

Mutual linearity of nonequilibrium network currents

Sara Dal Cengio, joint work with Pedro Harunari, Matteo Polettini, Vivien Lecomte

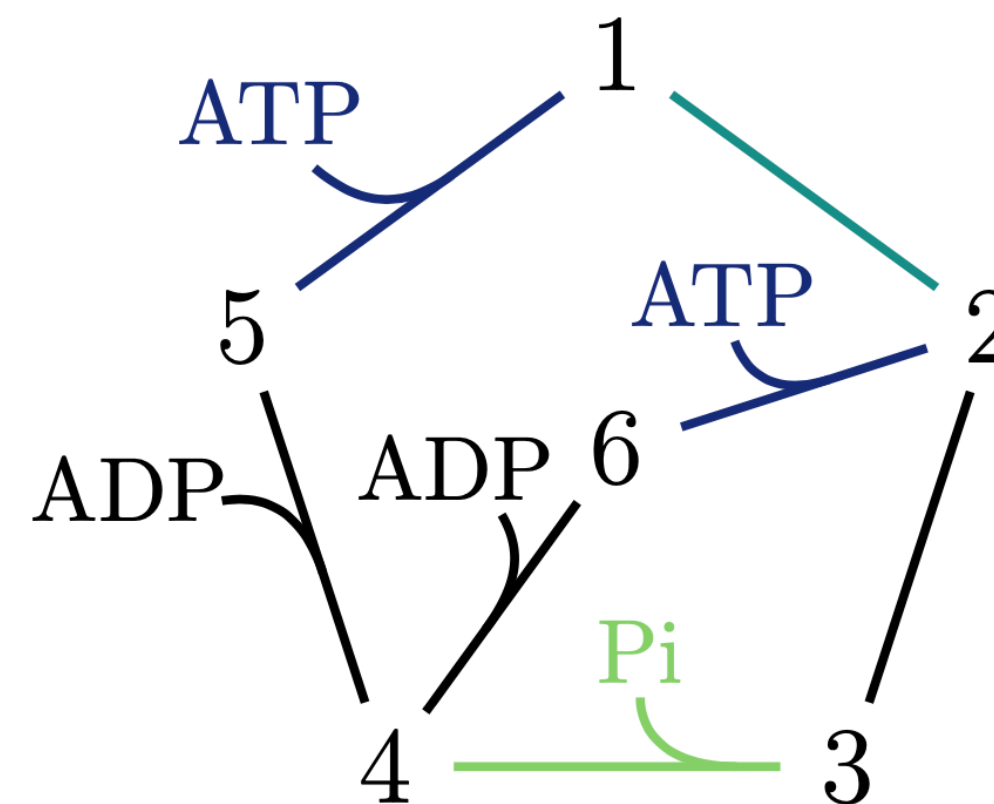
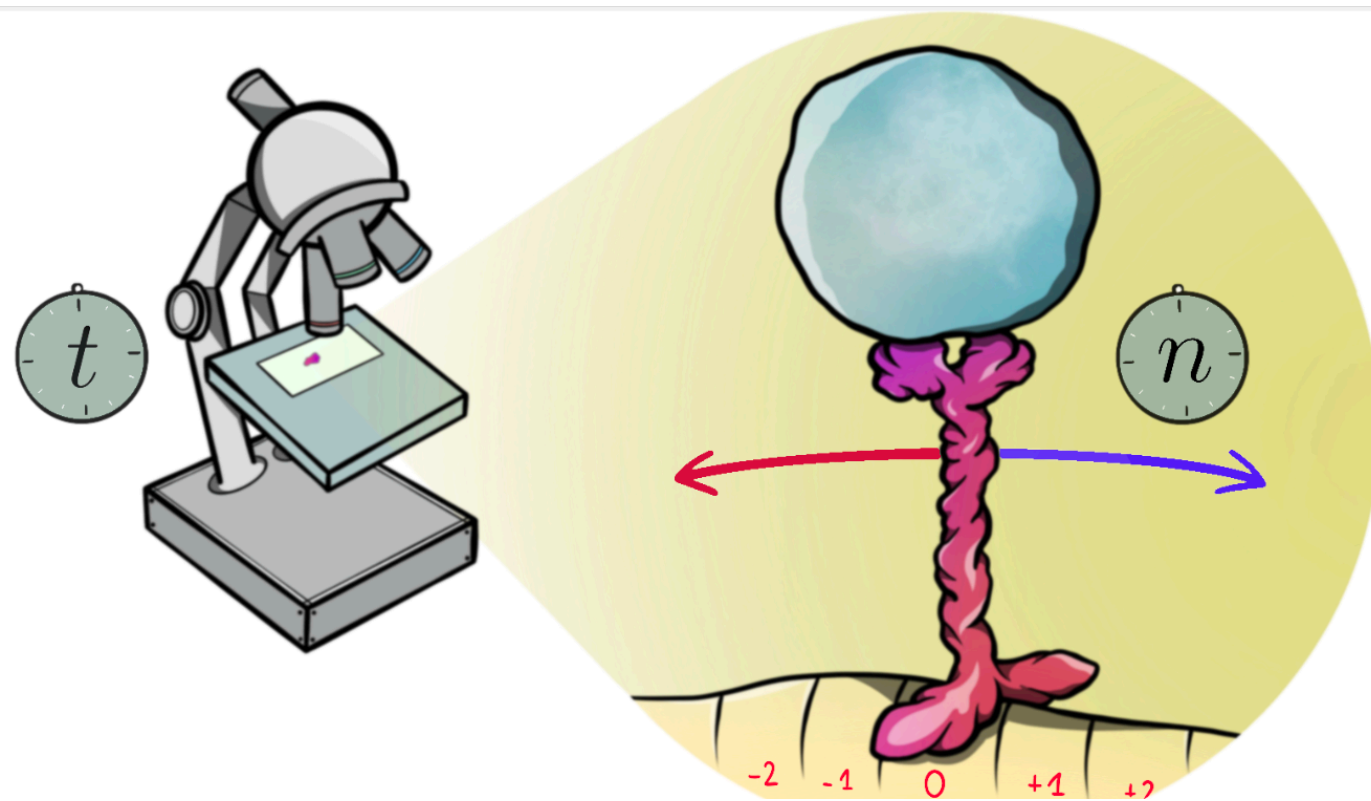
October 10, 2024



