



Sampling the flux space of microbial metabolic networks

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

Haris Zafeiropoulos

Genome-scale metabolic reconstruction

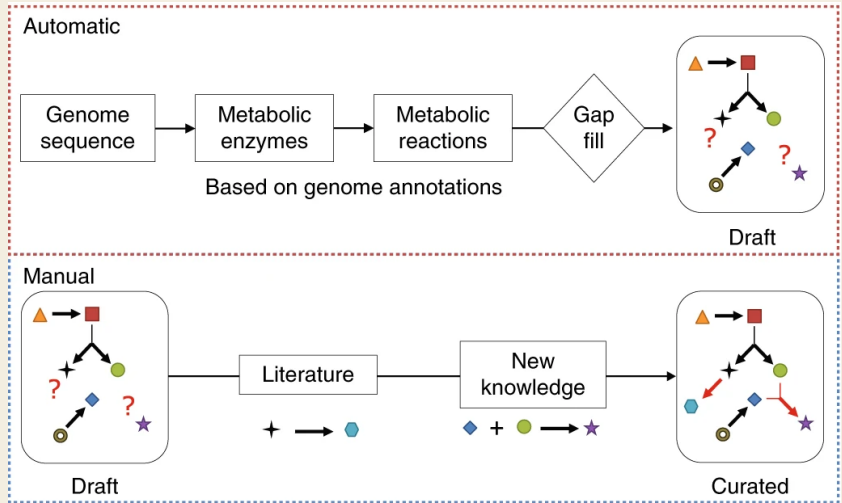










Figure from: Heirendt, Laurent, et al. "Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v. 3.0. Nature protocols 14.3 (2019): 639-702."

From a stoichiometric matrix to a constraint-based model

		Reactions						
		R ₁	R ₂	R ₃	R ₄	R ₅		
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 :

$$lb_i \leq v_i \leq ub_i$$

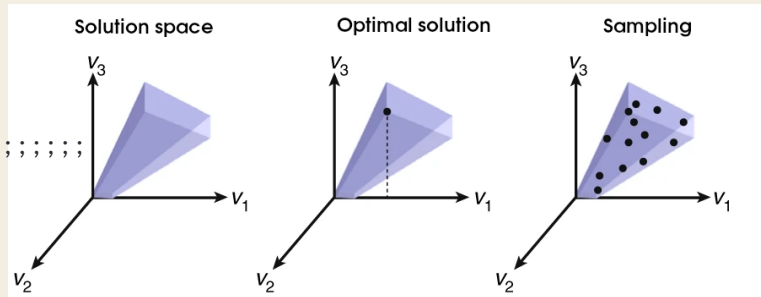
where lb : lower bound,

ub : upper bound and

S : the stoichiometric matrix

Flux sampling

an alternative approach



- enables the analysis of GSMMs without the need of an objective function
- determines the feasible solution spaces for fluxes in a network based on a set of conditions as well as the probability of obtaining a solution

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."

Thank you for your attention

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

email : haris-zaf@hcmr.gr

Twitter : [haris_zaf](#)

web-site : <https://hariszaf.github.io/>

