mu \underbrace{\left(S x_{\mathsf{Mac}} + x_{\mathsf{Met}}\right)}_{\hat{x}_{\mathsf{Met}}}$$

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Biomass “reaction”:

$$\sum_{i \in \mathsf{Met}} \hat{x}_{\mathsf{Met}} \cdot i \rightarrow \frac{1\,\mathsf{mol}}{1\,\mathsf{g}} \cdot \mathsf{BM}$$

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$\Longrightarrow$

$$0 = \underbrace{\begin{pmatrix} N & -n_{\mathsf{bm}} \end{pmatrix}}_{N_{\mathsf{bm}}} \begin{pmatrix} v_{\mathsf{Met}} \\ v_{\mathsf{bm}} \end{pmatrix}$$

$$n_{\mathsf{bm}} = \hat{x}_{\mathsf{Met}} \frac{\mathsf{g}}{\mathsf{mol}}, \quad v_{\mathsf{bm}} = \mu \frac{\mathsf{mol}}{\mathsf{g}}$$

Multiple species

$$0 = N^i_{\mathsf{bm}} \begin{pmatrix} v^i \\ \mu_i \, \frac{\mathsf{mol}}{\mathsf{g}} \end{pmatrix}$$

for $i = 1, \ldots, \#\mathsf{species}$

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Exchange metabolites (in medium):

$$\begin{pmatrix} ? \\ N^i \end{pmatrix} = \begin{matrix} & \text{RExc} & \text{RInt} \\ \text{SExc} & N_{\text{ext}}^i & 0 \\ \text{SMet} & N_{\text{exc}}^i & N_{\text{int}}^i \end{matrix}$$

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Dynamics (in medium):

$$\frac{\mathsf{d}X_{\mathsf{SExc}}}{\mathsf{d}t} = M \sum_i \gamma_i \, N^i_{\mathsf{ext}} v^i_{\mathsf{exc}} - \Phi$$

$$M = \sum_i M_i, \; \gamma_i = \frac{M_i}{M}$$

Community model in μ, γ and v^i

$$0 = N^i_{\mathsf{bm}} \begin{pmatrix} v^i \\ \mu \, \frac{\mathsf{mol}}{\mathsf{g}} \end{pmatrix},$$

$$l^i \leq v^i \leq u^i,$$

$$\gamma_i \geq 0,$$

for $i = 1, \ldots, \#$species, and

$$\sum_i \gamma_i \, (N^i_{\mathsf{ext}} v^i_{\mathsf{exc}})_j \begin{cases} = 0, & \text{if } j \in \mathsf{SExc}_0, \\ \leq 0, & \text{if } j \in \mathsf{SExc}_{\mathsf{in}}, \\ \geq 0, & \text{if } j \in \mathsf{SExc}_{\mathsf{out}}, \end{cases}$$

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Introduce $\bar{v}^i = \gamma_i \, v^i = \frac{v^i}{M}$ (fluxes on community level)

Koch, ..., Klamt (2019), Plos Comp. Biol.

Community model in μ, γ and $\bar{v}^i$

$$0 = N^i_{\mathsf{bm}} \begin{pmatrix} \bar{v}^i \\ \gamma_i \, \mu \, \frac{\mathsf{mol}}{\mathsf{g}} \end{pmatrix},$$

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$$\sum_i \gamma_i = 1.$$

Project fluxes to exchange fluxes ($\bar{v}^i \to \bar{v}^i_{\mathsf{exc}}$)

Community model in μ, γ and $\bar{v}^i_{\text{exc}}$

$$A^i \, \bar{v}^i_{\text{exc}} + b^i(\mu)\, \gamma_i \geq 0,$$

$$\gamma_i \, l^i_{\text{exc}} \leq \bar{v}^i_{\text{exc}} \leq \gamma_i \, u^i_{\text{exc}},$$
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$$\sum_i \gamma_i = 1.$$

Fix μ (define polytope)