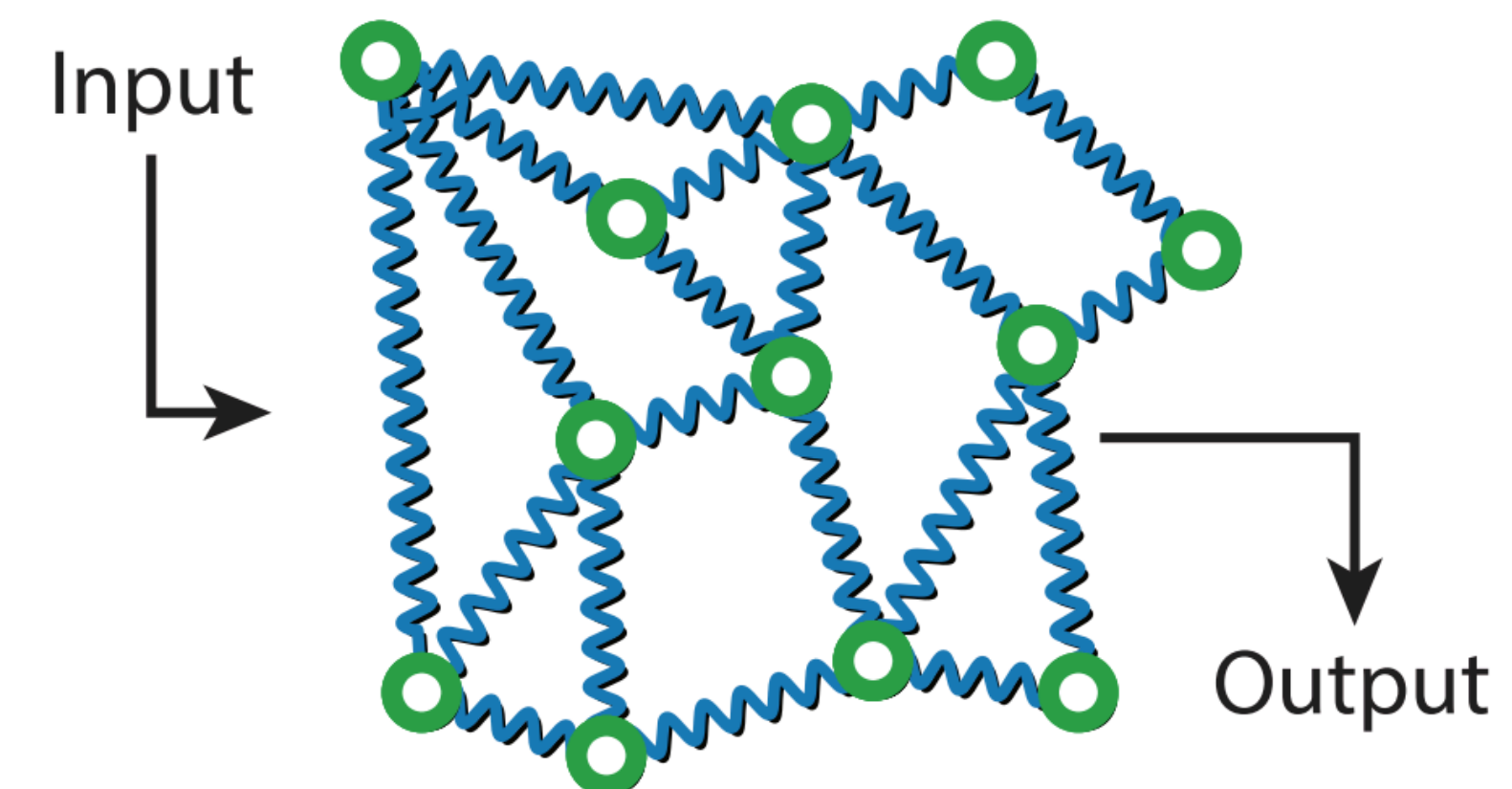
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Networks in the real world

