dingo: a Python package for metabolic flux sampling

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GeomScale

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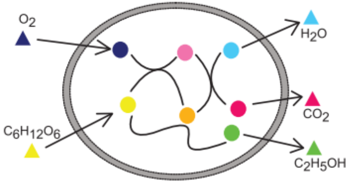
In our cells...



$$1\ C_6H_{12}O_6 + 6\ O_2 \longrightarrow 6\ CO_2 + 6\ H_2O \qquad (r_1)$$

$$1\ C_6H_{12}O_6 \longrightarrow 2\ C_2H_5OH + 2\ CO_2 \qquad (r_2)$$

We call both the inputs (reactants) and the outputs (products) of a chemical reaction, metabolites.

In every cell of our body
thousands of chemical reactions are taking place!

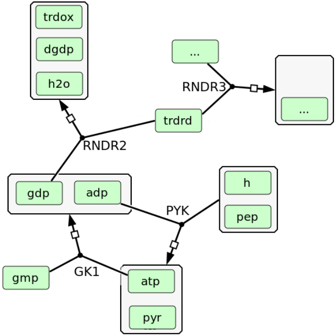
A network of reactions and metabolites

$$(\mathbf{GK1}):\ atp + pyr + gmp \longrightarrow gdp + adp$$

$$(\mathbf{PYK}):\ h + pep + adp \longrightarrow atp + pyr$$

$$(\mathbf{RNDR2}):\ gdp + trdrd \longrightarrow h2o + dgdp + trdox$$

$$(\mathbf{RNDR3}):\ trdrd + \cdots \longrightarrow \cdots + \ldots$$



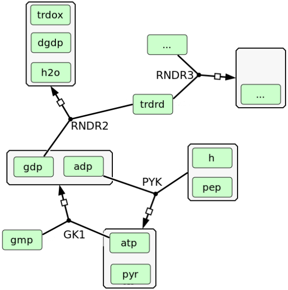
Reaction fluxes and steady states

$$(\mathbf{GK1}):\ \mathbf{v_1}\cdot atp + \mathbf{v_1}\cdot pyr + \mathbf{v_1}\cdot gmp \longrightarrow \mathbf{v_1}\cdot gdp + \mathbf{v_1}\cdot adp$$

$$(\mathbf{PYK}):\ \mathbf{v_2}\cdot h + \mathbf{v_2}\cdot pep + \mathbf{v_2}\cdot adp \longrightarrow \mathbf{v_2}\cdot atp + \mathbf{v_2}\cdot pyr$$

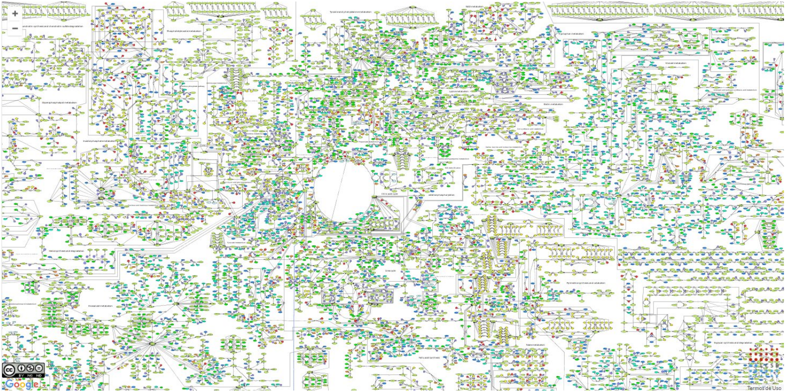
$$(\mathbf{RNDR2}):\ \mathbf{v_3}\cdot gdp + \mathbf{v_3}\cdot trdrd \longrightarrow \mathbf{v_3}\cdot h2o + \mathbf{v_3}\cdot dgdp + \mathbf{v_3}\cdot trdox$$

$$(\mathbf{RNDR3}):\ \mathbf{v_4}\cdot trdrd + \mathbf{v_4}\cdots \longrightarrow \mathbf{v_4}\cdots + \mathbf{v_4}\ldots$$



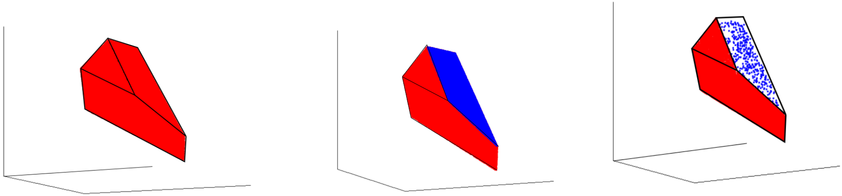
- The *i*-th reaction has a flux (rate) v_i that is *flowing*.
- The vector of fluxes that balances the network is a steady state.