Community model $\rightarrow$ community modes

Fix μ

$\downarrow$

composition & exchange flux polytope in $\gamma, \bar{v}_{\text{exc}}$

$\swarrow \quad \searrow$

composition polytope in γ exchange flux polytope in $\bar{v}_{\text{exc}}$

Community model → community modes

Fix μ

↓

composition & exchange flux polytope in $\gamma, \bar{v}_{\text{exc}}$

↙ ↘

composition polytope in γ exchange flux polytope in $\bar{v}_{\text{exc}}$

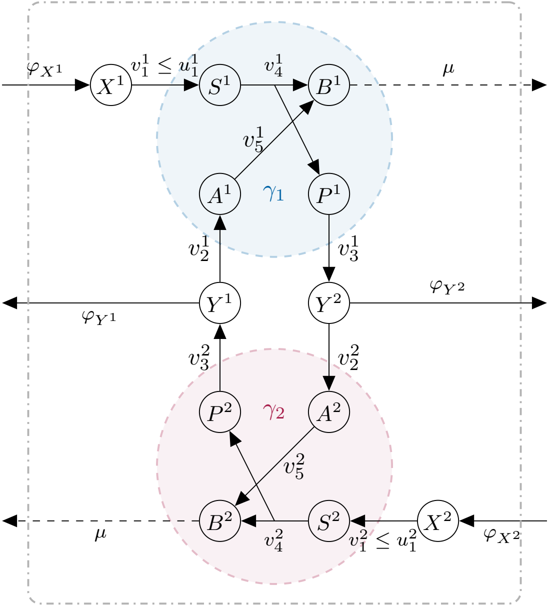
Conformally non-decomposable vectors:

eCXs

↙ ↘

eCOs eXFs

Example



φ_{X^1}
X^1
$v_1^1 \leq u_1^1$
S^1
v_4^1
B^1
μ
v_5^1
A^1
γ_1
P^1
v_2^1
v_3^1
φ_{Y^2}
Y^1
Y^2
φ_{Y^1}
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γ_2
A^2
v_5^2
B^2
S^2
X^2
φ_{X^2}
μ
v_4^2
$v_1^2 \leq u_1^2$

Example: elementary compositions & exchange fluxes

$\hat{\mu} \in [0,1]$:

$$
\begin{array}{lcccl}
 & \gamma_1, \gamma_2; & \hat{v}^1_1, \hat{v}^1_2, \hat{v}^1_3; & \hat{v}^2_1, \hat{v}^2_2, \hat{v}^2_3 & \\
\mathsf{eCX}_1 = (& 1, 0; & \hat{\mu}, 0, \hat{\mu}; & 0, 0, 0 &)^\top, \\
\mathsf{eCX}_2 = (& 0, 1; & 0, 0, 0; & \hat{\mu}, 0, \hat{\mu} &)^\top, \\
\mathsf{eCX}_3 = (& \frac{1}{2}, \frac{1}{2}; & \frac{\hat{\mu}}{2}, 0, \frac{\hat{\mu}}{2}; & 0, \frac{\hat{\mu}}{2}, 0 &)^\top, \\
\mathsf{eCX}_4 = (& \frac{1}{2}, \frac{1}{2}; & 0, \frac{\hat{\mu}}{2}, 0; & \frac{\hat{\mu}}{2}, 0, \frac{\hat{\mu}}{2} &)^\top.
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\mathsf{eCX}_4 = (& & \frac{1}{2}, \frac{1}{2}; & 0, \frac{\hat{\mu}}{2}, 0; & \frac{\hat{\mu}}{2}, 0, \frac{\hat{\mu}}{2} &)^\top.
\end{array}
$$

$\hat{\mu} \in [1, 2]$:

$$
\begin{array}{rcccl}
\mathsf{eCX}_5 = (& \frac{1}{\hat{\mu}}, \frac{\hat{\mu}-1}{\hat{\mu}}; & \frac{1}{\hat{\mu}}, \frac{\hat{\mu}-1}{\hat{\mu}}, \frac{1}{\hat{\mu}}; & \frac{\hat{\mu}-1}{\hat{\mu}}, \frac{(\hat{\mu}-1)^2}{\hat{\mu}}, \frac{\hat{\mu}-1}{\hat{\mu}} &)^\top, \\
\mathsf{eCX}_6 = (& \frac{\hat{\mu}-1}{\hat{\mu}}, \frac{1}{\hat{\mu}}; & \frac{\hat{\mu}-1}{\hat{\mu}}, \frac{(\hat{\mu}-1)^2}{\hat{\mu}}, \frac{\hat{\mu}-1}{\hat{\mu}}; & \frac{1}{\hat{\mu}}, \frac{\hat{\mu}-1}{\hat{\mu}}, \frac{1}{\hat{\mu}} &)^\top, \\
\mathsf{eCX}_7 = (& \frac{1}{2}, \frac{1}{2}; & \frac{1}{2}, \frac{\hat{\mu}-1}{2}, \frac{1}{2}; & \frac{\hat{\mu}-1}{2}, \frac{1}{2}, \frac{\hat{\mu}-1}{2} &)^\top, \\
\mathsf{eCX}_8 = (& \frac{1}{2}, \frac{1}{2}; & \frac{\hat{\mu}-1}{2}, \frac{1}{2}, \frac{\hat{\mu}-1}{2}; & \frac{1}{2}, \frac{\hat{\mu}-1}{2}, \frac{1}{2} &)^\top.
\end{array}
$$