Ex. Chemical reaction networks, metabolic networks

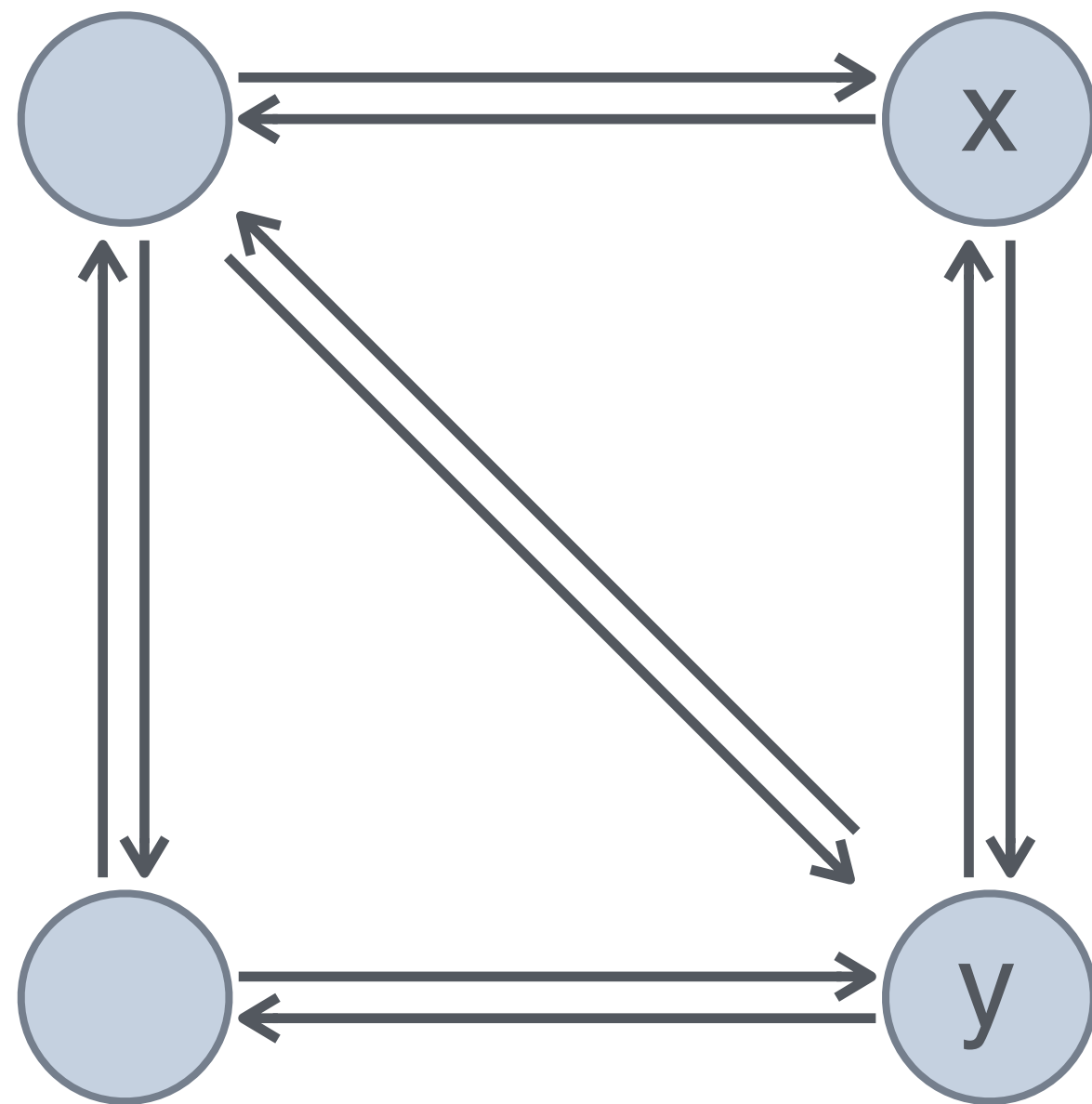


Ex. Pipe networks, resistor networks, elastic networks



Framework

Continuous-time Markov chain with rates $\mathbf{r} = \{r(x | y)\}$ on a network (state space)



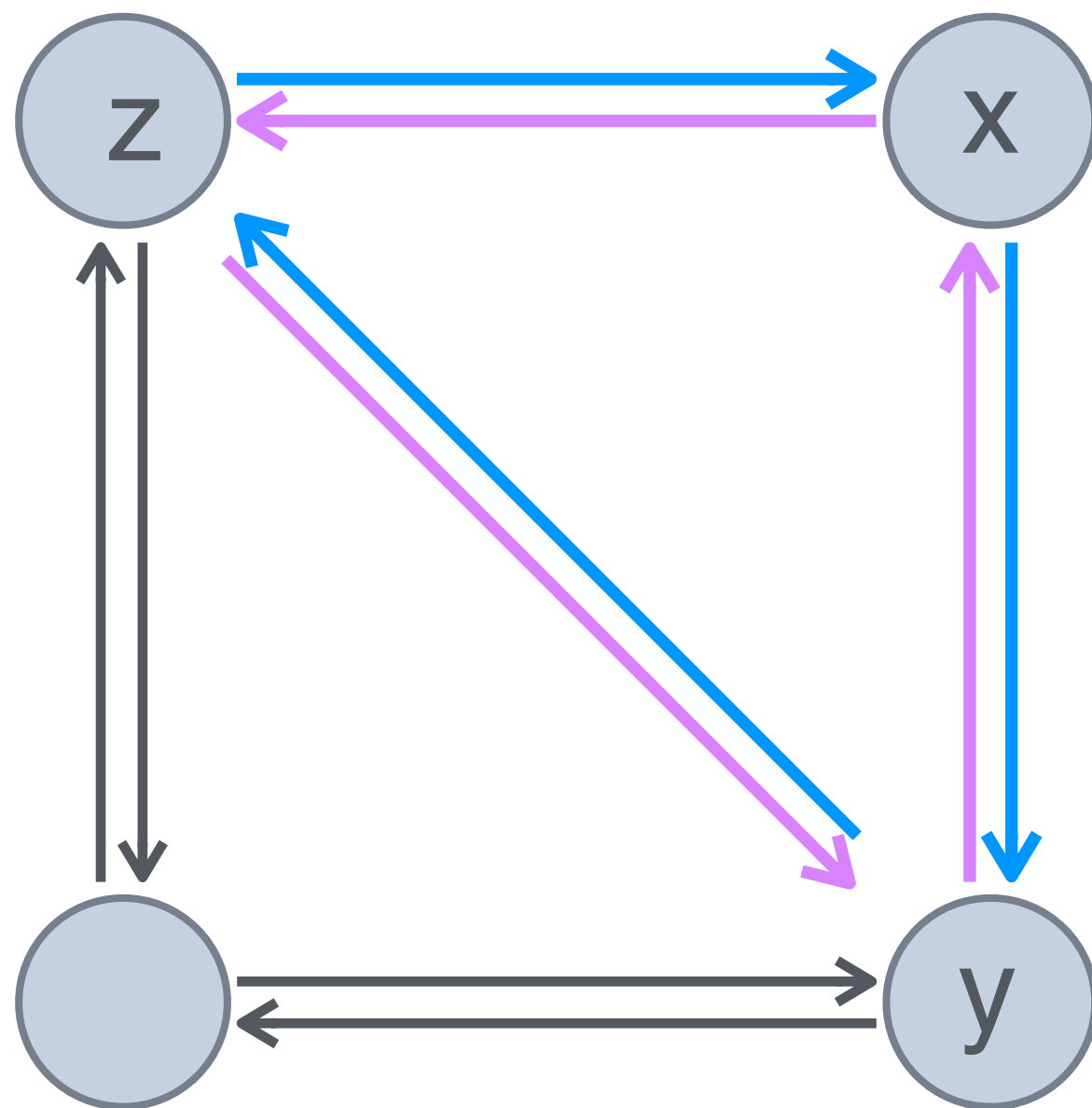
Cumulative edge current: $J_{x \leftarrow y}(t) = \#_{x \leftarrow y}(t) - \#_{y \leftarrow x}(t)$

Stationary edge current: $j_{xy} = \lim_{t \rightarrow \infty} \frac{\langle J_{x \leftarrow y}(t) \rangle}{t}$

(1) We assume that the system **reaches a stationary state** (ensured by Perron-Frobenius theorem for connected network)

Framework

If the transition rates fulfill the **Kolmogorov condition**, the stationary state is **equilibrium** with vanishing stationary currents $j_{xy} = 0 \ \forall (x,y)$