It is a complex problem



The complete human metabolic network Recon1 [Palsson et al.'07]

Geometry of metabolic networks



1. The set of steady states is represented by a convex polytope.
2. The optimal steady states (wrt the biomass objective function) belong to a facet of the polytope (FBA).
3. Sampling efficiently explore the space of allowable metabolic flux distributions.

dingo package

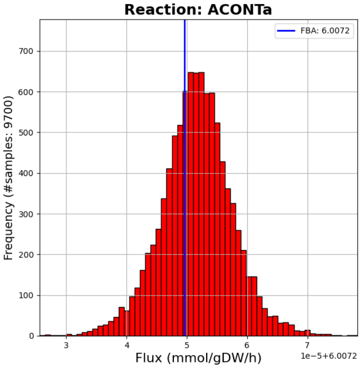
- Python package for sampling in metabolic networks
- Several sampling and rounding algorithms available
- Based on C++ volesti library
- FBA, FVA, loading standard models, copulas, ploting utilities
- publised in Bioinformatics Advances

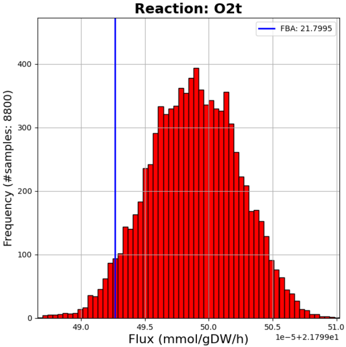
People / main contributors

- Apostolos Chalkis
- Vissarion Fisikopoulos
- Elias Tsigaridas
- Haris Zafeiropoulos

dingo example (FBA vs sampling)

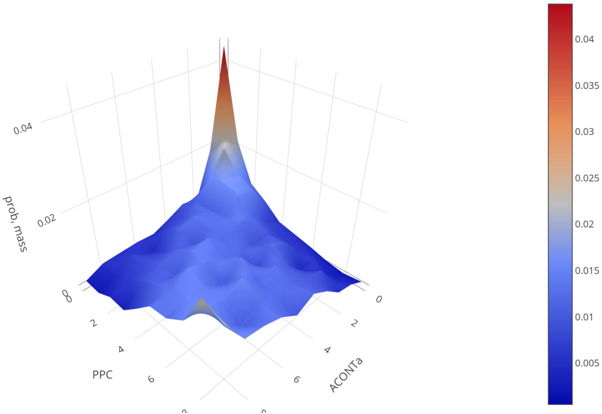
```
from dingo import MetabolicNetwork, PolytopeSampler

model = MetabolicNetwork.from_json('ext_data/ecoli_core.json')
fba_sol, fba_value = model.fba()
sampler = PolytopeSampler(model)
steady_states = sampler.generate_steady_states(ess = 3000)
reactions = model.reactions
plot_histogram(steady_states[13], reactions[13])
```





Analyse dependencies between reactions

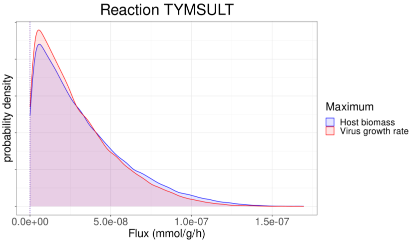
```
mod = MetabolicNetwork.from_json(’path/to/e_coli_core.json’)
sampler = PolytopeSampler(mod)
steady_states = sampler.generate_steady_states(ess = 3000)
reactions = model.reactions
data_flux2=[steady_states[12],reactions[12]]
data_flux1=[steady_states[13],reactions[13]]
plot_copula(data_flux1, data_flux2, n=10)
```



Copula between ACONTa and PPC

Reaction targeting

- [Renz,Widerspick,Dräger'20,'21] generate a host-virus network.
- two objective functions: (a) human biomass maintenance, (b) virus growth rate.
- Check diffs in FBA for each obj. function.
- Alternative: check if the flux distribution of reactions changes.
- Find possible anti-viral targets and study further.
- Could flux sampling lead to more accurate results than FBA?

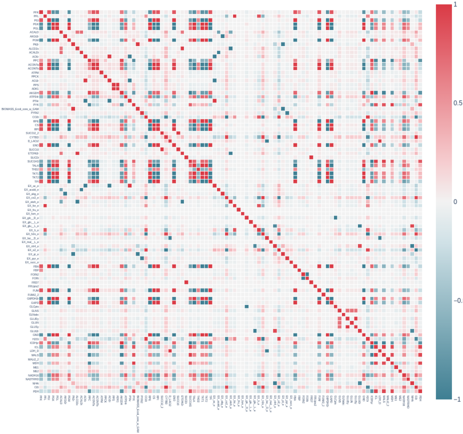


flux does not change

flux does change

Current and future development

- Sampling from the boundary of polytopes (Iva Janković - GSoC 2025)
- Statistical analysis of flux sampling datasets (Sotirios Touliopoulos - GSoC 2024-25)



Resources

- dingo repository:
- Colab notebook:
- PyPi package:

Thank you — Questions?