Example: elementary compositions

$\hat{\mu} \in [0, 1]$:

$$\gamma_1, \gamma_2$$

$$\mathsf{eCO}_1 = (1, 0)^\top,$$
$$\mathsf{eCO}_2 = (0, 1)^\top.$$

$\hat{\mu} \in [1, 2]$:

$$\mathsf{eCO}_5 = (\tfrac{1}{\hat{\mu}}, \tfrac{\hat{\mu}-1}{\hat{\mu}})^\top,$$
$$\mathsf{eCO}_6 = (\tfrac{\hat{\mu}-1}{\hat{\mu}}, \tfrac{1}{\hat{\mu}})^\top.$$

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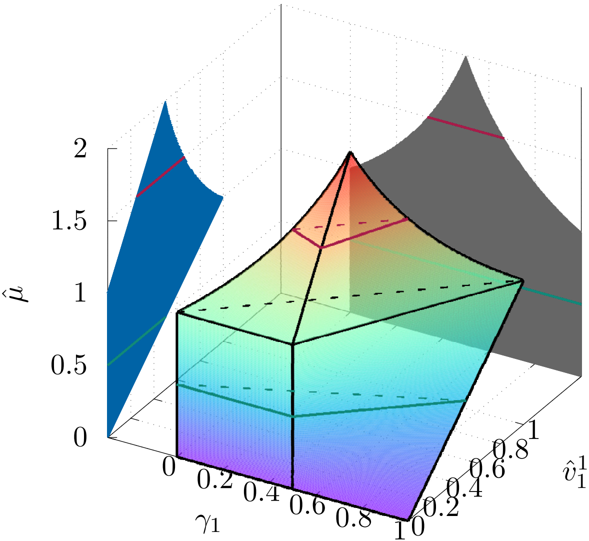
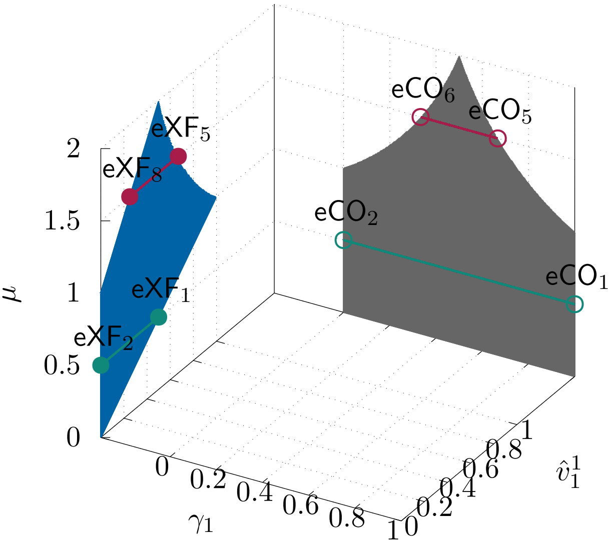
analogously for elementary exchange fluxes (eXFs)

Example: projection to μ, γ_1, v_1^1



Example: eCOs and eXFs



Biological interpretation

	$\hat{\mu} \in [0,1]$				$\hat{\mu} \in (1,2]$			
eCX	1	2	3	4	5	6	7	8
specialization	✓	✓						
commensalism			✓	✓				
mutualism					✓	✓	✓	✓
maximum uptake					✓	✓		
maximum yield			✓	✓			✓	✓
nonlinear in $\hat{\mu}$					✓	✓		

Next steps

- Applications:

  small communities (with small/large metabolic models)
  ecology?

- Computation:

  projection, EV enumeration
  `DD`, `lrs`

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- Metabolic Pathway Analysis (MPA) 2025 Vienna
- Economic Principles in Cell Biology
  Online seminar
  A collaborative open-access textbook
  `https://principlescellphysiology.org`
- Mathematics of Reaction Networks (MoRN)
  Online seminar
  `https://researchseminars.org/seminar/MoRN`

Thank you for your attention!