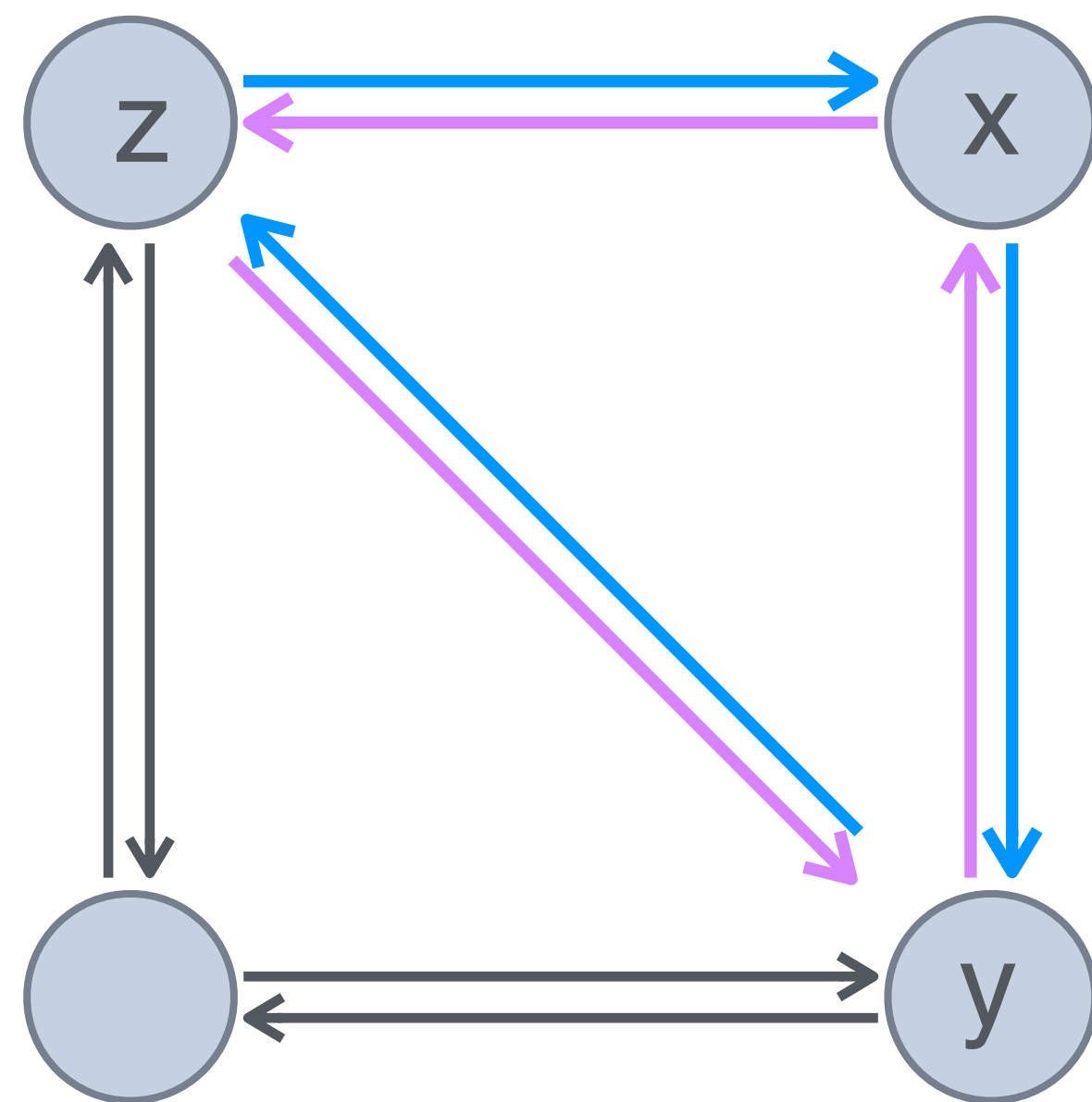
\forall cycle:

$$r(z|x)r(y|z)r(x|y) = r(y|x)r(z|y)r(x|z)$$

- \Leftrightarrow Detailed Balance (stat. mech.)
- \Leftrightarrow Wegscheider condition (chemistry)
- \Leftrightarrow Kirchhoff's voltage law (electric circuits)

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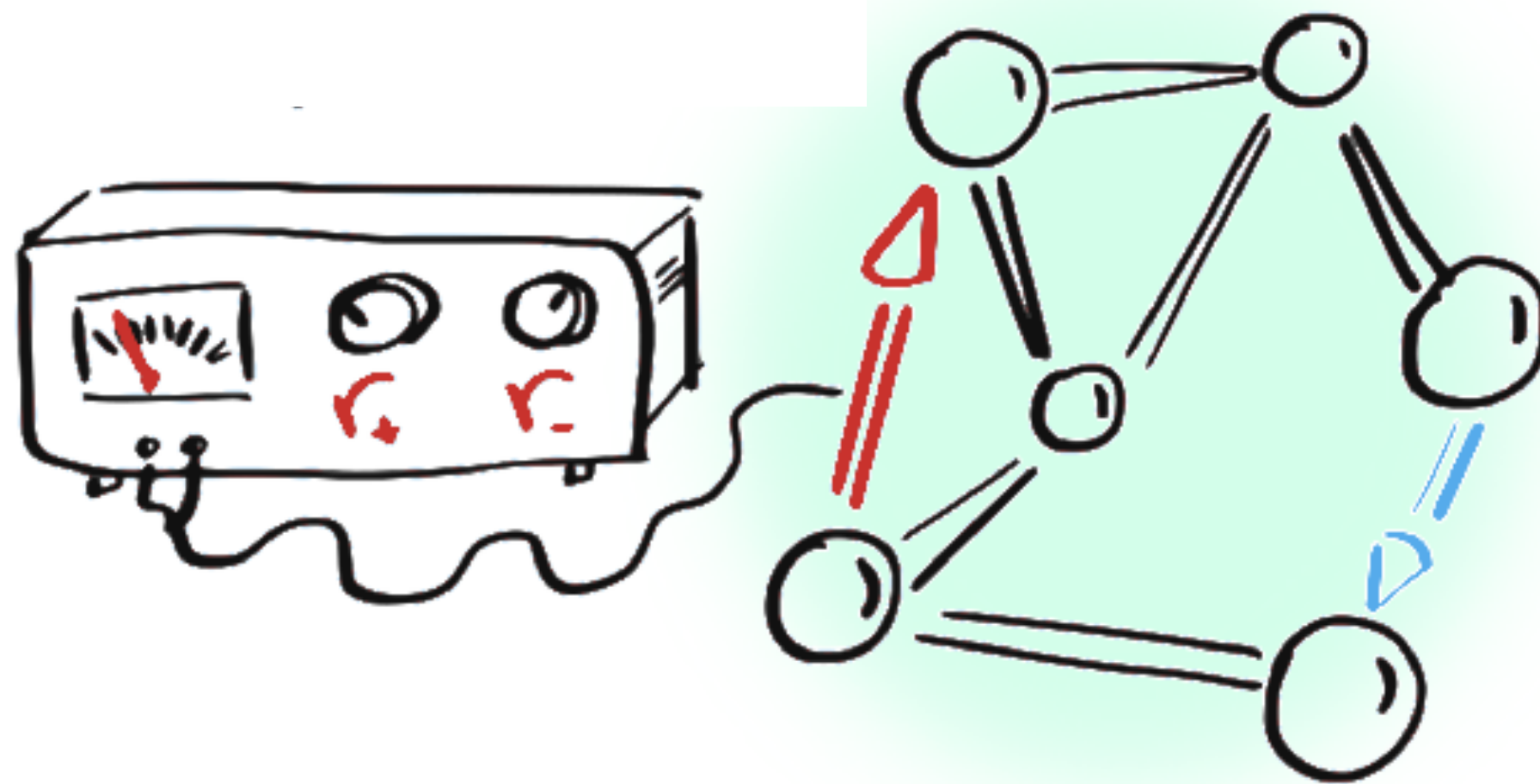
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- \Leftrightarrow Detailed Balance (stat. mech.)
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(2) We take arbitrary transition rates \Leftrightarrow **far-from-equilibrium**

