



# Sampling the flux space of microbial metabolic networks

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the example of SARS-CoV-2 on the human alveolar macrophage metabolic network

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# Genome-scale metabolic reconstruction

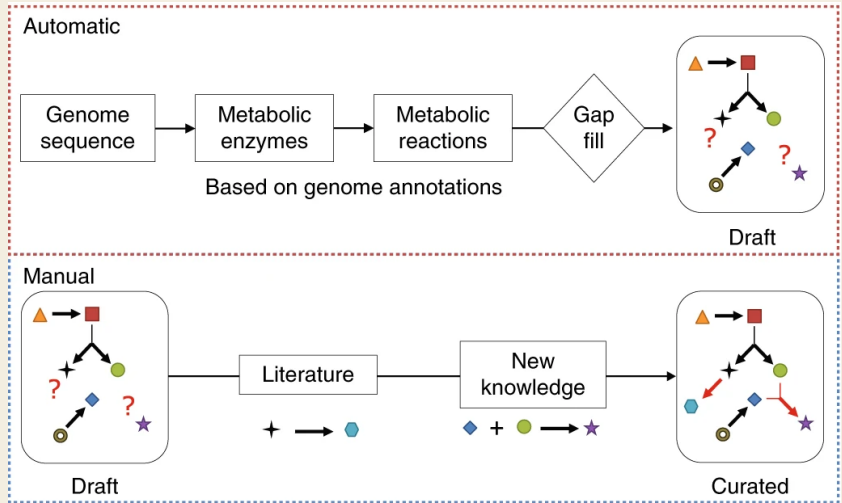










Figure from: Heirendt, Laurent, et al. "Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v. 3.0. Nature protocols 14.3 (2019): 639-702."

# From a stoichiometric matrix to a constraint-based model

		Reactions						
		R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>		
Metabolites		-1	0	0	0	0	$\times$	$=$
		1	-1	0	0	0		
		0	1	-1	0	0		
		0	1	0	0	-1		
		0	0	1	0	0		
		0	0	0	-1	0		
		0	0	0	1	-1		
		0	0	0	0	1		
		S-matrix					Flux vector	

## Flux Balance Analysis

Maximize minimize an  
objective function:

$$\psi = c_1 v_1 + c_2 v_2 + \dots + c_5 v_5$$

such that:

$$S * v = 0$$

and for each reaction  $i$ :

$$lb_i \leq v_i \leq ub_i$$

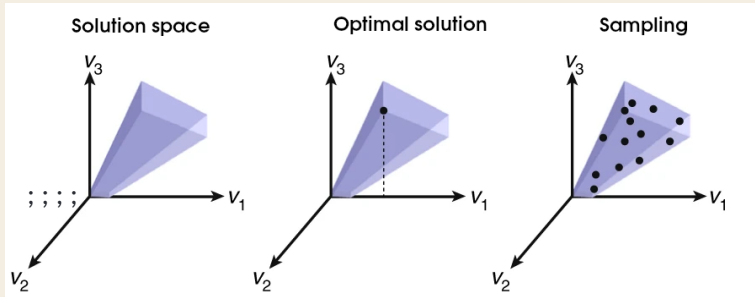
where  $lb$ : lower bound,

$ub$ : upper bound and

$S$ : the stoichiometric matrix

# Flux sampling

*an alternative approach*



Allows for:

- analysis of GSMMs without the need of an objective function

# Thank you for your attention

GitHub repository : <https://github.com/GeomScale/dingo/>

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