Questions

- How do currents respond to other currents in nonequilibrium steady-states?
- Can we establish **current-to-current relationships** when controlling the transition rates of one (or more) “input” current?

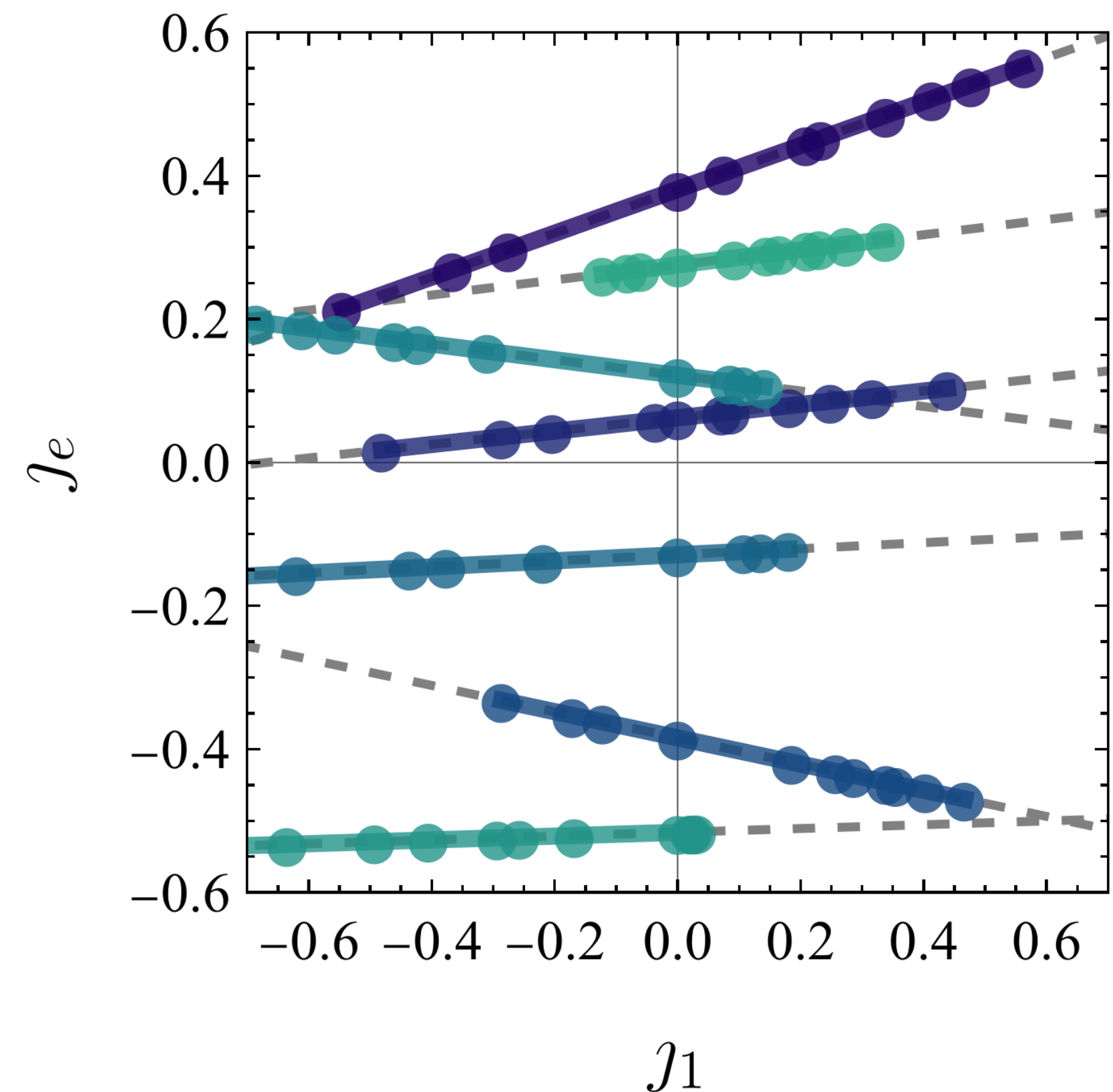
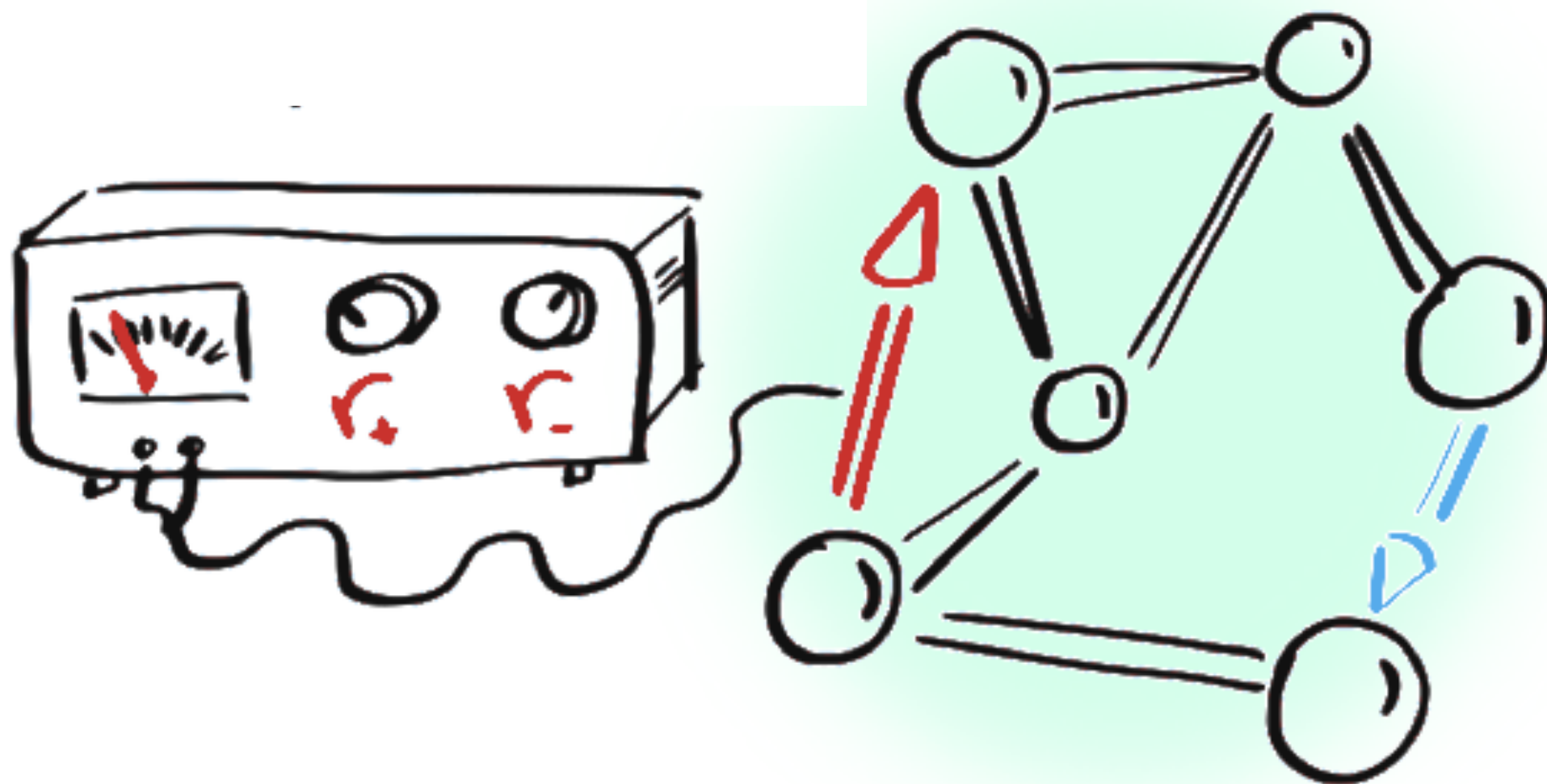


Ex. Metabolic reconstruction...

The case of one input current

Main result: Control rates $r_{\pm i}$ and fix every other rate. Then $\forall j_{e \neq i}$ there exist two constants (independent on $r_{\pm i}$) such that there is a **linear-affine relation**

$$j_e(r_{\pm i}) = \lambda_e^0 + \lambda_e^1 j_i(r_{\pm i})$$



Path to the proofs

$$j_e(r_{\pm i}) = \lambda_e^0 + \lambda_e^1 j_i(r_{\pm i})$$

- The affine parameter λ_e^0 is the value of the **current “at stalling”**, when we set the input rates to zero
- The linear parameter λ_e^1 is the **current-to-current susceptibility**:
 $\lambda_e^1 = \partial_{r_{\pm i}} j_e / \partial_{r_{\pm i}} j_i$

The difficult part of the proof is to show that $\partial_{r_{\pm i}} j_e / \partial_{r_{\pm i}} j_i$ does not depend on the input rates...

Path to the proofs

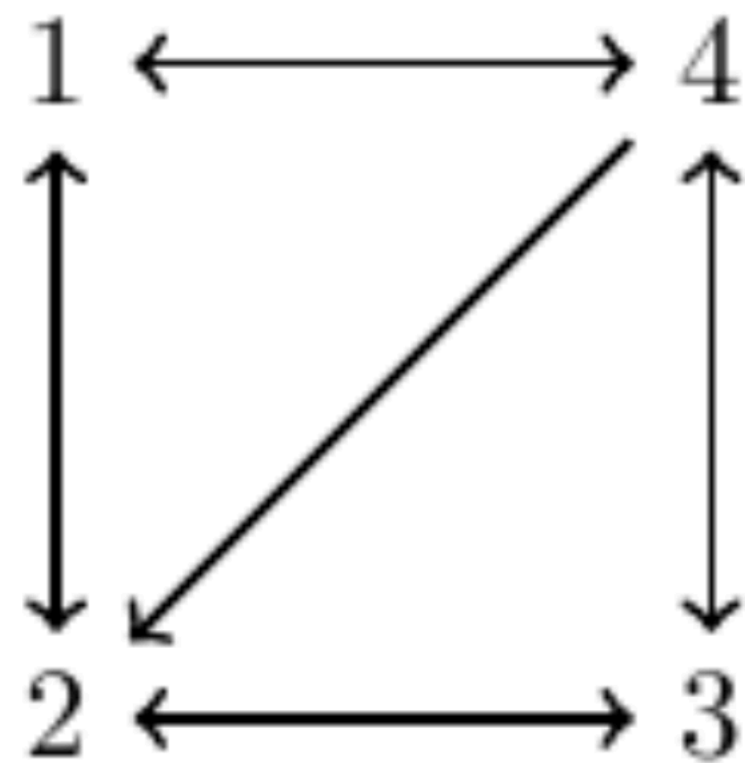
You can either...

- Use graph theory
- Expand the rate matrix
- Use Laplace transform (go to frequency domain)

Spanning tree ensembles

- Use graph theory

Idea: Current in terms of **spanning trees** (Markov chain tree theorem)

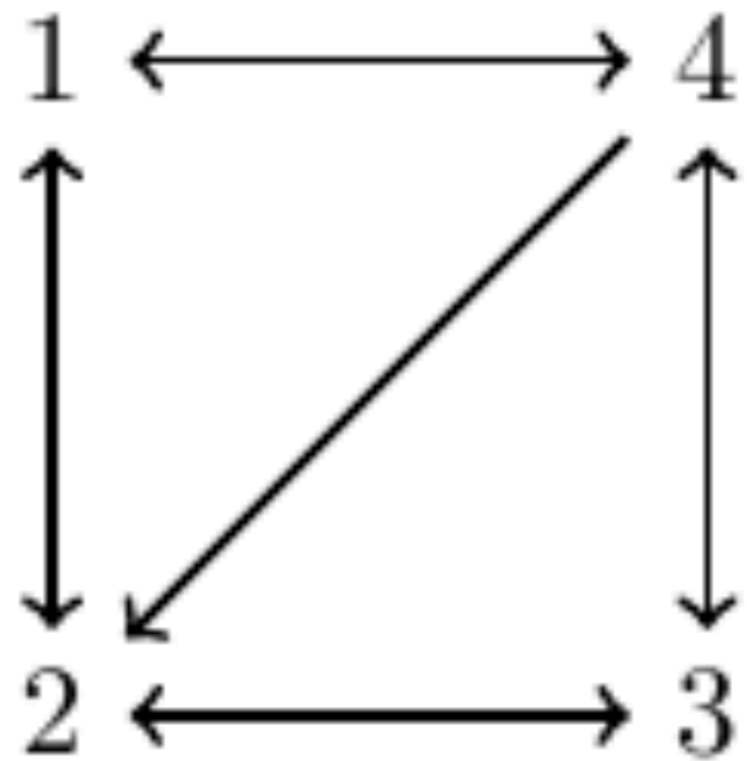


$$\begin{aligned}\tau_1 &= \begin{array}{c} \leftarrow \\ \uparrow \end{array} \begin{array}{c} \leftarrow \\ \uparrow \end{array} + \begin{array}{c} \leftarrow \\ \rightarrow \end{array} \begin{array}{c} \leftarrow \\ \uparrow \end{array} + \begin{array}{c} \leftarrow \\ \rightarrow \end{array} \begin{array}{c} \leftarrow \\ \rightarrow \end{array} + \begin{array}{c} \leftarrow \\ \nearrow \end{array} + \begin{array}{c} \leftarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \leftarrow \\ \rightarrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \leftarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \leftarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} \\ \tau_4 &= \begin{array}{c} \rightarrow \\ \uparrow \end{array} \begin{array}{c} \rightarrow \\ \uparrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \uparrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} \\ \tau_3 &= \begin{array}{c} \rightarrow \\ \uparrow \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} \\ \tau_2 &= \begin{array}{c} \leftarrow \\ \downarrow \end{array} \begin{array}{c} \leftarrow \\ \uparrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \uparrow \\ \rightarrow \end{array} + \begin{array}{c} \rightarrow \\ \nearrow \end{array} \begin{array}{c} \downarrow \\ \rightarrow \end{array}\end{aligned}$$

Spanning tree ensembles

- Use graph theory

Idea: Current in terms of **spanning trees** (Markov chain tree theorem)



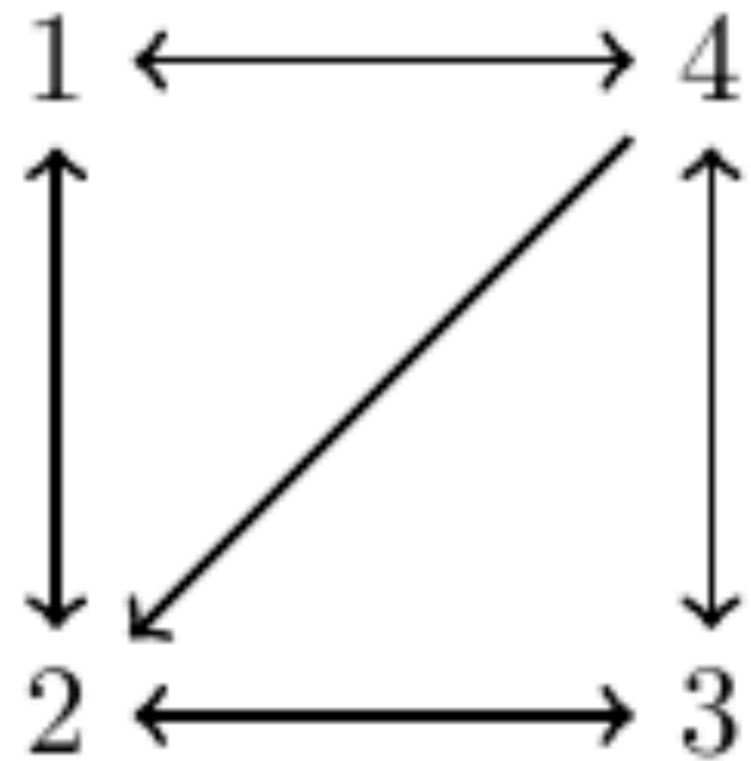
$$j_{xy} = \frac{r_{xy}\tau_y - r_{yx}\tau_x}{\sum_Z \tau_Z}$$

Currents are highly nonlinear in the rates!

Spanning tree ensembles

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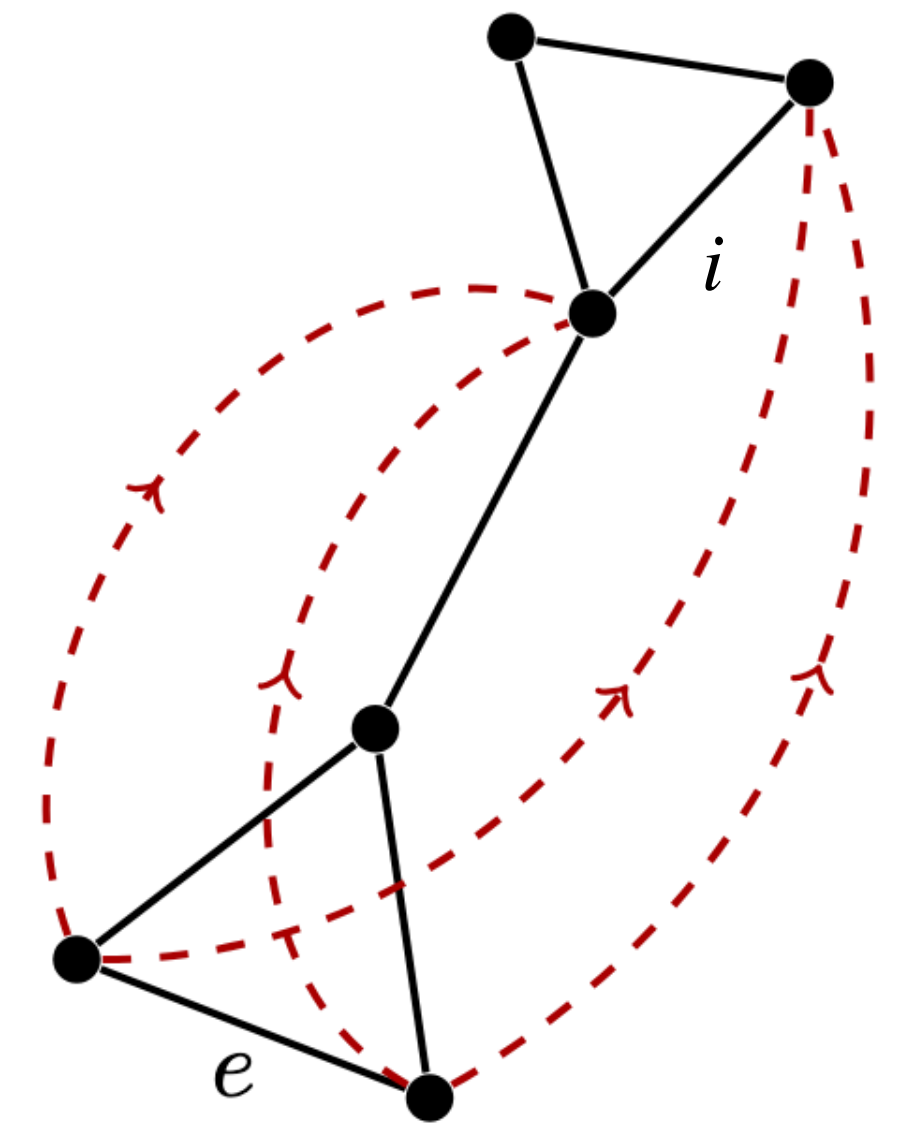
Currents are highly nonlinear in the rates!

Lambda's in terms of spanning trees?

Spanning tree ensembles

- λ_e^0 is simple! Current from the spanning trees **pruned by the input edge**

$$\lambda_{xy}^0 = \frac{r_{xy} \tau_y^{\setminus i} - r_{yx} \tau_x^{\setminus i}}{\sum_Z \tau_Z^{\setminus i}}$$

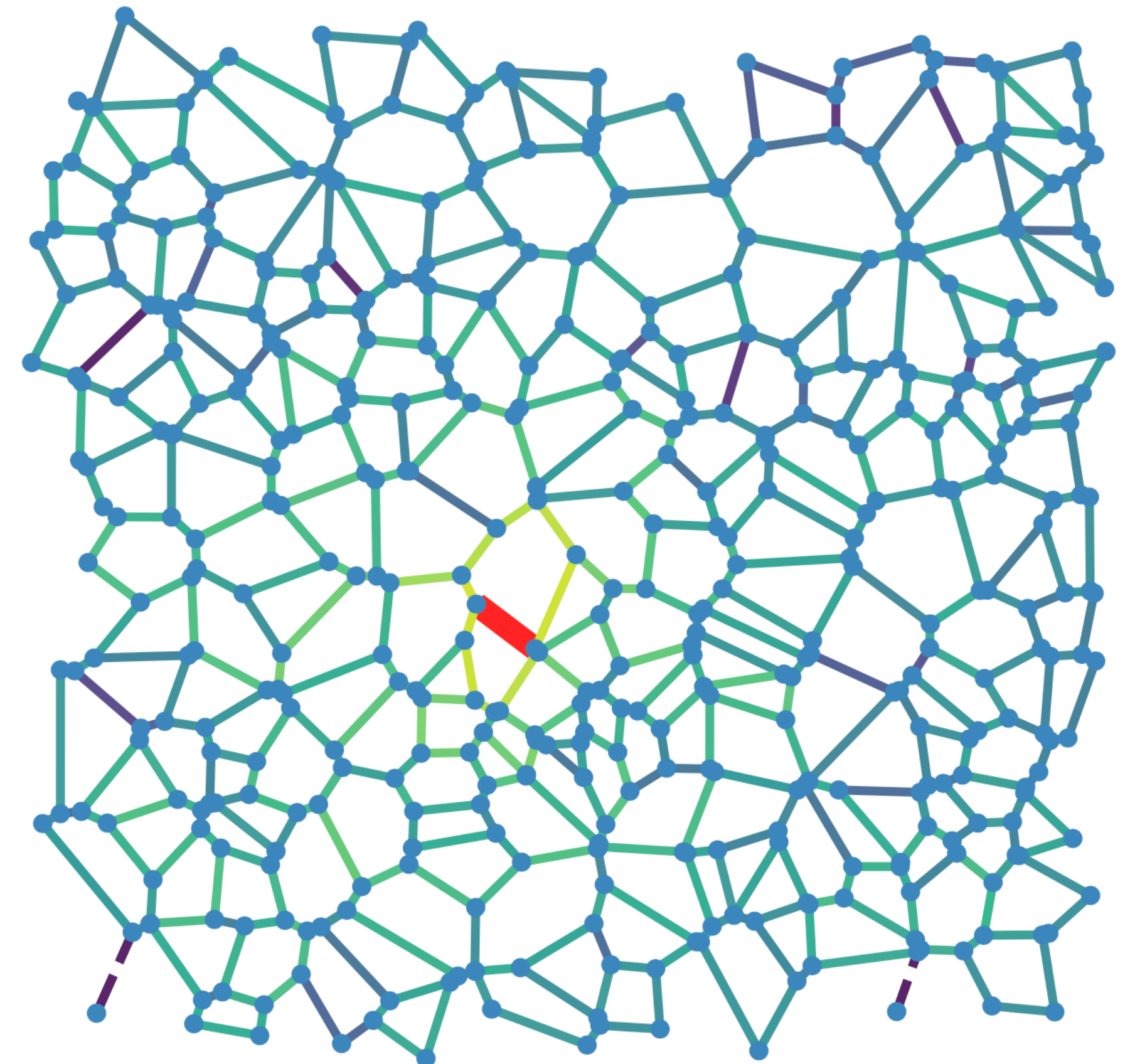


- λ_e^1 again a ratio of spanning trees, but in a **different ensemble...**

See —> Harunari, Dal Cengio, Lecomte, Polettini, PRL (2024)

More to come...

- A linear relationship arbitrarily far from equilibrium: any connection to **fluctuation theorems**?
- The result applies **beyond Markov chains**



Susceptibility map

More to come...

- A linear relationship arbitrarily far from equilibrium: any connection to **fluctuation theorems**?
- The result applies **beyond Markov chains**
- Does the linearity survive when we control **more than one input current**?

Yes! But you cannot control any arbitrary currents...

(Soon to appear on the ArXiv...)

Thank you for the attention!

- A linear relationship arbitrarily far from equilibrium: any connection to **fluctuation theorems**?
- The result applies **beyond Markov chains**
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The End